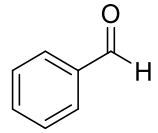
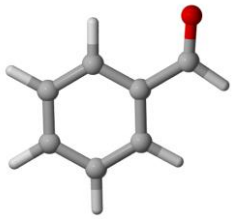
B3LYP/6-311+G**	**PhCHO**

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

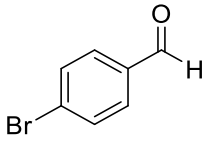
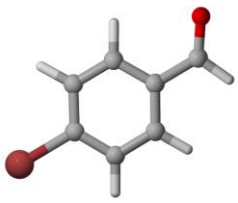
C	-0.0383310000	-1.1045640000	0.0000000000
C	-0.5344010000	0.2062400000	0.0000000000
C	0.3549540000	1.2867630000	0.0000000000
C	1.7294860000	1.0637480000	0.0000000000
C	2.2168840000	-0.2425590000	0.0000000000
C	1.3327730000	-1.3258940000	0.0000000000
H	-0.0347550000	2.3003790000	0.0000000000
H	2.4177120000	1.9012860000	0.0000010000
H	3.2869220000	-0.4189500000	0.0000010000
H	1.7192970000	-2.3388390000	0.0000000000
H	-0.7431110000	-1.9279290000	-0.0000010000
C	-1.9920600000	0.4631800000	-0.0000010000
H	-2.2699220000	1.5389750000	0.0000020000
O	-2.8489970000	-0.3920510000	0.0000010000

thermodynamic data

Zero-point correction= 0.109369 (Hartree/Particle)
Thermal correction to Energy= 0.115702
Thermal correction to Enthalpy= 0.116647
Thermal correction to Gibbs Free Energy= 0.078777
Sum of electronic and zero-point Energies= -345.559703
Sum of electronic and thermal Energies= -345.553370
Sum of electronic and thermal Enthalpies= -345.552426
Sum of electronic and thermal Free Energies= -345.590295

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.604	23.944	79.703

B3LYP/6-311+G**	***p*-Br-PhCHO**

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

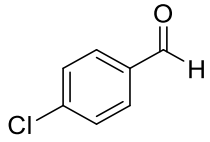
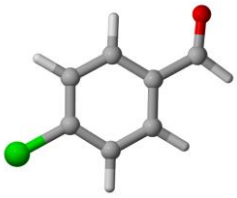
C	-1.4913430000	-1.0478040000	0.0000040000
C	-2.1201120000	0.2043800000	0.0000060000
C	-1.3433000000	1.3668470000	0.0000050000
C	0.0465100000	1.2927930000	0.0000020000
C	0.6489950000	0.0373580000	0.0000000000
C	-0.1067220000	-1.1373250000	0.0000020000
H	-1.8280350000	2.3381490000	0.0000060000
H	0.6503390000	2.1907530000	0.0000010000
H	0.3856500000	-2.1010560000	0.0000000000
H	-2.1041960000	-1.9415890000	0.0000050000
C	-3.5969310000	0.3090090000	0.0000100000
H	-3.9865050000	1.3488530000	-0.0000080000
O	-4.3563330000	-0.6337330000	-0.0000080000
Br	2.5574520000	-0.0833370000	-0.0000030000

thermodynamic data

Zero-point correction= 0.099081 (Hartree/Particle)
Thermal correction to Energy= 0.106858
Thermal correction to Enthalpy= 0.107802
Thermal correction to Gibbs Free Energy= 0.065148
Sum of electronic and zero-point Energies= -2919.111807
Sum of electronic and thermal Energies= -2919.104031
Sum of electronic and thermal Enthalpies= -2919.103086
Sum of electronic and thermal Free Energies= -2919.145741

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.054	28.282	89.773

B3LYP/6-311+G**	***p*-Cl-PhCHO**

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

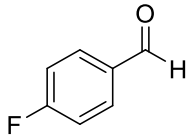
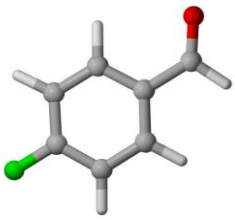
C	-0.8332430000	-1.0565030000	0.0000190000
C	-1.4396040000	0.2069510000	0.0000280000
C	-0.6418340000	1.3552520000	0.0000190000
C	0.7459170000	1.2558700000	0.0000040000
C	1.3255250000	-0.0098120000	-0.0000030000
C	0.5490090000	-1.1706750000	0.0000040000
H	-1.1089210000	2.3350170000	0.0000250000
H	1.3700640000	2.1399110000	-0.0000030000
H	1.0286720000	-2.1409580000	-0.0000030000
H	-1.4624000000	-1.9387750000	0.0000250000
C	-2.9139360000	0.3381930000	0.0000500000
H	-3.2844630000	1.3850040000	-0.0000500000
O	-3.6908030000	-0.5903420000	-0.0000420000
Cl	3.0724980000	-0.1513600000	-0.0000220000

thermodynamic data

Zero-point correction= 0.099752 (Hartree/Particle)
Thermal correction to Energy= 0.107266
Thermal correction to Enthalpy= 0.108210
Thermal correction to Gibbs Free Energy= 0.066939
Sum of electronic and zero-point Energies= -805.191644
Sum of electronic and thermal Energies= -805.184130
Sum of electronic and thermal Enthalpies= -805.183186
Sum of electronic and thermal Free Energies= -805.224457

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.310	27.799	86.862

B3LYP/6-311+G**	***p*-F-PhCHO**

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

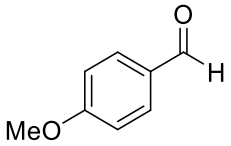
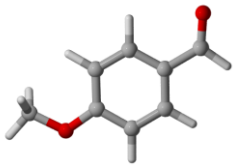
C	-0.4203990000	-1.0703940000	0.0000060000
C	-0.9897390000	0.2113190000	0.0000100000
C	-0.1603670000	1.3383440000	0.0000070000
C	1.2237970000	1.2007200000	0.0000010000
C	1.7515990000	-0.0821300000	-0.0000030000
C	0.9578030000	-1.2247310000	0.0000000000
H	-0.6019680000	2.3297170000	0.0000100000
H	1.8874360000	2.0560330000	-0.0000010000
H	1.4260830000	-2.2010510000	-0.0000030000
H	-1.0765750000	-1.9325890000	0.0000090000
C	-2.4585620000	0.3841180000	0.0000180000
H	-2.7988660000	1.4413620000	-0.0000190000
O	-3.2628490000	-0.5211750000	-0.0000180000
F	3.0935430000	-0.2297280000	-0.0000090000

thermodynamic data

Zero-point correction= 0.101102 (Hartree/Particle)
Thermal correction to Energy= 0.108240
Thermal correction to Enthalpy= 0.109185
Thermal correction to Gibbs Free Energy= 0.069226
Sum of electronic and zero-point Energies= -444.836729
Sum of electronic and thermal Energies= -444.829591
Sum of electronic and thermal Enthalpies= -444.828647
Sum of electronic and thermal Free Energies= -444.868605

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.922	26.931	84.100

B3LYP/6-311+G**	***p*-OMe-PhCHO**

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

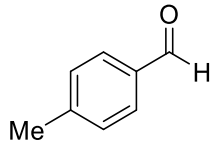
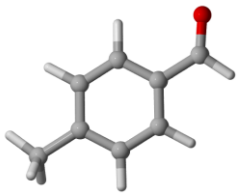
C	0.7329080000	-1.0012980000	-0.0000080000
C	1.4816770000	0.1808780000	-0.0000810000
C	0.8072220000	1.4115990000	-0.0000940000
C	-0.5753330000	1.4631220000	-0.0000360000
C	-1.3160720000	0.2718680000	0.0000360000
C	-0.6548290000	-0.9664440000	0.0000500000
H	1.3792240000	2.3344720000	-0.0001490000
H	-1.1093930000	2.4053130000	-0.0000450000
H	-1.2123900000	-1.8931950000	0.0001020000
H	1.2585640000	-1.9491960000	0.0000000000
C	2.9541510000	0.1471810000	-0.0001450000
H	3.4367790000	1.1482580000	-0.0001650000
O	3.6321360000	-0.8591920000	-0.0001010000
O	-2.6644690000	0.4178920000	0.0000860000
C	-3.4875890000	-0.7454440000	0.0002170000
H	-4.5126950000	-0.3801640000	0.0002820000
H	-3.3171930000	-1.3519840000	-0.8947600000
H	-3.3170440000	-1.3518860000	0.8952320000

thermodynamic data

Zero-point correction= 0.141691 (Hartree/Particle)
Thermal correction to Energy= 0.150607
Thermal correction to Enthalpy= 0.151551
Thermal correction to Gibbs Free Energy= 0.107577
Sum of electronic and zero-point Energies= -460.086341
Sum of electronic and thermal Energies= -460.077425
Sum of electronic and thermal Enthalpies= -460.076481
Sum of electronic and thermal Free Energies= -460.120455

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	94.507	33.217	92.551

B3LYP/6-311+G**	***p*-Me-PhCHO**

xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

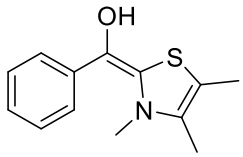
C	-0.4630580000	-1.0676050000	0.0001130000
C	-1.0460310000	0.2053250000	0.0001630000
C	-0.2203870000	1.3356600000	0.0001170000
C	1.1619530000	1.1970550000	0.0000390000
C	1.7541150000	-0.0728680000	-0.0000060000
C	0.9188540000	-1.1995650000	0.0000330000
H	-0.6674770000	2.3252600000	0.0001520000
H	1.7915450000	2.0809670000	0.0000110000
H	1.3627320000	-2.1894930000	0.0000000000
H	-1.1090780000	-1.9379090000	0.0001480000
C	-2.5144520000	0.3708250000	0.0002790000
H	-2.8585530000	1.4274050000	-0.0004460000
O	-3.3185460000	-0.5358330000	-0.0004240000
C	3.2557920000	-0.2155180000	-0.0000920000
H	3.6951860000	0.2623870000	-0.8808170000
H	3.5580090000	-1.2641450000	-0.0001360000
H	3.6952820000	0.2623410000	0.8806080000

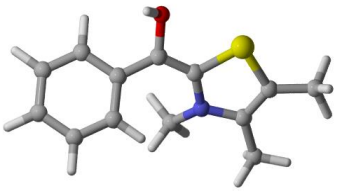
thermodynamic data

Zero-point correction= 0.136435 (Hartree/Particle)
Thermal correction to Energy= 0.143778
Thermal correction to Enthalpy= 0.144722
Thermal correction to Gibbs Free Energy= 0.104446
Sum of electronic and zero-point Energies= -384.861189
Sum of electronic and thermal Energies= -384.853846
Sum of electronic and thermal Enthalpies= -384.852902
Sum of electronic and thermal Free Energies= -384.893178

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.222	28.069	84.769

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.5869560000	-0.5271150000	-0.0790160000
N	-1.0030820000	0.7897130000	-0.2824830000
C	-2.3898190000	0.9790670000	-0.0779180000
C	-3.0725700000	-0.1536830000	0.1761280000
S	-2.0030220000	-1.5760720000	0.1716730000
C	-4.5278450000	-0.3557800000	0.4558280000
C	-2.9438510000	2.3713650000	-0.1327310000
C	0.6713630000	-1.0440370000	-0.0902360000
H	-2.3515060000	3.0533310000	0.4850740000
H	-3.9676830000	2.3889470000	0.2380880000
H	-2.9583560000	2.7767780000	-1.1498030000
H	-4.6950350000	-0.7631350000	1.4586930000
H	-4.9689170000	-1.0601950000	-0.2577790000
H	-5.0820400000	0.5805940000	0.3778640000
C	-0.2261920000	1.6972840000	-1.1249490000
H	0.3966540000	1.1089760000	-1.8012200000
H	0.4324620000	2.3489030000	-0.5440010000
H	-0.8977850000	2.3152530000	-1.7191630000
C	1.9541740000	-0.3544630000	0.0293570000
C	3.1117730000	-0.9051120000	-0.5598380000
C	4.3544240000	-0.3013240000	-0.3994230000
C	4.4849780000	0.8632040000	0.3576250000
C	3.3530430000	1.4098200000	0.9641550000
C	2.1085120000	0.8089680000	0.8112610000
H	3.0207150000	-1.8008440000	-1.1630920000
H	5.2260880000	-0.7399570000	-0.8733130000
H	3.4445820000	2.2991900000	1.5786760000
H	1.2489660000	1.2168610000	1.3301150000
O	0.7115350000	-2.4387700000	-0.2055060000
H	1.3287500000	-2.7858050000	0.4503040000
H	5.4545500000	1.3312560000	0.4827630000

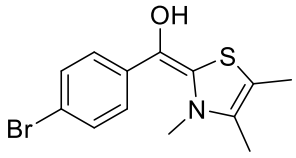
thermodynamic data

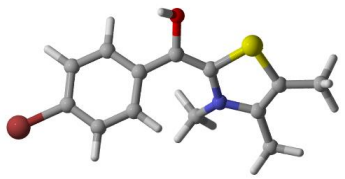
Zero-point correction= 0.250872 (Hartree/Particle)
Thermal correction to Energy= 0.267121
Thermal correction to Enthalpy= 0.268065
Thermal correction to Gibbs Free Energy= 0.207357
Sum of electronic and zero-point Energies= -1032.491596
Sum of electronic and thermal Energies= -1032.475348
Sum of electronic and thermal Enthalpies= -1032.474403

Sum of electronic and thermal Free Energies= -1032.535112

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.621	61.262	127.772

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

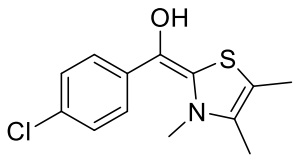
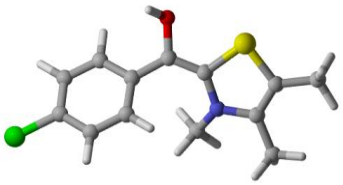
C	2.0505110000	-0.5713740000	0.0824360000
N	2.2554690000	0.7835940000	0.3388980000
C	3.5779290000	1.2127200000	0.0777390000
C	4.4219080000	0.2222880000	-0.2697460000
S	3.6012620000	-1.3561110000	-0.2932660000
C	5.8728160000	0.2787720000	-0.6286100000
C	3.8958970000	2.6741720000	0.1810210000
C	0.8945480000	-1.2907540000	0.1207270000
H	3.1662400000	3.2738010000	-0.3717290000
H	4.8808530000	2.8802840000	-0.2354580000
H	3.8987320000	3.0302100000	1.2162670000
H	6.0479300000	-0.0448930000	-1.6601160000
H	6.4621300000	-0.3766280000	0.0216710000
H	6.2691620000	1.2894110000	-0.5225160000
C	1.3851170000	1.5118810000	1.2608060000
H	0.8799630000	0.7956330000	1.9104740000
H	0.6186110000	2.0952650000	0.7429770000
H	1.9793840000	2.1830300000	1.8796990000
C	-0.4852330000	-0.8181080000	0.0876770000
C	-1.5127210000	-1.5869420000	0.6733270000
C	-2.8450150000	-1.1963230000	0.5987080000
C	-3.1783500000	-0.0249440000	-0.0754860000
C	-2.1935030000	0.7479110000	-0.6856930000
C	-0.8646480000	0.3481040000	-0.6088400000
H	-1.2554410000	-2.4906090000	1.2128820000
H	-3.6152800000	-1.7951010000	1.0682010000
Br	-5.0149090000	0.5218150000	-0.1805240000
H	-2.4630740000	1.6412510000	-1.2349300000
H	-0.1109580000	0.9274450000	-1.1284860000
O	1.0880010000	-2.6764420000	0.1698050000
H	0.5355470000	-3.0928880000	-0.5034650000

thermodynamic data

Zero-point correction= 0.240493 (Hartree/Particle)
Thermal correction to Energy= 0.258346
Thermal correction to Enthalpy= 0.259290
Thermal correction to Gibbs Free Energy= 0.193354
Sum of electronic and zero-point Energies= -3606.045154
Sum of electronic and thermal Energies= -3606.027301
Sum of electronic and thermal Enthalpies= -3606.026357
Sum of electronic and thermal Free Energies= -3606.092293

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.115	65.629	138.775

B3LYP/6-311+G**		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3607480000	-0.5672570000	0.0856290000
N	1.6233940000	0.7807550000	0.3276290000
C	2.9674350000	1.1459170000	0.0787450000
C	3.7701620000	0.1137800000	-0.2441250000
S	2.8794870000	-1.4267550000	-0.2569040000
C	5.2260410000	0.0991710000	-0.5862880000
C	3.3491930000	2.5931330000	0.1651330000
C	0.1722010000	-1.2309690000	0.1151120000
H	2.6567910000	3.2155250000	-0.4100320000
H	4.3495940000	2.7484810000	-0.2363500000
H	3.3498480000	2.9657020000	1.1945540000
H	5.3977450000	-0.2461160000	-1.6113700000
H	5.7772300000	-0.5737450000	0.0793710000
H	5.6675410000	1.0918560000	-0.4889230000
C	0.7787220000	1.5572000000	1.2342120000
H	0.2340210000	0.8713620000	1.8847330000
H	0.0457970000	2.1713620000	0.7034230000
H	1.3976840000	2.2052320000	1.8535620000
C	-1.1828890000	-0.6923690000	0.0557410000
C	-2.2550910000	-1.3999400000	0.6381590000
C	-3.5646200000	-0.9442310000	0.5390880000

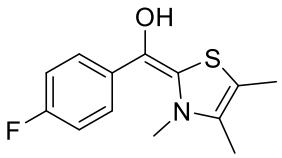
C	-3.8300880000	0.2317970000	-0.1560270000
C	-2.7998330000	0.9448870000	-0.7632100000
C	-1.4941810000	0.4805840000	-0.6626180000
H	-2.0505770000	-2.3072830000	1.1937820000
H	-4.3734520000	-1.4936650000	1.0044980000
Cl	-5.4863650000	0.8163260000	-0.2832520000
H	-3.0215690000	1.8419970000	-1.3278390000
H	-0.7053490000	1.0139240000	-1.1793090000
O	0.2980590000	-2.6235060000	0.1834950000
H	-0.2639230000	-3.0215330000	-0.4930240000

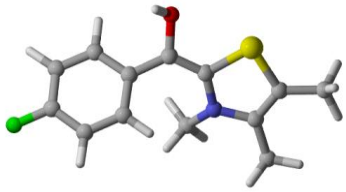
thermodynamic data

Zero-point correction= 0.241185 (Hartree/Particle)
Thermal correction to Energy= 0.258721
Thermal correction to Enthalpy= 0.259665
Thermal correction to Gibbs Free Energy= 0.195348
Sum of electronic and zero-point Energies= -1492.124644
Sum of electronic and thermal Energies= -1492.107108
Sum of electronic and thermal Enthalpies= -1492.106164
Sum of electronic and thermal Free Energies= -1492.170481

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.350	65.157	135.367

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9724660000	-0.5584320000	0.0844570000
N	1.2978190000	0.7807170000	0.3078450000
C	2.6636800000	1.0726120000	0.0799430000
C	3.4193080000	-0.0034380000	-0.2106360000
S	2.4536950000	-1.4989560000	-0.2136090000
C	4.8782730000	-0.0966980000	-0.5259540000
C	3.1173940000	2.4999460000	0.1501820000
C	-0.2467860000	-1.1604580000	0.1013260000
H	2.4657230000	3.1476110000	-0.4444010000
H	4.1300120000	2.5979700000	-0.2385580000

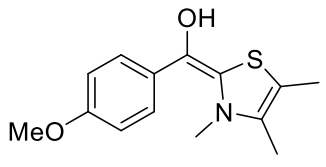
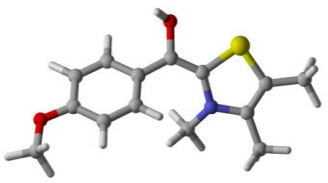
H	3.1226780000	2.8882710000	1.1738980000
H	5.0502010000	-0.4709430000	-1.5408400000
H	5.3838030000	-0.7825640000	0.1624530000
H	5.3674250000	0.8745540000	-0.4399150000
C	0.4789550000	1.6103470000	1.1902460000
H	-0.0867930000	0.9632730000	1.8628420000
H	-0.2347200000	2.2309330000	0.6408090000
H	1.1188240000	2.2578790000	1.7880420000
C	-1.5746530000	-0.5536670000	0.0180350000
C	-2.6824610000	-1.1851510000	0.6205200000
C	-3.9671820000	-0.6655150000	0.5003400000
C	-4.1524440000	0.4953330000	-0.2339350000
C	-3.0979400000	1.1414230000	-0.8606900000
C	-1.8185690000	0.6097480000	-0.7398200000
H	-2.5247060000	-2.0838040000	1.2045760000
H	-4.8163190000	-1.1447720000	0.9722790000
F	-5.4048400000	1.0088190000	-0.3539520000
H	-3.2866720000	2.0302250000	-1.4505390000
H	-0.9984670000	1.0822180000	-1.2668910000
O	-0.1955040000	-2.5571220000	0.1846990000
H	-0.7675020000	-2.9312590000	-0.4970400000

thermodynamic data

Zero-point correction= 0.242375 (Hartree/Particle)
Thermal correction to Energy= 0.259590
Thermal correction to Enthalpy= 0.260534
Thermal correction to Gibbs Free Energy= 0.197230
Sum of electronic and zero-point Energies= -1131.768410
Sum of electronic and thermal Energies= -1131.751195
Sum of electronic and thermal Enthalpies= -1131.750251
Sum of electronic and thermal Free Energies= -1131.813555

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.895	64.364	133.235

B3LYP/6-311+G**		

xyz-matrix

XYZ file generated by gabedit : coordinates in Angstrom

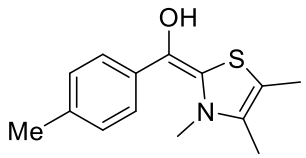
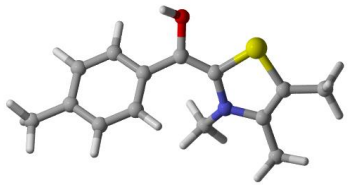
C	1.3731480000	-0.5727670000	0.0484040000
N	1.5887250000	0.7779780000	0.3463010000
C	2.9213090000	1.1947650000	0.1186360000
C	3.7573600000	0.2082310000	-0.2565920000
S	2.9226210000	-1.3625470000	-0.3408250000
C	5.2101260000	0.2620570000	-0.6080480000
C	3.2618580000	2.6468430000	0.2742260000
C	0.2137660000	-1.2791630000	0.0616550000
H	2.5397030000	3.2774630000	-0.2534620000
H	4.2486580000	2.8529260000	-0.1381430000
H	3.2747820000	2.9648850000	1.3220120000
H	5.3860870000	-0.0254700000	-1.6503740000
H	5.7897320000	-0.4242760000	0.0190080000
H	5.6183210000	1.2631930000	-0.4627680000
C	0.7223800000	1.4644490000	1.3020890000
H	0.3579750000	0.7467880000	2.0420910000
H	-0.1474500000	1.9193630000	0.8210320000
H	1.2831350000	2.2421630000	1.8168250000
C	-1.1671080000	-0.7921490000	0.0639800000
C	-2.1835630000	-1.5276870000	0.7123110000
C	-3.5061710000	-1.1202900000	0.6763730000
C	-3.8715710000	0.0413190000	-0.0160940000
C	-2.8882020000	0.7777940000	-0.6805700000
C	-1.5593850000	0.3544800000	-0.6438250000
H	-1.9166150000	-2.4215640000	1.2640750000
H	-4.2786710000	-1.6847140000	1.1854080000
H	-3.1418750000	1.6645750000	-1.2462640000
H	-0.8167600000	0.9125570000	-1.2025530000
O	0.3880400000	-2.6689860000	0.0419910000
H	-0.2029000000	-3.0448420000	-0.6220490000
O	-5.2005240000	0.3611590000	0.0108380000
C	-5.6315420000	1.5261740000	-0.6767130000
H	-6.7066260000	1.5873870000	-0.5148670000
H	-5.1536440000	2.4276400000	-0.2768400000
H	-5.4314110000	1.4551060000	-1.7516650000

thermodynamic data

Zero-point correction= 0.282864 (Hartree/Particle)
Thermal correction to Energy= 0.301869
Thermal correction to Enthalpy= 0.302813
Thermal correction to Gibbs Free Energy= 0.235436
Sum of electronic and zero-point Energies= -1147.014931
Sum of electronic and thermal Energies= -1146.995926
Sum of electronic and thermal Enthalpies= -1146.994982
Sum of electronic and thermal Free Energies= -1147.062359

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.426	70.634	141.808

B3LYP/6-311+G**	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.0026640000	-0.5583150000	0.0816310000
N	1.3154990000	0.7842550000	0.3084770000
C	2.6773600000	1.0895060000	0.0790180000
C	3.4437640000	0.0218620000	-0.2151550000
S	2.4939680000	-1.4841180000	-0.2192900000
C	4.9028900000	-0.0552530000	-0.5338600000
C	3.1175440000	2.5211440000	0.1501630000
C	-0.2104900000	-1.1711520000	0.1006830000
H	2.4574740000	3.1631420000	-0.4413470000
H	4.1280670000	2.6297810000	-0.2413740000
H	3.1220990000	2.9080960000	1.1744500000
H	5.0768310000	-0.4296690000	-1.5484430000
H	5.4181290000	-0.7340390000	0.1545620000
H	5.3813460000	0.9216760000	-0.4511440000
C	0.4891720000	1.6010140000	1.1955160000
H	-0.0532820000	0.9457030000	1.8797070000
H	-0.2467990000	2.1988140000	0.6505150000
H	1.1212760000	2.2681610000	1.7798800000
C	-1.5442490000	-0.5773200000	0.0204190000
C	-2.6474800000	-1.2165410000	0.6236750000
C	-3.9314520000	-0.7013300000	0.5017930000
C	-4.1861500000	0.4666600000	-0.2290140000
C	-3.0968880000	1.0911030000	-0.8446560000
C	-1.8067560000	0.5817860000	-0.7331830000
H	-2.4822850000	-2.1136950000	1.2091940000
H	-4.7546830000	-1.2142460000	0.9907420000
H	-3.2625220000	1.9834740000	-1.4408090000
H	-0.9946820000	1.0660910000	-1.2631630000
O	-0.1436470000	-2.5677360000	0.1781980000
H	-0.7473420000	-2.9424500000	-0.4749790000
C	-5.5860110000	1.0175910000	-0.3497280000
H	-5.6041790000	1.9272070000	-0.9538760000
H	-6.0038800000	1.2617200000	0.6324440000
H	-6.2618880000	0.2936980000	-0.8164630000

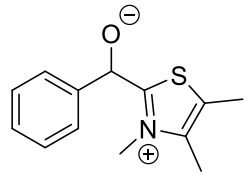
thermodynamic data

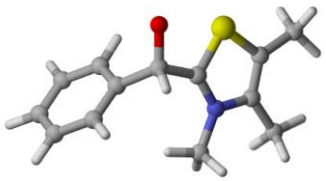
Zero-point correction= 0.277520 (Hartree/Particle)

Thermal correction to Energy= 0.295075
Thermal correction to Enthalpy= 0.296020
Thermal correction to Gibbs Free Energy= 0.231238
Sum of electronic and zero-point Energies= -1071.792142
Sum of electronic and thermal Energies= -1071.774586
Sum of electronic and thermal Enthalpies= -1071.773642
Sum of electronic and thermal Free Energies= -1071.838423

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	185.163	65.501	136.343

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.5739570000	-0.3036000000	0.5496120000
N	-1.0732670000	0.9255100000	0.4127600000
C	-2.3837580000	0.9674790000	-0.1039750000
C	-2.8592500000	-0.2819030000	-0.3539160000
S	-1.6677770000	-1.5191580000	0.0722720000
C	-4.1903390000	-0.6779860000	-0.9160820000
C	-3.0554620000	2.2897000000	-0.3132330000
C	0.7355830000	-0.9389760000	1.0772980000
H	-3.0903480000	2.8797660000	0.6075420000
H	-4.0810120000	2.1393620000	-0.6468850000
H	-2.5468680000	2.8896030000	-1.0746950000
H	-4.6718760000	-1.4338380000	-0.2897150000
H	-4.0851640000	-1.1036810000	-1.9186510000
H	-4.8675720000	0.1744060000	-0.9864710000
C	-0.3262170000	2.1287780000	0.7958870000
H	0.7093880000	1.8554600000	0.9767370000
H	-0.7567450000	2.5651640000	1.6994760000
H	-0.3607060000	2.8575750000	-0.0134780000
C	1.9506420000	-0.3656900000	0.3183410000
C	2.1168770000	-0.6516210000	-1.0411080000
C	3.2315770000	-0.1860590000	-1.7311210000
C	4.2094810000	0.5604590000	-1.0676410000
C	4.0648060000	0.8294220000	0.2905960000
C	2.9389460000	0.3673440000	0.9771430000
H	4.8312620000	1.3855660000	0.8200500000
H	2.8405590000	0.5587070000	2.0423450000

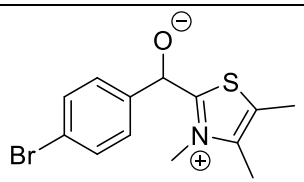
O	0.5612240000	-2.2540100000	0.9556970000
H	5.0834330000	0.9133140000	-1.6040670000
H	1.3795650000	-1.2717610000	-1.5393190000
H	3.3489190000	-0.4146450000	-2.7852370000
H	0.8211090000	-0.5590470000	2.1303070000

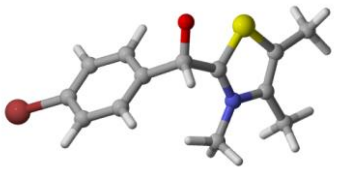
thermodynamic data

Zero-point correction= 0.249742 (Hartree/Particle)
Thermal correction to Energy= 0.265924
Thermal correction to Enthalpy= 0.266868
Thermal correction to Gibbs Free Energy= 0.204803
Sum of electronic and zero-point Energies= -1032.460244
Sum of electronic and thermal Energies= -1032.444062
Sum of electronic and thermal Enthalpies= -1032.443118
Sum of electronic and thermal Free Energies= -1032.505184

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	166.870	59.888	130.628

B3LYP/6-311+G**		





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0242420000	-0.4711530000	0.5059190000
N	-2.3406800000	0.8174870000	0.6395750000
C	-3.5061910000	1.2058790000	-0.0512400000
C	-4.0629220000	0.1570980000	-0.7144260000
S	-3.1334400000	-1.3263980000	-0.4635850000
C	-5.2910150000	0.1424680000	-1.5725960000
C	-3.9650070000	2.6303150000	0.0115290000
C	-0.9286930000	-1.4286810000	1.0410230000
H	-4.1354500000	2.9590970000	1.0411740000
H	-4.9022390000	2.7451080000	-0.5306430000
H	-3.2384040000	3.3127890000	-0.4407040000
H	-5.9659440000	-0.6656720000	-1.2781490000
H	-5.0360840000	-0.0118790000	-2.6254510000
H	-5.8441890000	1.0796340000	-1.4979410000
C	-1.5547390000	1.7463100000	1.4594760000
H	-0.6326230000	1.2571840000	1.7589200000

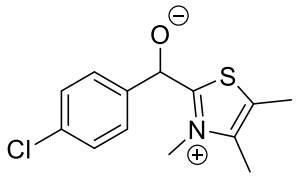
H	-2.1231960000	2.0357370000	2.3454140000
H	-1.3084990000	2.6344230000	0.8777970000
C	0.4708880000	-0.8995560000	0.6637560000
C	0.8713070000	-0.8980450000	-0.6762550000
C	2.1436750000	-0.4742800000	-1.0448380000
C	3.0343590000	-0.0631510000	-0.0535670000
C	2.6761930000	-0.0822470000	1.2876980000
C	1.3894970000	-0.5025430000	1.6350300000
H	3.3861780000	0.2116740000	2.0504010000
H	1.1127620000	-0.5415610000	2.6849350000
O	-1.2290500000	-2.6234570000	0.5379120000
Br	4.7969840000	0.5193650000	-0.5525900000
H	0.1845880000	-1.2672770000	-1.4299180000
H	2.4458990000	-0.4735190000	-2.0846080000
H	-1.0037080000	-1.3403910000	2.1574060000

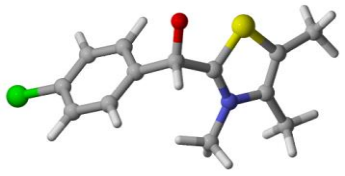
thermodynamic data

Zero-point correction= 0.239535 (Hartree/Particle)
Thermal correction to Energy= 0.257216
Thermal correction to Enthalpy= 0.258160
Thermal correction to Gibbs Free Energy= 0.191207
Sum of electronic and zero-point Energies= -3606.013988
Sum of electronic and thermal Energies= -3605.996307
Sum of electronic and thermal Enthalpies= -3605.995363
Sum of electronic and thermal Free Energies= -3606.062317

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.406	64.197	140.916

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3445890000	-0.4133520000	0.5434850000
N	-1.7238420000	0.8649920000	0.5632370000
C	-2.9403140000	1.1225250000	-0.1005720000
C	-3.4683180000	-0.0146860000	-0.6275400000
S	-2.4499080000	-1.4173170000	-0.2759510000
C	-4.7300070000	-0.1785760000	-1.4186840000

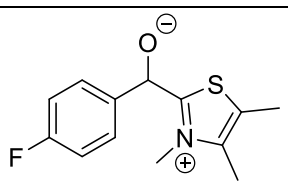
C	-3.4737380000	2.5210740000	-0.1533360000
C	-0.1758510000	-1.2553880000	1.1167420000
H	-3.5894230000	2.9503440000	0.8463190000
H	-4.4521270000	2.5302480000	-0.6311170000
H	-2.8210510000	3.1854770000	-0.7285580000
H	-5.3443640000	-0.9877780000	-1.0149050000
H	-4.5124840000	-0.4233690000	-2.4628130000
H	-5.3322950000	0.7309150000	-1.4093660000
C	-0.9508010000	1.9092110000	1.2450920000
H	0.0233900000	1.5084600000	1.5091020000
H	-1.4734150000	2.2332930000	2.1471770000
H	-0.8114930000	2.7598500000	0.5784740000
C	1.1744520000	-0.7050320000	0.6106500000
C	1.5098840000	-0.8349430000	-0.7408350000
C	2.7390060000	-0.3961630000	-1.2199620000
C	3.6535500000	0.1648330000	-0.3293640000
C	3.3606400000	0.2799270000	1.0227830000
C	2.1163380000	-0.1587390000	1.4822220000
H	4.0930370000	0.6912140000	1.7063140000
H	1.8920370000	-0.0930210000	2.5431810000
O	-0.4379350000	-2.5099440000	0.7589300000
Cl	5.2160170000	0.7198280000	-0.9298810000
H	0.8082260000	-1.3182230000	-1.4114830000
H	2.9954750000	-0.4964840000	-2.2673490000
H	-0.2004170000	-1.0504680000	2.2200330000

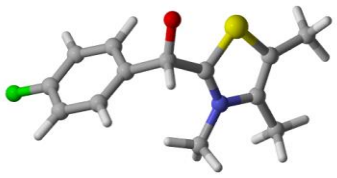
thermodynamic data

Zero-point correction= 0.240139 (Hartree/Particle)
Thermal correction to Energy= 0.257584
Thermal correction to Enthalpy= 0.258528
Thermal correction to Gibbs Free Energy= 0.192808
Sum of electronic and zero-point Energies= -1492.093611
Sum of electronic and thermal Energies= -1492.076166
Sum of electronic and thermal Enthalpies= -1492.075222
Sum of electronic and thermal Free Energies= -1492.140942

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.637	63.756	138.321

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

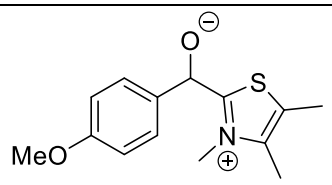
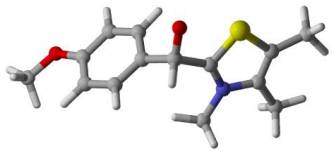
C	0.9574070000	-0.3577430000	-0.5605250000
N	1.3935480000	0.9003110000	-0.4849090000
C	2.6579720000	1.0436240000	0.1221720000
C	3.1626430000	-0.1590620000	0.5071920000
S	2.0614810000	-1.4795480000	0.0908770000
C	4.4618730000	-0.4497290000	1.1941860000
C	3.2581030000	2.4081520000	0.2686800000
C	-0.2800810000	-1.0929860000	-1.1360790000
H	3.3397690000	2.9214600000	-0.6940610000
H	4.2605840000	2.3335170000	0.6871390000
H	2.6690570000	3.0442840000	0.9371110000
H	5.0547600000	-1.1718550000	0.6258590000
H	4.2954870000	-0.8746270000	2.1885020000
H	5.0636490000	0.4518900000	1.3156020000
C	0.6311530000	2.0348370000	-1.0179720000
H	-0.3830110000	1.7078480000	-1.2285480000
H	1.0979680000	2.4037360000	-1.9335590000
H	0.5968290000	2.8343810000	-0.2787710000
C	-1.5742670000	-0.5330790000	-0.5086360000
C	-1.8410970000	-0.7667500000	0.8449210000
C	-3.0220550000	-0.3221430000	1.4296190000
C	-3.9451790000	0.3454940000	0.6350610000
C	-3.7329060000	0.5718670000	-0.7127760000
C	-2.5350340000	0.1243880000	-1.2773600000
H	-4.4923610000	1.0700150000	-1.3031250000
H	-2.3624330000	0.2717140000	-2.3396230000
O	-0.0579420000	-2.3851570000	-0.9079150000
F	-5.1039250000	0.7775070000	1.2008680000
H	-1.1255440000	-1.3346130000	1.4288710000
H	-3.2422610000	-0.4964660000	2.4759700000
H	-0.3033590000	-0.7882210000	-2.2164230000

thermodynamic data

Zero-point correction= 0.241391 (Hartree/Particle)
Thermal correction to Energy= 0.258467
Thermal correction to Enthalpy= 0.259411
Thermal correction to Gibbs Free Energy= 0.194943
Sum of electronic and zero-point Energies= -1131.737842
Sum of electronic and thermal Energies= -1131.720765
Sum of electronic and thermal Enthalpies= -1131.719821
Sum of electronic and thermal Free Energies= -1131.784290

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.191	62.907	135.686

B3LYP/6-311+G**	

xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

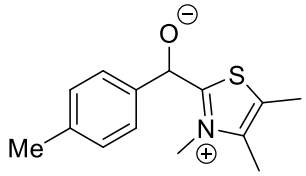
C	1.3617240000	-0.3963210000	-0.5409930000
N	1.7100700000	0.8910090000	-0.5310830000
C	2.9517890000	1.1537530000	0.0817180000
C	3.5312570000	0.0115900000	0.5389490000
S	2.5269670000	-1.4031340000	0.1868180000
C	4.8344840000	-0.1483760000	1.2606220000
C	3.4550540000	2.5623990000	0.1611050000
C	0.1853050000	-1.2429510000	-1.0838260000
H	3.5086310000	3.0315690000	-0.8258610000
H	4.4563890000	2.5780400000	0.5886250000
H	2.8179650000	3.1886190000	0.7939390000
H	5.4454770000	-0.9290420000	0.7994410000
H	4.6758100000	-0.4328690000	2.3053780000
H	5.4155490000	0.7749540000	1.2525360000
C	0.8767460000	1.9374950000	-1.1332710000
H	-0.1043750000	1.5221820000	-1.3465020000
H	1.3356230000	2.2978420000	-2.0563130000
H	0.7635070000	2.7660640000	-0.4346250000
C	-1.1510330000	-0.7261750000	-0.5167110000
C	-1.4200410000	-0.8364820000	0.8552280000
C	-2.6348840000	-0.4304420000	1.3811690000
C	-3.6316670000	0.0837990000	0.5382580000
C	-3.3928960000	0.1786330000	-0.8319850000
C	-2.1529430000	-0.2282930000	-1.3423200000
O	0.4905110000	-2.5024570000	-0.7717690000
H	-2.8478060000	-0.5158610000	2.4405180000
H	0.1640860000	-1.0102720000	-2.1824720000
O	-4.7984230000	0.4502720000	1.1528080000
C	-5.8637710000	0.9306500000	0.3478510000
H	-6.6828430000	1.1452460000	1.0328130000
H	-5.5854550000	1.8492350000	-0.1815370000
H	-6.1877490000	0.1776700000	-0.3792540000
H	-0.6711370000	-1.2791400000	1.5030100000
H	-1.9839710000	-0.1731730000	-2.4143960000
H	-4.1531120000	0.5438270000	-1.5098910000

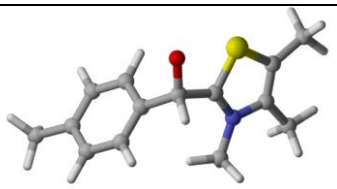
thermodynamic data

Zero-point correction= 0.281896 (Hartree/Particle)
Thermal correction to Energy= 0.300772
Thermal correction to Enthalpy= 0.301716
Thermal correction to Gibbs Free Energy= 0.232928
Sum of electronic and zero-point Energies= -1146.983891
Sum of electronic and thermal Energies= -1146.965015
Sum of electronic and thermal Enthalpies= -1146.964071
Sum of electronic and thermal Free Energies= -1147.032859

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.737	69.147	144.776

B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9884970000	-0.3754460000	0.5494300000
N	-1.4072590000	0.8898030000	0.5017670000
C	-2.6655150000	1.0642280000	-0.1099350000
C	-3.1824010000	-0.1217560000	-0.5287420000
S	-2.0998750000	-1.4672980000	-0.1394990000
C	-4.4803440000	-0.3783810000	-1.2315560000
C	-3.2477680000	2.4396210000	-0.2246470000
C	0.2341020000	-1.1400000000	1.1124090000
H	-3.3234240000	2.9307550000	0.7500670000
H	-4.2507920000	2.3879230000	-0.6453170000
H	-2.6498020000	3.0838800000	-0.8772560000
H	-5.0929110000	-1.0957300000	-0.6780200000
H	-4.3124900000	-0.7946430000	-2.2293000000
H	-5.0635160000	0.5360910000	-1.3483740000
C	-0.6317300000	1.9989040000	1.0683190000
H	0.3818740000	1.6563820000	1.2576950000
H	-1.0880200000	2.3386270000	2.0005350000
H	-0.5973620000	2.8238090000	0.3575850000
C	1.5389270000	-0.5727480000	0.5165070000
C	1.8178600000	-0.7466990000	-0.8435280000
C	3.0107870000	-0.2876660000	-1.3879780000
C	3.9780490000	0.3455210000	-0.5922960000
C	3.7038390000	0.4997160000	0.7670840000

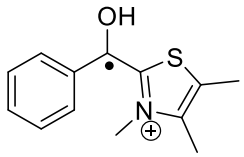
C	2.5003470000	0.0453500000	1.3139630000
O	-0.0029440000	-2.4235550000	0.8444140000
H	3.2056120000	-0.4323540000	-2.4468730000
H	0.2492480000	-0.8694120000	2.2020120000
H	1.1011690000	-1.2765150000	-1.4617820000
H	2.3211100000	0.1556510000	2.3803000000
H	4.4419120000	0.9673840000	1.4120050000
C	5.2874420000	0.8057400000	-1.1875660000
H	5.8202680000	1.4750690000	-0.5084180000
H	5.1331410000	1.3356230000	-2.1320260000
H	5.9457670000	-0.0442500000	-1.3973170000

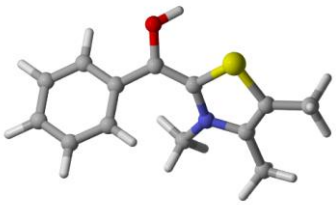
thermodynamic data

Zero-point correction= 0.276810 (Hartree/Particle)
Thermal correction to Energy= 0.294922
Thermal correction to Enthalpy= 0.295867
Thermal correction to Gibbs Free Energy= 0.228625
Sum of electronic and zero-point Energies= -1071.760371
Sum of electronic and thermal Energies= -1071.742258
Sum of electronic and thermal Enthalpies= -1071.741314
Sum of electronic and thermal Free Energies= -1071.808556

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	185.067	65.983	141.522

(u)B3LYP/6-311+G**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

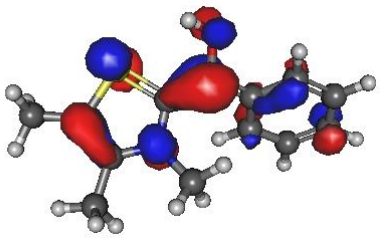
C	0.5922470000	-0.5360480000	0.1412290000
N	1.0220600000	0.7362230000	0.4018800000
C	2.3798870000	0.9501240000	0.1540360000
C	3.0396160000	-0.1738120000	-0.2518210000
S	1.9373370000	-1.5256020000	-0.3737550000
C	4.4830810000	-0.3684740000	-0.5923240000

C	2.9724590000	2.3082530000	0.3659870000
C	-0.7092350000	-1.0683410000	0.2371780000
H	2.3820170000	3.0819420000	-0.1303200000
H	3.9799950000	2.3484600000	-0.0421970000
H	3.0370390000	2.5607850000	1.4287020000
H	4.6072050000	-0.6799980000	-1.6330690000
H	4.9349550000	-1.1362710000	0.0415910000
H	5.0452430000	0.5531330000	-0.4483710000
C	0.2015300000	1.7523240000	1.0851130000
H	-0.6350920000	1.2662260000	1.5775410000
H	-0.1814830000	2.4859550000	0.3752180000
H	0.8144690000	2.2521240000	1.8321650000
C	-1.9584340000	-0.3695640000	0.0066860000
C	-3.1377710000	-0.8322780000	0.6276320000
C	-4.3491310000	-0.2038800000	0.3777190000
C	-4.4124070000	0.8759930000	-0.5052680000
C	-3.2556330000	1.3247740000	-1.1477220000
C	-2.0376700000	0.7102770000	-0.8975290000
H	-3.0884690000	-1.6752330000	1.3045730000
H	-5.2484250000	-0.5574540000	0.8673370000
H	-5.3621690000	1.3582380000	-0.7037240000
H	-3.3123390000	2.1400060000	-1.8590300000
H	-1.1551460000	1.0297080000	-1.4396760000
O	-0.8435750000	-2.3998860000	0.4394890000
H	-0.0722450000	-2.7885500000	0.8747770000

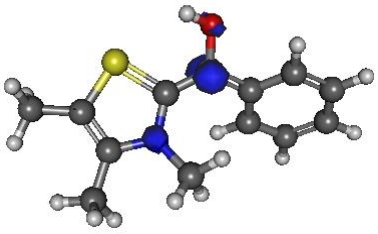
thermodynamic data

Zero-point correction= 0.252142 (Hartree/Particle)
Thermal correction to Energy= 0.268223
Thermal correction to Enthalpy= 0.269167
Thermal correction to Gibbs Free Energy= 0.207584
Sum of electronic and zero-point Energies= -1032.275215
Sum of electronic and thermal Energies= -1032.259135
Sum of electronic and thermal Enthalpies= -1032.258190
Sum of electronic and thermal Free Energies= -1032.319773

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	168.313	60.601	129.612

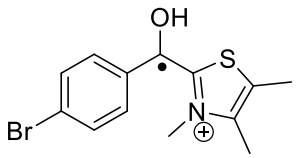
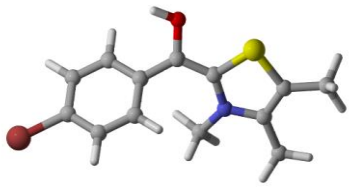


Alpha-HOMO (6311)



Spin-density (6311)

(u)B3LYP/6-311+G**	

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

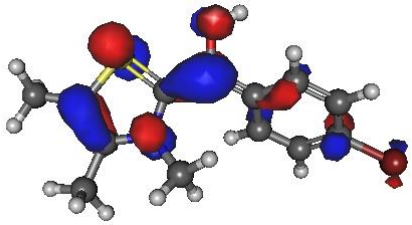
C	2.0630350000	-0.5591970000	0.1012950000
N	2.2857030000	0.7594010000	0.3936520000
C	3.5880840000	1.1882340000	0.1390690000
C	4.4080800000	0.1846380000	-0.2973020000
S	3.5418200000	-1.3245620000	-0.4127510000
C	5.8594700000	0.2339700000	-0.6579200000
C	3.9658420000	2.6179170000	0.3688300000
C	0.8752760000	-1.3013260000	0.1725070000
H	3.2527000000	3.2997760000	-0.1003320000
H	4.9457350000	2.8215160000	-0.0576720000
H	4.0142120000	2.8587390000	1.4352720000
H	6.0055250000	0.0850160000	-1.7316950000
H	6.4183480000	-0.5470600000	-0.1361470000
H	6.2997320000	1.1924450000	-0.3864360000
C	1.3150050000	1.6211630000	1.0900910000
H	0.6039360000	1.0003170000	1.6267930000
H	0.7767420000	2.2557430000	0.3849020000
H	1.8483260000	2.2439220000	1.8046050000
C	-0.4981020000	-0.8206550000	0.1194770000
C	-1.4949580000	-1.4584620000	0.8863720000
C	-2.8214170000	-1.0615410000	0.7974070000
C	-3.1733720000	-0.0280430000	-0.0735450000
C	-2.2053450000	0.6063580000	-0.8568590000
C	-0.8794000000	0.2121580000	-0.7588310000
H	-1.2261650000	-2.2427380000	1.5857530000
H	-3.5767100000	-1.5440020000	1.4039720000
Br	-4.9862790000	0.5141800000	-0.2026730000
H	-2.4933520000	1.3862350000	-1.5498060000
H	-0.1414000000	0.6766480000	-1.4025500000
O	1.0996970000	-2.6359640000	0.2389760000
H	0.3123110000	-3.1292440000	-0.0299950000

thermodynamic data

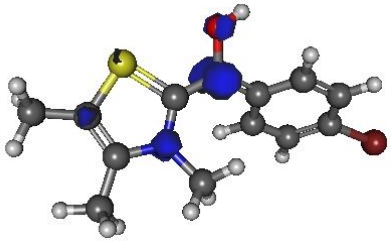
Zero-point correction= 0.241987 (Hartree/Particle)
Thermal correction to Energy= 0.259575
Thermal correction to Enthalpy= 0.260519

Thermal correction to Gibbs Free Energy= 0.193863
Sum of electronic and zero-point Energies= -3605.829883
Sum of electronic and thermal Energies= -3605.812295
Sum of electronic and thermal Enthalpies= -3605.811351
Sum of electronic and thermal Free Energies= -3605.878006

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.886	64.722	140.288

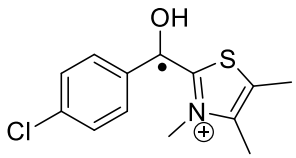


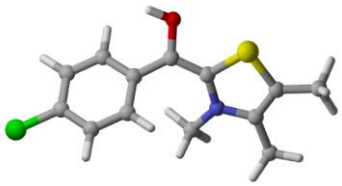
Alpha-HOMO (6311)



Spin-density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

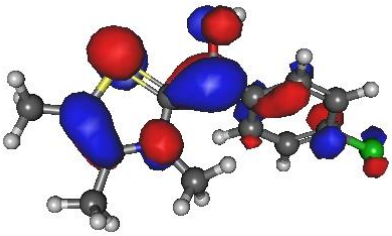
C	-1.3771130000	0.5517820000	0.1027940000
N	-1.6565690000	-0.7602680000	0.3755350000
C	-2.9821780000	-1.1224530000	0.1387300000
C	-3.7616030000	-0.0735260000	-0.2644820000
S	-2.8270610000	1.3948490000	-0.3703420000
C	-5.2197690000	-0.0485310000	-0.5993250000
C	-3.4237050000	-2.5364020000	0.3515610000
C	-0.1549020000	1.2362080000	0.1660990000
H	-2.7547830000	-3.2429170000	-0.1454990000
H	-4.4214230000	-2.6847510000	-0.0560680000
H	-3.4601000000	-2.7945330000	1.4144350000
H	-5.3767820000	0.0989110000	-1.6718500000
H	-5.7268450000	0.7655880000	-0.0754450000
H	-5.7056360000	-0.9797430000	-0.3109720000
C	-0.7158590000	-1.6810410000	1.0364510000
H	0.0415540000	-1.1062940000	1.5606040000

H	-0.2314440000	-2.3350050000	0.3100950000
H	-1.2632940000	-2.2832530000	1.7580260000
C	1.1937590000	0.6925820000	0.0834830000
C	2.2293530000	1.2655240000	0.8502750000
C	3.5335630000	0.8080100000	0.7350380000
C	3.8234160000	-0.2216020000	-0.1624700000
C	2.8172390000	-0.7925650000	-0.9460400000
C	1.5135900000	-0.3379550000	-0.8216820000
H	2.0065480000	2.0464540000	1.5691290000
H	4.3224100000	1.2370610000	1.3392300000
Cl	5.4566650000	-0.7942130000	-0.3145790000
H	3.0640530000	-1.5698320000	-1.6577580000
H	0.7455940000	-0.7527630000	-1.4640890000
O	-0.3149530000	2.5784920000	0.2583720000
H	0.4906790000	3.0388600000	-0.0148380000

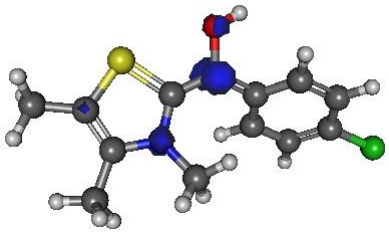
thermodynamic data

Zero-point correction= 0.242607 (Hartree/Particle)
Thermal correction to Energy= 0.259941
Thermal correction to Enthalpy= 0.260885
Thermal correction to Gibbs Free Energy= 0.195703
Sum of electronic and zero-point Energies= -1491.909524
Sum of electronic and thermal Energies= -1491.892190
Sum of electronic and thermal Enthalpies= -1491.891246
Sum of electronic and thermal Free Energies= -1491.956429

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.115	64.276	137.188

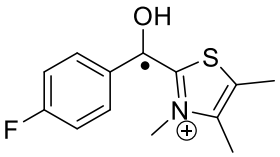


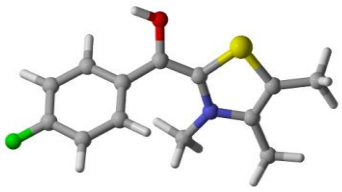
Alpha-HOMO (6311)



Spin-density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

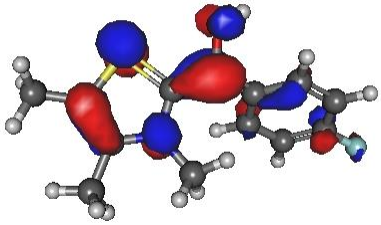
31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9917850000	-0.5423540000	0.1045970000
N	1.3295200000	0.7609700000	0.3548950000
C	2.6754800000	1.0531690000	0.1385390000
C	3.4110280000	-0.0407790000	-0.2260200000
S	2.4087320000	-1.4645860000	-0.3203860000
C	4.8726440000	-0.1431560000	-0.5296910000
C	3.1808870000	2.4486490000	0.3304150000
C	-0.2624890000	-1.1654280000	0.1551010000
H	2.5587650000	3.1751320000	-0.1977080000
H	4.1935230000	2.5390090000	-0.0567820000
H	3.2058870000	2.7293380000	1.3878980000
H	5.0434190000	-0.3239220000	-1.5950070000
H	5.3296190000	-0.9674920000	0.0234880000
H	5.3969560000	0.7706760000	-0.2533110000
C	0.4219010000	1.7431950000	0.9718670000
H	-0.3801110000	1.2207940000	1.4840130000
H	-0.0052120000	2.4082140000	0.2199250000
H	0.9809940000	2.3291900000	1.6979140000
C	-1.5831970000	-0.5579060000	0.0433920000
C	-2.6502930000	-1.0556280000	0.8204830000
C	-3.9295940000	-0.5376280000	0.6817720000
C	-4.1414380000	0.4725320000	-0.2496490000
C	-3.1187510000	0.9770910000	-1.0465100000
C	-1.8414730000	0.4585960000	-0.8973130000
H	-2.4691610000	-1.8250460000	1.5628200000
H	-4.7554800000	-0.8957190000	1.2832280000
F	-5.3733270000	0.9736270000	-0.3900560000
H	-3.3393950000	1.7438820000	-1.7783450000
H	-1.0468710000	0.8124210000	-1.5435740000
O	-0.1705940000	-2.5122930000	0.2684720000
H	-0.9935230000	-2.9363020000	-0.0118380000

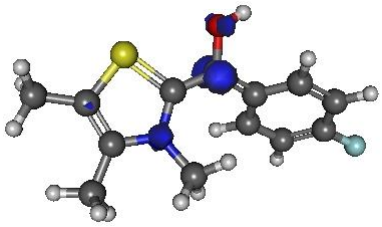
thermodynamic data

Zero-point correction= 0.243933 (Hartree/Particle)
Thermal correction to Energy= 0.260903
Thermal correction to Enthalpy= 0.261847
Thermal correction to Gibbs Free Energy= 0.197817
Sum of electronic and zero-point Energies= -1131.554073
Sum of electronic and thermal Energies= -1131.537103
Sum of electronic and thermal Enthalpies= -1131.536159
Sum of electronic and thermal Free Energies= -1131.600188

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.719	63.442	134.761

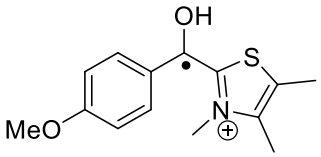


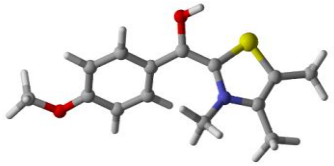
Alpha-HOMO (6311)



Spin-density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

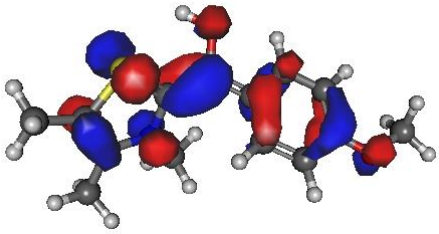
C	1.3731270000	-0.5645710000	-0.1463540000
N	1.7048010000	0.7314470000	-0.4389470000
C	3.0301850000	1.0693160000	-0.1474640000
C	3.7652310000	0.0222340000	0.3225820000
S	2.7777660000	-1.4182200000	0.4525500000
C	5.2044630000	-0.0356740000	0.7262040000
C	3.5106990000	2.4668860000	-0.3859990000
C	0.1260090000	-1.2086480000	-0.2664120000
H	2.8383230000	3.2005670000	0.0651400000
H	3.5896630000	2.6927820000	-1.4536450000
H	4.4961270000	2.6081320000	0.0528010000
H	5.7365570000	-0.8111540000	0.1685720000
H	5.3103730000	-0.2598600000	1.7913530000
H	5.7031350000	0.9128430000	0.5310240000
C	0.8421350000	1.6370610000	-1.2168590000
H	0.3927040000	2.3966090000	-0.5763300000
H	0.0525650000	1.0606410000	-1.6889500000
H	1.4416360000	2.1191270000	-1.9868680000
C	-1.1763130000	-0.6228520000	-0.0935100000
C	-1.3824580000	0.5191270000	0.7206990000
C	-2.6447860000	1.0238840000	0.9259230000
C	-3.7639280000	0.4069860000	0.3275610000
C	-3.5821280000	-0.7397190000	-0.4656260000

C	-2.3095440000	-1.2468090000	-0.6600830000
H	-4.4259220000	-1.2347960000	-0.9258800000
H	-2.1772440000	-2.1344160000	-1.2650180000
H	-2.8125300000	1.8801950000	1.5670980000
O	-4.9460090000	0.9788030000	0.5861170000
C	-6.1503820000	0.4088280000	0.0528220000
H	-6.9544380000	1.0445340000	0.4144390000
H	-6.1348430000	0.4208660000	-1.0399550000
H	-6.2927450000	-0.6104090000	0.4203690000
O	0.1238550000	-2.5579520000	-0.4323170000
H	0.9270300000	-2.8721240000	-0.8690990000
H	-0.5448970000	0.9747520000	1.2354750000

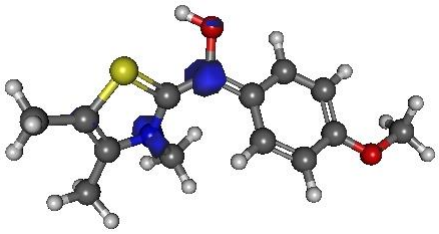
thermodynamic data

Zero-point correction= 0.284691 (Hartree/Particle)
Thermal correction to Energy= 0.303371
Thermal correction to Enthalpy= 0.304315
Thermal correction to Gibbs Free Energy= 0.236997
Sum of electronic and zero-point Energies= -1146.806376
Sum of electronic and thermal Energies= -1146.787696
Sum of electronic and thermal Enthalpies= -1146.786752
Sum of electronic and thermal Free Energies= -1146.854070

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.368	69.872	141.683

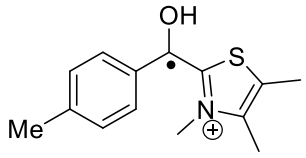


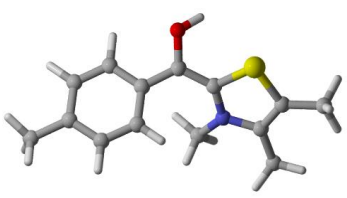
Alpha-HOMO (6311)



Spin-density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

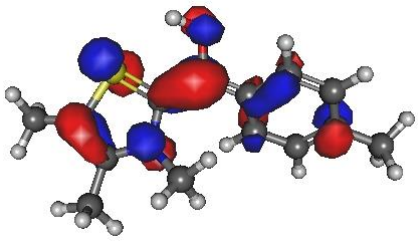
34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.0040070000	-0.5650640000	0.1404580000
N	1.3454930000	0.7263230000	0.4372730000
C	2.6739200000	1.0533930000	0.1527350000
C	3.4019260000	0.0001340000	-0.3180100000
S	2.4017500000	-1.4285920000	-0.4569140000
C	4.8422670000	-0.0694430000	-0.7155910000
C	3.1675530000	2.4451330000	0.3976430000
C	-0.2493580000	-1.1990600000	0.2563840000
H	2.5039000000	3.1871720000	-0.0525640000
H	4.1555840000	2.5779910000	-0.0378500000
H	3.2457960000	2.6656760000	1.4664710000
H	4.9504010000	-0.2924550000	-1.7807330000
H	5.3651630000	-0.8505470000	-0.1571920000
H	5.3480870000	0.8743930000	-0.5164930000
C	0.4813820000	1.6449300000	1.1994140000
H	-0.3125030000	1.0779680000	1.6753540000
H	0.0381020000	2.3962490000	0.5452170000
H	1.0796170000	2.1347960000	1.9652230000
C	-1.5514230000	-0.5945500000	0.0896590000
C	-2.6816820000	-1.1863440000	0.6942740000
C	-3.9423760000	-0.6497410000	0.4973000000
C	-4.1384510000	0.4764830000	-0.3179100000
C	-3.0153480000	1.0436240000	-0.9422670000
C	-1.7467640000	0.5247210000	-0.7471550000
H	-2.5548850000	-2.0616110000	1.3182360000
H	-4.7965630000	-1.1135260000	0.9779580000
C	-5.5097030000	1.0619950000	-0.5103380000
H	-3.1480200000	1.8881900000	-1.6093030000
H	-0.9092490000	0.9511600000	-1.2872750000
H	-5.5897630000	1.5927900000	-1.4605060000
H	-5.7332200000	1.7798400000	0.2870100000
H	-6.2812860000	0.2905290000	-0.4773270000
O	-0.2702420000	-2.5452480000	0.4137380000
H	0.5386290000	-2.8806870000	0.8240070000

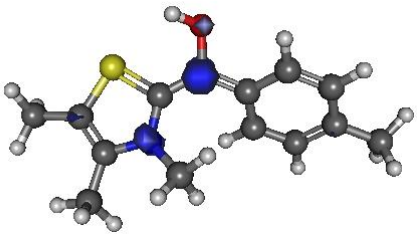
thermodynamic data

Zero-point correction= 0.279432 (Hartree/Particle)
Thermal correction to Energy= 0.297332
Thermal correction to Enthalpy= 0.298276
Thermal correction to Gibbs Free Energy= 0.232354
Sum of electronic and zero-point Energies= -1071.578934
Sum of electronic and thermal Energies= -1071.561034
Sum of electronic and thermal Enthalpies= -1071.560090
Sum of electronic and thermal Free Energies= -1071.626012

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.579	66.662	138.744

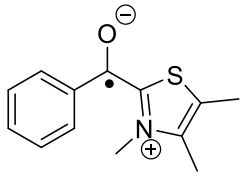


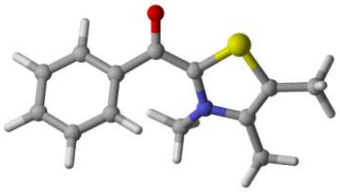
Alpha-HOMO (6311)



Spin-density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

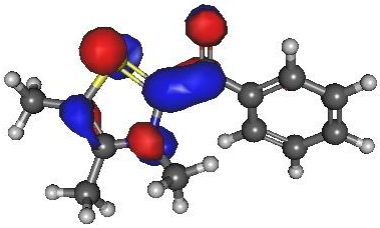
C	0.5894880000	-0.5647310000	0.1274050000
N	0.9764230000	0.7549680000	0.3073470000
C	2.3495000000	0.9685010000	0.0932100000
C	3.0397400000	-0.1601930000	-0.1946140000
S	1.9842840000	-1.5773540000	-0.1994270000
C	4.4941570000	-0.3354230000	-0.5002520000
C	2.8884650000	2.3638240000	0.1902260000
C	-0.6955680000	-1.1944170000	0.1293220000
H	2.3731540000	3.0362850000	-0.5029380000
H	3.9485970000	2.3815050000	-0.0567860000
H	2.7769170000	2.7788090000	1.1966810000
H	4.6488110000	-0.6875520000	-1.5252640000
H	4.9476040000	-1.0733390000	0.1690970000
H	5.0428520000	0.5996550000	-0.3819420000
C	0.2194830000	1.6940120000	1.1445020000
H	-0.7745030000	1.3013540000	1.3251230000
H	0.1227130000	2.6610690000	0.6483560000
H	0.7243220000	1.8306670000	2.1061050000
O	-0.7448150000	-2.4423850000	0.2068020000
C	-1.9682100000	-0.4177720000	-0.0284980000
C	-3.1184180000	-0.8833640000	0.6233620000
C	-4.3402080000	-0.2419910000	0.4467790000
C	-4.4388690000	0.8595820000	-0.4046700000
C	-3.3065110000	1.3131040000	-1.0802460000
C	-2.0792840000	0.6813880000	-0.8910970000
H	-3.0358270000	-1.7589750000	1.2558920000
H	-5.2200020000	-0.6061540000	0.9658880000
H	-5.3934460000	1.3529930000	-0.5496530000

H	-3.3814520000	2.1522570000	-1.7633200000
H	-1.2072940000	1.0282490000	-1.4348200000

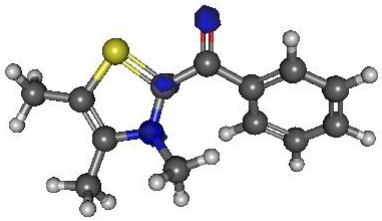
thermodynamic data

Zero-point correction= 0.239152 (Hartree/Particle)
Thermal correction to Energy= 0.255097
Thermal correction to Enthalpy= 0.256042
Thermal correction to Gibbs Free Energy= 0.194541
Sum of electronic and zero-point Energies= -1031.897965
Sum of electronic and thermal Energies= -1031.882020
Sum of electronic and thermal Enthalpies= -1031.881075
Sum of electronic and thermal Free Energies= -1031.942576

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.076	59.202	129.440

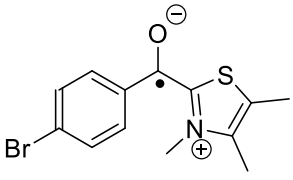


Alpha-HOMO (6311)



spin density (6311)

(u)B3LYP/6-311+G**	



xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

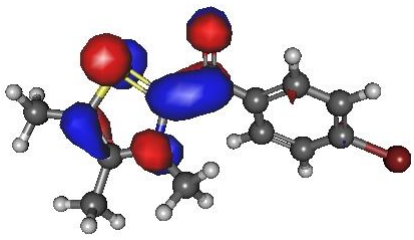
C	-2.2838960000	-0.6434190000	0.8183700000
C	-3.2042010000	0.0402550000	0.0288960000
C	-2.8143160000	1.1265780000	-0.7552580000
C	-1.4804420000	1.5205830000	-0.7497040000
C	-0.5205190000	0.8310560000	0.0098730000
C	-0.9467950000	-0.2435720000	0.8048770000
C	0.8835910000	1.3618060000	-0.0189060000

C	1.9896590000	0.4491780000	0.0490240000
O	1.0444450000	2.6029520000	-0.1466150000
S	1.8710750000	-1.2945610000	-0.2059970000
C	3.6266820000	-1.4662200000	-0.1937270000
C	4.2249280000	-0.2625540000	0.0007020000
N	3.3302400000	0.8016910000	0.1336490000
C	5.6992780000	0.0039450000	0.0777160000
C	4.2282040000	-2.8235750000	-0.3876190000
C	3.7876510000	2.1358690000	0.5381900000
Br	-5.0374770000	-0.5074130000	0.0319380000
H	-2.6067880000	-1.4681430000	1.4445000000
H	-3.5464390000	1.6559220000	-1.3555610000
H	-1.1596520000	2.3779830000	-1.3319780000
H	-0.2440680000	-0.7605560000	1.4506870000
H	6.0309530000	0.6703570000	-0.7279170000
H	5.9783250000	0.4734840000	1.0282110000
H	6.2611170000	-0.9271990000	-0.0105180000
H	5.3181430000	-2.7891520000	-0.3111180000
H	3.8643620000	-3.5324340000	0.3669840000
H	3.9773780000	-3.2385940000	-1.3721070000
H	4.1112270000	2.1266390000	1.5865820000
H	4.6261690000	2.4434520000	-0.0914820000
H	2.9575760000	2.8256290000	0.4046080000

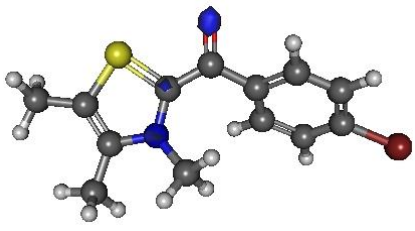
thermodynamic data

Zero-point correction= 0.228871 (Hartree/Particle)
Thermal correction to Energy= 0.246291
Thermal correction to Enthalpy= 0.247235
Thermal correction to Gibbs Free Energy= 0.180816
Sum of electronic and zero-point Energies= -3605.469027
Sum of electronic and thermal Energies= -3605.451606
Sum of electronic and thermal Enthalpies= -3605.450662
Sum of electronic and thermal Free Energies= -3605.517081

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	154.550	63.477	139.791

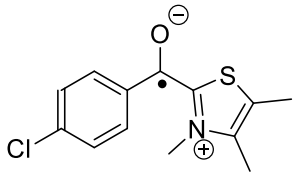
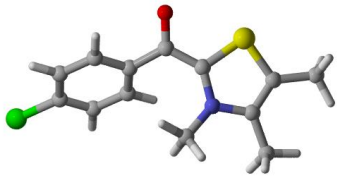


Alpha-HOMO (6311)



spin density (6311)

(u)B3LYP/6-311+G**	

xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

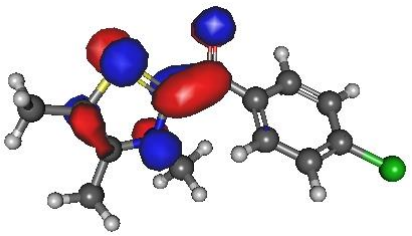
C	1.3731010000	-0.6025920000	-0.1073070000
N	1.6130510000	0.7349400000	-0.3683300000
C	2.9377470000	1.1303620000	-0.1239680000
C	3.7459230000	0.1107450000	0.2554820000
S	2.8652280000	-1.4178970000	0.3179080000
C	5.2021000000	0.1286680000	0.6001560000
C	3.3192860000	2.5695720000	-0.2983250000
C	0.1754600000	-1.3841890000	-0.1412110000
H	2.6286020000	3.2316350000	0.2316660000
H	3.3264170000	2.8711440000	-1.3507280000
H	4.3176450000	2.7470000000	0.0981470000
H	5.7627830000	-0.5670760000	-0.0322180000
H	5.3716890000	-0.1677530000	1.6402490000
H	5.6327010000	1.1207530000	0.4603840000
C	0.6909120000	1.5775100000	-1.1339030000
H	0.1210160000	2.2497130000	-0.4882270000
H	-0.0099460000	0.9437220000	-1.6713940000
H	1.2517930000	2.1675800000	-1.8585080000
O	0.2778590000	-2.6321950000	-0.1736280000
C	-1.1848020000	-0.7633860000	-0.0641290000
C	-1.4768280000	0.3102010000	0.7867150000
C	-2.7752840000	0.7992040000	0.9081520000
C	-3.7918970000	0.2087070000	0.1647690000
C	-3.5346050000	-0.8729910000	-0.6745950000
C	-2.2366750000	-1.3603740000	-0.7726670000
Cl	-5.4337800000	0.8278870000	0.3010190000
H	-4.3414880000	-1.3289130000	-1.2343200000
H	-2.0225220000	-2.2205520000	-1.3953080000
H	-2.9990620000	1.6180640000	1.5802450000
H	-0.6898880000	0.7513170000	1.3884950000

thermodynamic data

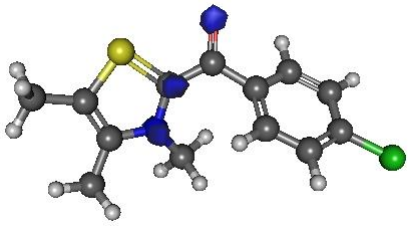
Zero-point correction= 0.229446 (Hartree/Particle)
Thermal correction to Energy= 0.246714
Thermal correction to Enthalpy= 0.247658
Thermal correction to Gibbs Free Energy= 0.182144
Sum of electronic and zero-point Energies= -1491.530995

Sum of electronic and thermal Energies= -1491.513727
Sum of electronic and thermal Enthalpies= -1491.512783
Sum of electronic and thermal Free Energies= -1491.578297

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	154.815	63.092	137.887

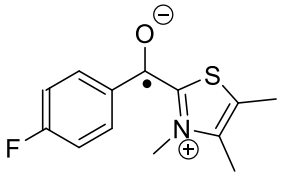


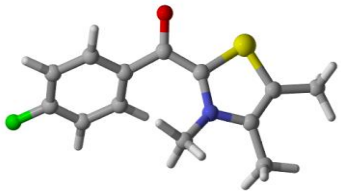
Alpha-HOMO (6311)



spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

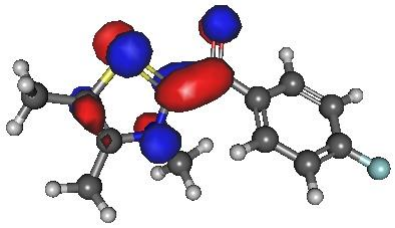
C	0.9818420000	-0.5970220000	-0.1224950000
N	1.2852170000	0.7336440000	-0.3565560000
C	2.6307040000	1.0565890000	-0.1167410000
C	3.3906210000	-0.0095260000	0.2323290000
S	2.4359540000	-1.4948770000	0.2697860000
C	4.8478080000	-0.0714570000	0.5669480000
C	3.0775530000	2.4803200000	-0.2599900000
C	-0.2564080000	-1.3128880000	-0.1435750000
H	2.4400520000	3.1564920000	0.3172220000
H	3.0591090000	2.8169560000	-1.3013770000
H	4.0975520000	2.5964460000	0.1025800000
H	5.3674570000	-0.7857660000	-0.0796250000
H	5.0085790000	-0.3920500000	1.6012960000
H	5.3286490000	0.8990160000	0.4390450000
C	0.4205890000	1.6263000000	-1.1337500000
H	-0.0351640000	2.3959670000	-0.5065620000
H	-0.3728780000	1.0449320000	-1.5939530000

H	1.0024150000	2.1056570000	-1.9223670000
O	-0.2218880000	-2.5634370000	-0.1962680000
C	-1.5797450000	-0.6196720000	-0.0323880000
C	-1.7909780000	0.4700150000	0.8226760000
C	-3.0584120000	1.0274990000	0.9767660000
C	-4.1110900000	0.4809070000	0.2600630000
C	-3.9473000000	-0.6085050000	-0.5834640000
C	-2.6787090000	-1.1625960000	-0.7136140000
F	-5.3470570000	1.0231280000	0.3979460000
H	-4.8018000000	-1.0115540000	-1.1130460000
H	-2.5231790000	-2.0334890000	-1.3384630000
H	-3.2381430000	1.8584230000	1.6478200000
H	-0.9646620000	0.8710640000	1.3987870000

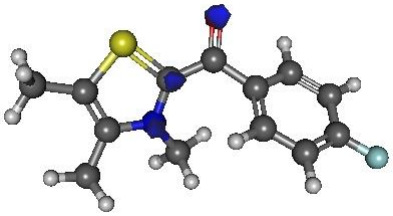
thermodynamic data

Zero-point correction= 0.230864 (Hartree/Particle)
Thermal correction to Energy= 0.247696
Thermal correction to Enthalpy= 0.248640
Thermal correction to Gibbs Free Energy= 0.184685
Sum of electronic and zero-point Energies= -1131.175209
Sum of electronic and thermal Energies= -1131.158377
Sum of electronic and thermal Enthalpies= -1131.157433
Sum of electronic and thermal Free Energies= -1131.221388

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	155.431	62.198	134.604

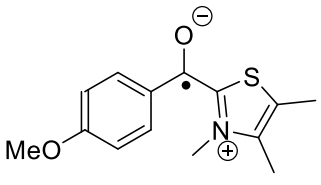


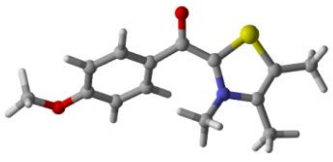
Alpha-HOMO (6311)



spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

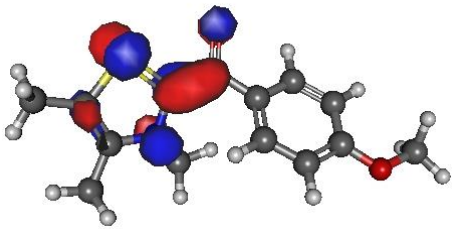
C	1.3821010000	-0.6014590000	-0.1379450000
N	1.6466200000	0.7463130000	-0.3435290000
C	2.9874890000	1.0932330000	-0.0969320000
C	3.7713850000	0.0432440000	0.2426920000
S	2.8558510000	-1.4692350000	0.2551840000
C	5.2243210000	0.0153500000	0.5998750000
C	3.3961600000	2.5300380000	-0.2201440000
C	0.1573370000	-1.3439190000	-0.1482720000
H	2.8019590000	3.1682770000	0.4416350000
H	3.2718380000	2.9055010000	-1.2403710000
H	4.4432060000	2.6543380000	0.0511040000
H	5.7650570000	-0.7048860000	-0.0222700000
H	5.3752950000	-0.2788780000	1.6436420000
H	5.6901210000	0.9911550000	0.4571510000
C	0.8500350000	1.5655320000	-1.2666680000
H	0.6963080000	2.5643470000	-0.8559570000
H	-0.1196910000	1.1048750000	-1.4174280000
H	1.3571410000	1.6464520000	-2.2341500000
O	0.2216780000	-2.5918430000	-0.2073050000
C	-1.1763190000	-0.6772050000	-0.0228770000
C	-1.3951080000	0.4529210000	0.7823000000
C	-2.6667730000	0.9774880000	0.9519420000
C	-3.7625160000	0.3845770000	0.3115750000
C	-3.5662530000	-0.7489520000	-0.4840230000
C	-2.2841390000	-1.2737400000	-0.6314240000
H	-4.3969020000	-1.2328270000	-0.9803110000
H	-2.1303830000	-2.1708600000	-1.2190810000
H	-2.8404750000	1.8380320000	1.5870650000
H	-0.5621530000	0.9126960000	1.3026300000
O	-4.9711700000	0.9776260000	0.5308550000
C	-6.1280020000	0.4095960000	-0.0695660000
H	-6.9625750000	1.0340100000	0.2450890000
H	-6.0580090000	0.4219280000	-1.1626190000
H	-6.2930680000	-0.6170870000	0.2740280000

thermodynamic data

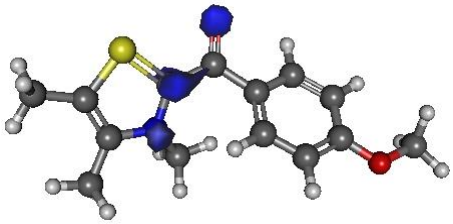
Zero-point correction= 0.271541 (Hartree/Particle)
Thermal correction to Energy= 0.290056
Thermal correction to Enthalpy= 0.291000
Thermal correction to Gibbs Free Energy= 0.223687
Sum of electronic and zero-point Energies= -1146.422555
Sum of electronic and thermal Energies= -1146.404041
Sum of electronic and thermal Enthalpies= -1146.403096
Sum of electronic and thermal Free Energies= -1146.470409

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	182.013	68.399	141.672

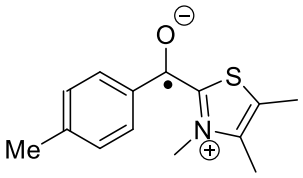


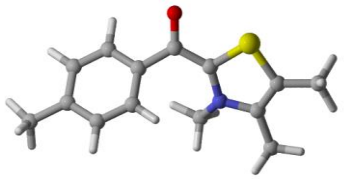
Alpha-HOMO (6311)



spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

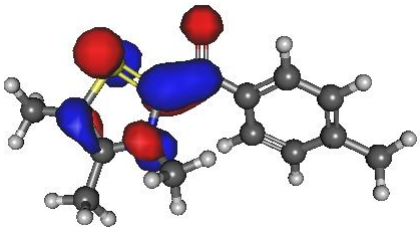
C	1.3821010000	-0.6014590000	-0.1379450000
N	1.6466200000	0.7463130000	-0.3435290000
C	2.9874890000	1.0932330000	-0.0969320000
C	3.7713850000	0.0432440000	0.2426920000
S	2.8558510000	-1.4692350000	0.2551840000
C	5.2243210000	0.0153500000	0.5998750000
C	3.3961600000	2.5300380000	-0.2201440000
C	0.1573370000	-1.3439190000	-0.1482720000
H	2.8019590000	3.1682770000	0.4416350000
H	3.2718380000	2.9055010000	-1.2403710000
H	4.4432060000	2.6543380000	0.0511040000
H	5.7650570000	-0.7048860000	-0.0222700000
H	5.3752950000	-0.2788780000	1.6436420000
H	5.6901210000	0.9911550000	0.4571510000
C	0.8500350000	1.5655320000	-1.2666680000
H	0.6963080000	2.5643470000	-0.8559570000
H	-0.1196910000	1.1048750000	-1.4174280000
H	1.3571410000	1.6464520000	-2.2341500000
O	0.2216780000	-2.5918430000	-0.2073050000
C	-1.1763190000	-0.6772050000	-0.0228770000
C	-1.3951080000	0.4529210000	0.7823000000
C	-2.6667730000	0.9774880000	0.9519420000
C	-3.7625160000	0.3845770000	0.3115750000

C	-3.5662530000	-0.7489520000	-0.4840230000
C	-2.2841390000	-1.2737400000	-0.6314240000
H	-4.3969020000	-1.2328270000	-0.9803110000
H	-2.1303830000	-2.1708600000	-1.2190810000
H	-2.8404750000	1.8380320000	1.5870650000
H	-0.5621530000	0.9126960000	1.3026300000
O	-4.9711700000	0.9776260000	0.5308550000
C	-6.1280020000	0.4095960000	-0.0695660000
H	-6.9625750000	1.0340100000	0.2450890000
H	-6.0580090000	0.4219280000	-1.1626190000
H	-6.2930680000	-0.6170870000	0.2740280000

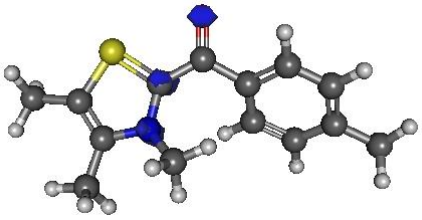
thermodynamic data

Zero-point correction= 0.266271 (Hartree/Particle)
Thermal correction to Energy= 0.283218
Thermal correction to Enthalpy= 0.284162
Thermal correction to Gibbs Free Energy= 0.220415
Sum of electronic and zero-point Energies= -1071.198501
Sum of electronic and thermal Energies= -1071.181555
Sum of electronic and thermal Enthalpies= -1071.180611
Sum of electronic and thermal Free Energies= -1071.244357

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.722	63.275	134.167

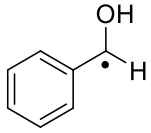


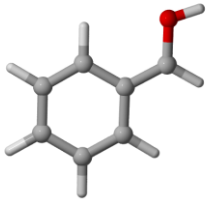
Alpha-HOMO (6311)



spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

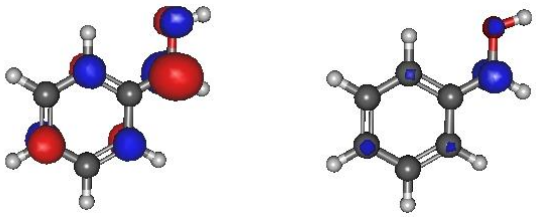
15
XYZ file generated by gabedit : coordinates in Angstrom

C	0.0192430000	-1.0810320000	0.0000000000
C	0.4927470000	0.2607070000	0.0000720000
C	-0.4718980000	1.3071230000	0.0000320000
C	-1.8257470000	1.0231210000	-0.0001000000
C	-2.2758540000	-0.3038820000	-0.0001910000
C	-1.3406630000	-1.3452970000	-0.0001290000
H	-0.1344840000	2.3386980000	0.0001010000
H	-2.5431140000	1.8365930000	-0.0001370000
H	-3.3374470000	-0.5210720000	-0.0003070000
H	-1.6829230000	-2.3746770000	-0.0001720000
H	0.7366380000	-1.8917490000	0.0000650000
C	1.8632660000	0.5697420000	0.0001310000
H	2.2302910000	1.5890750000	0.0006190000
O	2.7863260000	-0.4365260000	0.0001230000
H	3.6738690000	-0.0675590000	-0.0000440000

thermodynamic data

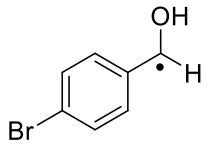
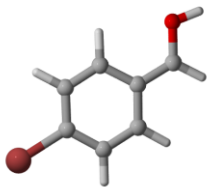
Zero-point correction= 0.119224 (Hartree/Particle)
Thermal correction to Energy= 0.126256
Thermal correction to Enthalpy= 0.127200
Thermal correction to Gibbs Free Energy= 0.087580
Sum of electronic and zero-point Energies= -346.116365
Sum of electronic and thermal Energies= -346.109333
Sum of electronic and thermal Enthalpies= -346.108388
Sum of electronic and thermal Free Energies= -346.148008

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.227	27.197	83.387



Alpha-HOMO (6311) spin density (6311)

(u)B3LYP/6-311+G**	

xyz-matrix

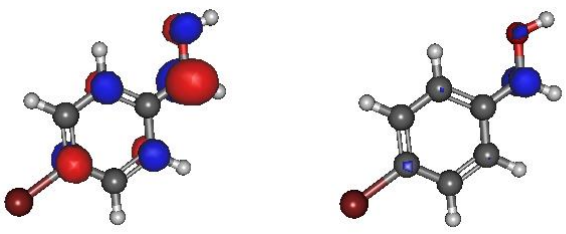
15
XYZ file generated by gabedit : coordinates in Angstrom

C	1.4591400000	-1.0082170000	0.0000950000
C	2.0955770000	0.2647110000	0.0001640000
C	1.2642580000	1.4197210000	0.0001630000
C	-0.1136740000	1.3118420000	0.0000590000
C	-0.7054200000	0.0439050000	-0.0000300000
C	0.0789150000	-1.1124620000	-0.0000030000
H	1.7198130000	2.4043770000	0.0002330000
H	-0.7318530000	2.2006010000	0.0000450000
H	-0.3929340000	-2.0869430000	-0.0000480000
H	2.0674780000	-1.9034670000	0.0001240000
C	3.4918210000	0.4014790000	0.0001950000
H	3.9820030000	1.3674720000	0.0006250000
Br	-2.6146950000	-0.1073360000	-0.0001960000
O	4.2798180000	-0.7114490000	0.0003100000
H	5.2075750000	-0.4595700000	-0.0004500000

thermodynamic data

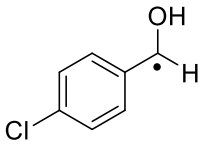
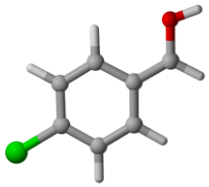
Zero-point correction= 0.109064 (Hartree/Particle)
Thermal correction to Energy= 0.117560
Thermal correction to Enthalpy= 0.118504
Thermal correction to Gibbs Free Energy= 0.074019
Sum of electronic and zero-point Energies= -2919.669934
Sum of electronic and thermal Energies= -2919.661438
Sum of electronic and thermal Enthalpies= -2919.660494
Sum of electronic and thermal Free Energies= -2919.704979

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.770	31.491	93.627



Alpha-HOMO (6311) spin density (6311)

(u)B3LYP/6-311+G**	

xyz-matrix

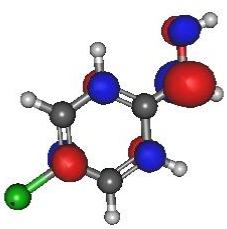
15
XYZ file generated by gabedit : coordinates in Angstrom

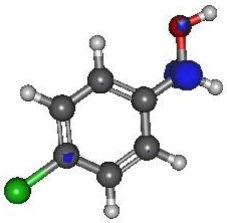
C	0.8006470000	-1.0202730000	0.0000300000
C	1.4086380000	0.2666030000	0.0001010000
C	0.5516670000	1.4027650000	0.0001130000
C	-0.8231090000	1.2635750000	0.0000140000
C	-1.3863520000	-0.0167230000	-0.0000800000
C	-0.5767200000	-1.1549300000	-0.0000630000
H	0.9852030000	2.3972460000	0.0001910000
H	-1.4648510000	2.1356020000	0.0000100000
H	-1.0310320000	-2.1379200000	-0.0001100000
H	1.4290860000	-1.9014580000	0.0000510000
C	2.8015890000	0.4348250000	0.0001170000
H	3.2697580000	1.4116550000	0.0005750000
Cl	-3.1353060000	-0.1935470000	-0.0002190000
O	3.6146800000	-0.6603220000	0.0002900000
H	4.5364340000	-0.3872950000	-0.0006960000

thermodynamic data

Zero-point correction= 0.109694 (Hartree/Particle)
Thermal correction to Energy= 0.117932
Thermal correction to Enthalpy= 0.118876
Thermal correction to Gibbs Free Energy= 0.075772
Sum of electronic and zero-point Energies= -805.749489
Sum of electronic and thermal Energies= -805.741251
Sum of electronic and thermal Enthalpies= -805.740307
Sum of electronic and thermal Free Energies= -805.783411

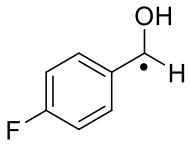
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.004	31.030	90.721

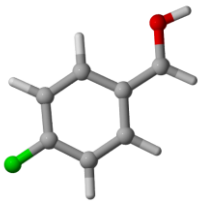




Alpha-HOMO (6311) spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

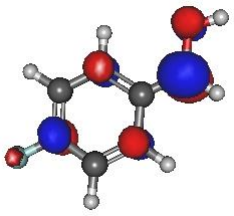
15
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.3940120000	-1.0370160000	0.0001380000
C	-0.9546270000	0.2710730000	0.0000260000
C	-0.0598750000	1.3777990000	-0.0001070000
C	1.3106670000	1.1907660000	-0.0000770000
C	1.8120910000	-0.1080300000	0.0000480000
C	0.9794170000	-1.2208590000	0.0001550000
H	-0.4601680000	2.3859420000	-0.0002220000
H	1.9959010000	2.0295590000	-0.0001640000
H	1.4144640000	-2.2129650000	0.0002480000
H	-1.0548560000	-1.8939110000	0.0002430000
C	-2.3431940000	0.4876490000	0.0000320000
H	-2.7790280000	1.4791190000	-0.0001850000
F	3.1579570000	-0.2912850000	0.0000660000
O	-3.1920610000	-0.5819490000	-0.0004210000
H	-4.1042360000	-0.2788770000	0.0015530000

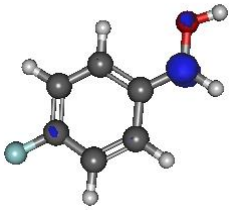
thermodynamic data

Zero-point correction= 0.110836 (Hartree/Particle)
Thermal correction to Energy= 0.118750
Thermal correction to Enthalpy= 0.119695
Thermal correction to Gibbs Free Energy= 0.077801
Sum of electronic and zero-point Energies= -445.392986
Sum of electronic and thermal Energies= -445.385071
Sum of electronic and thermal Enthalpies= -445.384127
Sum of electronic and thermal Free Energies= -445.426021

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.517	30.311	88.173

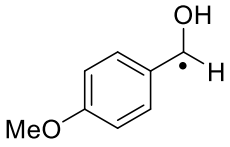


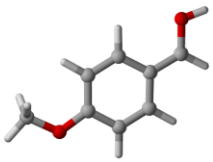
Alpha-HOMO (6311)



spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

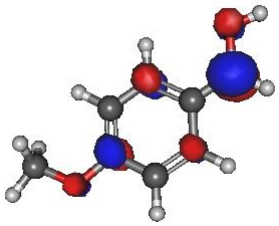
19
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7061280000	-0.9594460000	-0.0000580000
C	-1.4509250000	0.2483830000	-0.0000200000
C	-0.7133430000	1.4683520000	0.0000170000
C	0.6630720000	1.4729860000	0.0000160000
C	1.3812150000	0.2627660000	-0.0000220000
C	0.6836040000	-0.9503860000	-0.0000620000
H	-1.2491780000	2.4120510000	0.0000500000
H	1.2194400000	2.4028780000	0.0000460000
H	1.2135170000	-1.8939710000	-0.0001020000
H	-1.2351200000	-1.9038500000	-0.0000910000
C	-2.8546940000	0.2694720000	-0.0000170000
H	-3.4260030000	1.1896010000	0.0000150000
O	2.7434350000	0.3811640000	-0.0000380000
C	3.5264440000	-0.8031070000	0.0001460000
H	4.5646470000	-0.4745810000	0.0002530000
H	3.3379270000	-1.4078140000	0.8942230000
H	3.3381590000	-1.4079420000	-0.8938960000
O	-3.5491090000	-0.9107910000	-0.0000050000
H	-4.4934640000	-0.7334660000	-0.0001500000

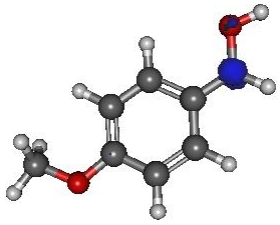
thermodynamic data

Zero-point correction= 0.151230 (Hartree/Particle)
Thermal correction to Energy= 0.160994
Thermal correction to Enthalpy= 0.161938
Thermal correction to Gibbs Free Energy= 0.115787
Sum of electronic and zero-point Energies= -460.639938
Sum of electronic and thermal Energies= -460.630174
Sum of electronic and thermal Enthalpies= -460.629230
Sum of electronic and thermal Free Energies= -460.675381

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.025	36.690	97.134

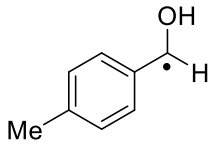
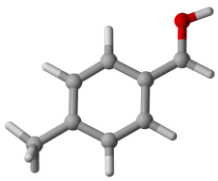


Alpha-HOMO (6311)



spin density (6311)

(u)B3LYP/6-311+G**	

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

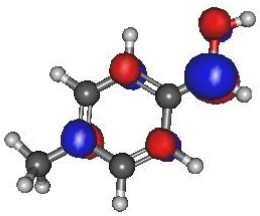
C	-0.4320870000	-1.0336990000	-0.0001000000
C	-1.0100170000	0.2645260000	-0.0000170000
C	-0.1209650000	1.3762990000	-0.0000950000
C	1.2473020000	1.1923110000	-0.0001780000
C	1.8179870000	-0.0950160000	-0.0001660000
C	0.9449520000	-1.1925140000	-0.0001760000
H	-0.5297130000	2.3818990000	-0.0001530000
H	1.8984260000	2.0614850000	-0.0002790000
H	1.3590750000	-2.1962390000	-0.0002870000
H	-1.0817920000	-1.8997650000	-0.0001720000
C	-2.3984810000	0.4718500000	0.0000910000

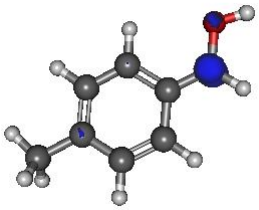
H	-2.8398600000	1.4611850000	-0.0002150000
C	3.3146930000	-0.2747960000	0.0003990000
H	3.7745720000	0.1926650000	-0.8770280000
H	3.5882820000	-1.3320420000	-0.0051080000
H	3.7726820000	0.1828000000	0.8840560000
O	-3.2455590000	-0.6010050000	-0.0000150000
H	-4.1575050000	-0.2977070000	0.0007680000

thermodynamic data

Zero-point correction= 0.146139 (Hartree/Particle)
Thermal correction to Energy= 0.155185
Thermal correction to Enthalpy= 0.156129
Thermal correction to Gibbs Free Energy= 0.109568
Sum of electronic and zero-point Energies= -385.416818
Sum of electronic and thermal Energies= -385.407772
Sum of electronic and thermal Enthalpies= -385.406828
Sum of electronic and thermal Free Energies= -385.453389

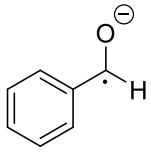
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	97.380	33.374	97.997

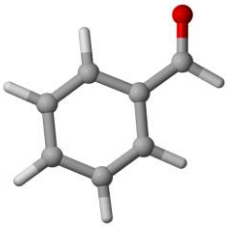




Alpha-HOMO (6311) spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

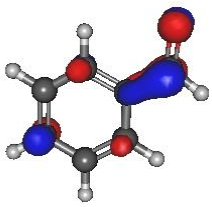
C	-1.3318030000	-1.3273330000	-0.0000150000

C	-2.2534090000	-0.2593330000	0.0000820000
C	-1.7397750000	1.0594040000	0.0000160000
C	-0.3789920000	1.2938970000	-0.0000340000
C	0.5731260000	0.2238120000	-0.0000300000
C	0.0329790000	-1.1081630000	-0.0000590000
C	1.9781220000	0.4705740000	-0.0000120000
O	2.8994020000	-0.3949200000	0.0000650000
H	-1.7043230000	-2.3504080000	0.0000000000
H	-3.3228410000	-0.4424820000	0.0000500000
H	-2.4272870000	1.9030220000	-0.0000250000
H	-0.0079000000	2.3172700000	-0.0000890000
H	0.7331470000	-1.9363260000	-0.0001600000
H	2.2525060000	1.5511420000	0.0000180000

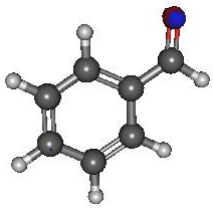
thermodynamic data

Zero-point correction= 0.105458 (Hartree/Particle)
Thermal correction to Energy= 0.111981
Thermal correction to Enthalpy= 0.112925
Thermal correction to Gibbs Free Energy= 0.074246
Sum of electronic and zero-point Energies= -345.580594
Sum of electronic and thermal Energies= -345.574071
Sum of electronic and thermal Enthalpies= -345.573126
Sum of electronic and thermal Free Energies= -345.611805

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.269	25.383	81.407

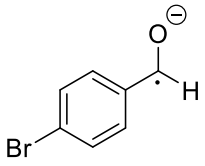


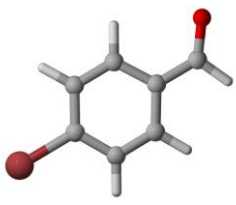
Alpha-HOMO (6311)



spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

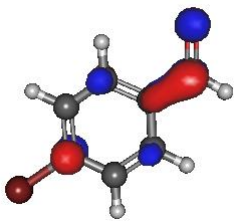
14
XYZ file generated by gabedit : coordinates in Angstrom

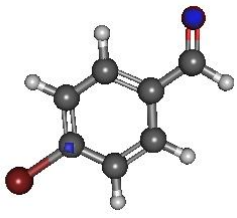
C	0.1213910000	-1.1376390000	-0.0083560000
C	-0.6517960000	0.0349580000	-0.0138390000
C	-0.0345990000	1.3027800000	-0.0064540000
C	1.3434860000	1.3809770000	-0.0011010000
C	2.1754780000	0.2166230000	0.0001530000
C	1.5003000000	-1.0522410000	-0.0032620000
C	3.5984680000	0.3124660000	0.0041850000
O	4.4167030000	-0.6459700000	0.0063040000
Br	-2.5873090000	-0.0869440000	0.0038860000
H	-0.3661590000	-2.1068240000	-0.0102710000
H	-0.6382390000	2.2036140000	-0.0075300000
H	1.8167470000	2.3603390000	0.0010880000
H	2.1066990000	-1.9507720000	-0.0031610000
H	3.9867870000	1.3569020000	0.0054740000

thermodynamic data

Zero-point correction= 0.095215 (Hartree/Particle)
Thermal correction to Energy= 0.103540
Thermal correction to Enthalpy= 0.104484
Thermal correction to Gibbs Free Energy= 0.059275
Sum of electronic and zero-point Energies= -2919.144965
Sum of electronic and thermal Energies= -2919.136640
Sum of electronic and thermal Enthalpies= -2919.135696
Sum of electronic and thermal Free Energies= -2919.180905

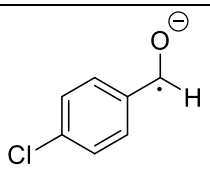
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	64.973	29.872	95.152

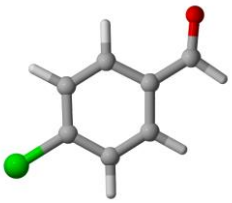




Alpha-HOMO (6311) spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

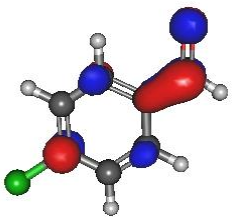
14
XYZ file generated by gabedit : coordinates in Angstrom

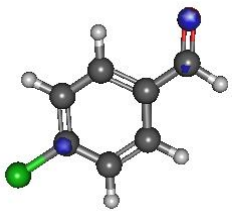
C	-0.5404010000	-1.1706550000	-0.0007840000
C	-1.3349320000	-0.0140940000	-0.0008760000
C	-0.7409690000	1.2635170000	-0.0003480000
C	0.6353730000	1.3688000000	-0.0001540000
C	1.4891190000	0.2200840000	-0.0001400000
C	0.8372120000	-1.0613350000	-0.0006580000
C	2.9101670000	0.3423230000	0.0001560000
O	3.7470310000	-0.6014190000	0.0010370000
Cl	-3.1153480000	-0.1580320000	0.0007330000
H	-1.0141680000	-2.1471920000	-0.0008750000
H	-1.3649070000	2.1508940000	-0.0010140000
H	1.0904350000	2.3567960000	-0.0004590000
H	1.4605420000	-1.9482060000	-0.0013610000
H	3.2793620000	1.3937650000	-0.0002260000

thermodynamic data

Zero-point correction= 0.095996 (Hartree/Particle)
Thermal correction to Energy= 0.103892
Thermal correction to Enthalpy= 0.104836
Thermal correction to Gibbs Free Energy= 0.062201
Sum of electronic and zero-point Energies= -805.222749
Sum of electronic and thermal Energies= -805.214853
Sum of electronic and thermal Enthalpies= -805.213909
Sum of electronic and thermal Free Energies= -805.256544

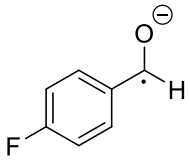
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.193	29.345	89.733

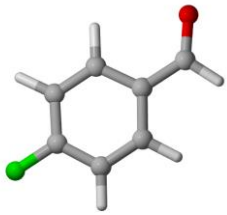




Alpha-HOMO (6311) spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

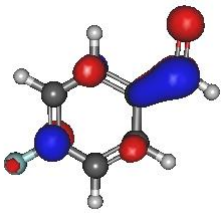
14
XYZ file generated by gabedit : coordinates in Angstrom

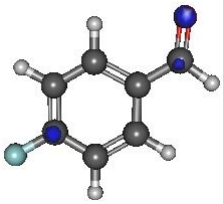
C	-0.9552970000	-1.2219270000	-0.0001320000
C	-1.7679760000	-0.0899520000	0.0003170000
C	-1.2262090000	1.2026510000	0.0002060000
C	0.1485780000	1.3507550000	-0.0001040000
C	1.0361150000	0.2272390000	-0.0000750000
C	0.4230150000	-1.0750100000	-0.0003320000
C	2.4532480000	0.3909160000	-0.0001780000
O	3.3178950000	-0.5323620000	0.0004690000
F	-3.1501360000	-0.2408410000	0.0000690000
H	-1.4146460000	-2.2062270000	-0.0000480000
H	-1.8882150000	2.0629090000	-0.0003140000
H	0.5755150000	2.3511110000	-0.0006550000
H	1.0736860000	-1.9415830000	-0.0010160000
H	2.7928750000	1.4522370000	-0.0005530000

thermodynamic data

Zero-point correction= 0.096977 (Hartree/Particle)
Thermal correction to Energy= 0.104477
Thermal correction to Enthalpy= 0.105421
Thermal correction to Gibbs Free Energy= 0.064264
Sum of electronic and zero-point Energies= -444.860830
Sum of electronic and thermal Energies= -444.853330
Sum of electronic and thermal Enthalpies= -444.852386
Sum of electronic and thermal Free Energies= -444.893543

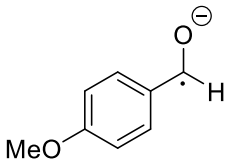
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.560	28.629	86.622

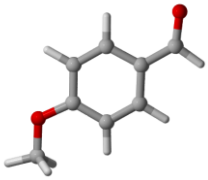




Alpha-HOMO (6311) spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

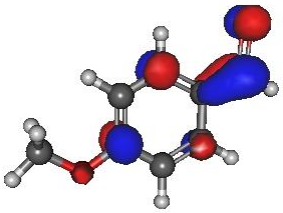
C	0.3744150000	1.3399640000	0.0006410000
C	1.3058240000	0.2852570000	0.0014240000
C	0.8352480000	-1.0413910000	0.0022080000
C	-0.5291200000	-1.2957250000	0.0016510000
C	-1.5038940000	-0.2498510000	0.0003030000
C	-0.9829850000	1.0912240000	0.0002020000
C	-2.9051850000	-0.5122600000	-0.0008860000
O	-3.8352780000	0.3486310000	-0.0020050000
O	2.6594430000	0.6551130000	0.0027030000
C	3.6093740000	-0.3776260000	-0.0042100000
H	0.7520940000	2.3589890000	0.0005870000
H	1.5253960000	-1.8782670000	0.0032220000
H	-0.8715870000	-2.3282640000	0.0021590000
H	-1.6952890000	1.9085300000	-0.0004050000
H	-3.1696960000	-1.5950240000	-0.0009010000
H	4.5911480000	0.1019470000	-0.0052170000
H	3.5291070000	-1.0212720000	0.8845110000
H	3.5234370000	-1.0141430000	-0.8975320000

thermodynamic data

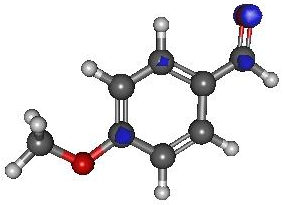
Zero-point correction= 0.136917 (Hartree/Particle)
Thermal correction to Energy= 0.145432
Thermal correction to Enthalpy= 0.146376
Thermal correction to Gibbs Free Energy= 0.102974
Sum of electronic and zero-point Energies= -460.099109

Sum of electronic and thermal Energies= -460.090594
Sum of electronic and thermal Enthalpies= -460.089650
Sum of electronic and thermal Free Energies= -460.133052

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.260	32.911	91.347

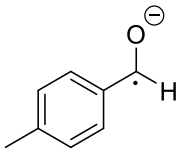


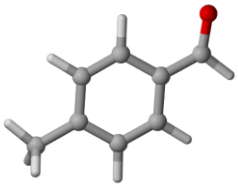
Alpha-HOMO (6311)



spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

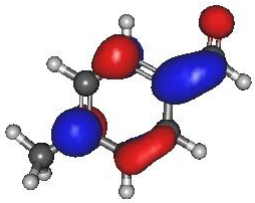
17
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9208730000	-1.1960200000	0.0000890000
C	-1.7814030000	-0.0795680000	0.0001760000
C	-1.1650680000	1.2005610000	0.0000690000
C	0.2069640000	1.3439420000	-0.0000220000
C	1.0881880000	0.2176760000	-0.0000070000
C	0.4583320000	-1.0729460000	-0.0000470000
C	2.5060290000	0.3767860000	0.0000340000
O	3.3712560000	-0.5438430000	-0.0000360000
C	-3.2803110000	-0.2217620000	-0.0000950000
H	-1.3600920000	-2.1935900000	0.0000980000
H	-1.7926020000	2.0911340000	-0.0001130000
H	0.6417670000	2.3419780000	-0.0002390000
H	1.0965210000	-1.9495580000	-0.0002490000
H	2.8465700000	1.4384370000	0.0001230000
H	-3.5740010000	-1.2770040000	0.0006180000
H	-3.7498880000	0.2443240000	0.8805770000
H	-3.7494770000	0.2430030000	-0.8817040000

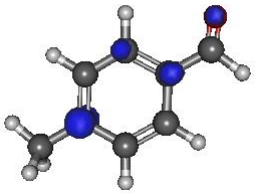
thermodynamic data

Zero-point correction= 0.132267 (Hartree/Particle)
Thermal correction to Energy= 0.140696
Thermal correction to Enthalpy= 0.141640
Thermal correction to Gibbs Free Energy= 0.097980
Sum of electronic and zero-point Energies= -384.879406
Sum of electronic and thermal Energies= -384.870977
Sum of electronic and thermal Enthalpies= -384.870033
Sum of electronic and thermal Free Energies= -384.913693

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	88.288	31.353	91.892

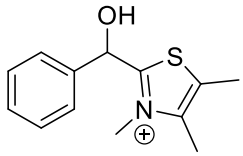


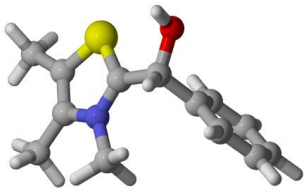
Alpha-HOMO (6311)



spin density (6311)

B3LYP/6-311+G**	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	0.5921860000	-0.3592830000	-0.5497820000
N	1.1020160000	0.8688780000	-0.4842920000
C	2.3984720000	0.9375750000	0.0565500000
C	2.8677920000	-0.2921790000	0.4083470000
S	1.6833090000	-1.5241720000	0.0450010000
C	4.1761500000	-0.6689180000	1.0329520000
C	3.0888550000	2.2574140000	0.1890480000
C	-0.7593050000	-0.7563470000	-1.1015150000
H	3.1349180000	2.7880750000	-0.7653280000
H	4.1100780000	2.1109530000	0.5351920000

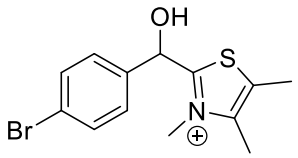
H	2.5872760000	2.9043140000	0.9149430000
H	4.5873990000	-1.5714120000	0.5760960000
H	4.0611440000	-0.8586220000	2.1039080000
H	4.9096220000	0.1275510000	0.9093150000
C	0.3983810000	2.0686210000	-0.9778790000
H	-0.6655990000	1.8630790000	-1.0435760000
H	0.7899440000	2.3456310000	-1.9579940000
H	0.5519960000	2.8862380000	-0.2772540000
C	-1.9331030000	-0.2551020000	-0.2741250000
C	-1.9749510000	-0.4414280000	1.1133330000
C	-3.0913160000	-0.0351100000	1.8379980000
C	-4.1725880000	0.5588790000	1.1854570000
C	-4.1388660000	0.7421260000	-0.1949950000
C	-3.0221000000	0.3356090000	-0.9237510000
H	-4.9801900000	1.1950930000	-0.7057180000
H	-3.0043150000	0.4707030000	-2.0009180000
H	-5.0406160000	0.8731910000	1.7526910000
H	-1.1461070000	-0.9156340000	1.6279720000
H	-3.1207110000	-0.1845000000	2.9107840000
H	-0.8406140000	-0.3357580000	-2.1138780000
O	-0.6960290000	-2.1761970000	-1.1796610000
H	-1.5906780000	-2.5358700000	-1.1687380000

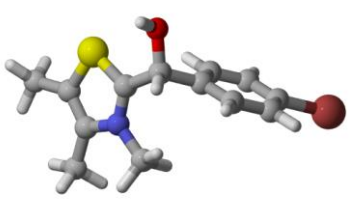
thermodynamic data

Zero-point correction= 0.264099 (Hartree/Particle)
Thermal correction to Energy= 0.280689
Thermal correction to Enthalpy= 0.281633
Thermal correction to Gibbs Free Energy= 0.218587
Sum of electronic and zero-point Energies= -1032.892492
Sum of electronic and thermal Energies= -1032.875903
Sum of electronic and thermal Enthalpies= -1032.874959
Sum of electronic and thermal Free Energies= -1032.938005

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	176.135	61.288	132.692

B3LYP/6-311+G**		





xyz-matrix

XYZ file generated by gabedit : coordinates in Angstrom

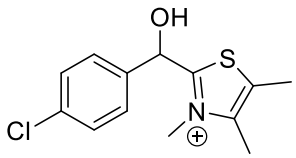
C	-2.0433560000	-0.5775760000	0.4108760000
N	-2.3854660000	0.6607180000	0.7609810000
C	-3.5225120000	1.1631780000	0.1032740000
C	-4.0424980000	0.2594630000	-0.7739760000
S	-3.1087360000	-1.2167120000	-0.7545570000
C	-5.2220840000	0.3896840000	-1.6879560000
C	-4.0160130000	2.5426620000	0.4024180000
C	-0.8939530000	-1.3951800000	0.9595000000
H	-4.1995520000	2.6845690000	1.4704710000
H	-4.9526220000	2.7253800000	-0.1206520000
H	-3.3043820000	3.3061800000	0.0743840000
H	-5.8138500000	-0.5278120000	-1.7036030000
H	-4.9038390000	0.6003560000	-2.7128960000
H	-5.8764960000	1.1993480000	-1.3657530000
C	-1.6734480000	1.4436420000	1.7897130000
H	-0.6840990000	1.0249180000	1.9449610000
H	-2.2405330000	1.4245890000	2.7216960000
H	-1.5666360000	2.4703200000	1.4464680000
C	0.4780780000	-0.8580480000	0.5850890000
C	0.7999120000	-0.5411880000	-0.7404930000
C	2.0799080000	-0.1140200000	-1.0744820000
C	3.0487390000	-0.0025620000	-0.0755290000
C	2.7499150000	-0.3206050000	1.2473420000
C	1.4642740000	-0.7481720000	1.5704850000
H	3.5094200000	-0.2412980000	2.0141610000
H	1.2380780000	-1.0052830000	2.6007440000
Br	4.8003660000	0.5855510000	-0.5287620000
H	0.0577890000	-0.6382820000	-1.5254170000
H	2.3262770000	0.1272060000	-2.1003990000
H	-0.9814920000	-1.3955240000	2.0552800000
O	-1.1382210000	-2.7051120000	0.4596030000
H	-0.3188550000	-3.2133720000	0.4788750000

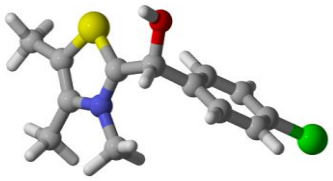
thermodynamic data

Zero-point correction= 0.253899 (Hartree/Particle)
Thermal correction to Energy= 0.271869
Thermal correction to Enthalpy= 0.272813
Thermal correction to Gibbs Free Energy= 0.205642
Sum of electronic and zero-point Energies= -3606.441143
Sum of electronic and thermal Energies= -3606.423173
Sum of electronic and thermal Enthalpies= -3606.422229
Sum of electronic and thermal Free Energies= -3606.489400

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	170.600	65.512	141.373

B3LYP/6-311+G**	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3640850000	-0.3178740000	-0.7111320000
N	1.8192890000	-0.7822700000	0.4503530000
C	2.9046630000	-0.0657770000	0.9862650000
C	3.2864780000	0.9711200000	0.1881940000
S	2.2748370000	1.0252320000	-1.2324030000
C	4.3802190000	1.9763240000	0.3737740000
C	3.5068790000	-0.4787210000	2.2917180000
C	0.1699560000	-0.8044090000	-1.5175720000
H	2.7543240000	-0.5332660000	3.0820430000
H	4.2578820000	0.2443660000	2.6027530000
H	3.9972500000	-1.4537900000	2.2188150000
H	3.9728930000	2.9782080000	0.5335460000
H	5.0340280000	2.0143650000	-0.5007140000
H	4.9963710000	1.7224670000	1.2352950000
C	1.2405430000	-1.9447280000	1.1593870000
H	2.0496560000	-2.5187750000	1.6038820000
H	0.7150090000	-2.5644970000	0.4426290000
H	0.5630440000	-1.5924200000	1.9380730000
C	-1.1543150000	-0.3973170000	-0.8674620000
C	-1.6149770000	0.9153740000	-1.0159360000
C	-2.8147160000	1.3188810000	-0.4419440000
C	-3.5683930000	0.3959270000	0.2823700000
C	-3.1354300000	-0.9196560000	0.4259660000
C	-1.9273350000	-1.3103840000	-0.1465120000
H	-3.7398020000	-1.6319240000	0.9728540000
H	-1.6086680000	-2.3404760000	-0.0470590000
Cl	-5.0781660000	0.8915120000	1.0012930000
H	-1.0466100000	1.6356040000	-1.5962060000
H	-3.1715350000	2.3332600000	-0.5647230000
H	0.2426120000	-0.2874470000	-2.4822510000
O	0.3334020000	-2.2008270000	-1.6992760000
H	-0.3132050000	-2.5151530000	-2.3434320000

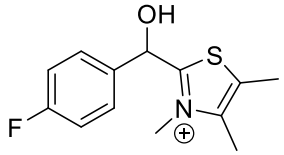
thermodynamic data

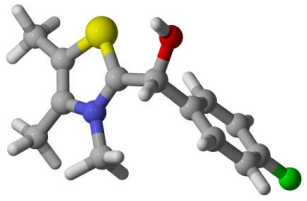
Zero-point correction= 0.255157 (Hartree/Particle)
Thermal correction to Energy= 0.272601

Thermal correction to Enthalpy= 0.273545
Thermal correction to Gibbs Free Energy= 0.208139
Sum of electronic and zero-point Energies= -1492.516509
Sum of electronic and thermal Energies= -1492.499065
Sum of electronic and thermal Enthalpies= -1492.498121
Sum of electronic and thermal Free Energies= -1492.563527

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.060	64.816	137.658

B3LYP/6-311+G**	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9753900000	-0.4377440000	-0.5356170000
N	1.4269720000	0.8141200000	-0.5818720000
C	2.6721610000	1.0115950000	0.0410940000
C	3.1617000000	-0.1425380000	0.5751650000
S	2.0623140000	-1.4667980000	0.2772390000
C	4.4299730000	-0.3745700000	1.3380400000
C	3.2972520000	2.3698320000	0.0621650000
C	-0.3088590000	-0.9658040000	-1.1378330000
H	3.3947930000	2.7864120000	-0.9435230000
H	4.2939610000	2.3140340000	0.4954550000
H	2.7169320000	3.0722920000	0.6677970000
H	4.8889710000	-1.3260130000	1.0624070000
H	4.2434130000	-0.3926320000	2.4156020000
H	5.1555700000	0.4129770000	1.1348140000
C	0.7171840000	1.9101800000	-1.2695020000
H	-0.3323370000	1.6525680000	-1.3732670000
H	1.1635350000	2.0774760000	-2.2511280000
H	0.7958160000	2.8156270000	-0.6722540000
C	-1.5671120000	-0.4383880000	-0.4681910000
C	-1.7192240000	-0.4722920000	0.9246360000
C	-2.9037720000	-0.0515810000	1.5164900000
C	-3.9324400000	0.4019180000	0.6987260000
C	-3.8183360000	0.4432040000	-0.6831610000
C	-2.6258330000	0.0175270000	-1.2619620000
H	-4.6483150000	0.7951670000	-1.2825430000

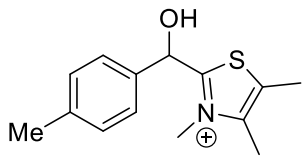
H	-2.5280450000	0.0352020000	-2.3427800000
F	-5.0755500000	0.8116180000	1.2677490000
H	-0.9181960000	-0.8406190000	1.5559300000
H	-3.0426860000	-0.0728680000	2.5900080000
H	-0.3254130000	-0.6666950000	-2.1954820000
O	-0.1733450000	-2.3796300000	-1.0433710000
H	-1.0456350000	-2.7885410000	-1.0868180000

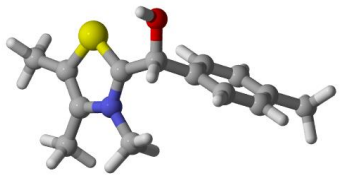
thermodynamic data

Zero-point correction= 0.256042 (Hartree/Particle)
Thermal correction to Energy= 0.273338
Thermal correction to Enthalpy= 0.274282
Thermal correction to Gibbs Free Energy= 0.209767
Sum of electronic and zero-point Energies= -1132.165496
Sum of electronic and thermal Energies= -1132.148200
Sum of electronic and thermal Enthalpies= -1132.147256
Sum of electronic and thermal Free Energies= -1132.211771

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.522	64.130	135.783

B3LYP/6-311+G**





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	1.0086480000	-0.4591550000	-0.5180120000
N	1.4491450000	0.7940480000	-0.6069140000
C	2.6862750000	1.0269620000	0.0203400000
C	3.1815180000	-0.1013350000	0.6012980000
S	2.0966480000	-1.4469680000	0.3432550000
C	4.4445900000	-0.2939050000	1.3833160000
C	3.2958580000	2.3922320000	-0.0031110000
C	-0.2647000000	-1.0211240000	-1.1104690000
H	3.4008820000	2.7715890000	-1.0227380000
H	4.2877280000	2.3649570000	0.4436270000
H	2.6998970000	3.1101920000	0.5681070000
H	4.9380700000	-1.2297480000	1.1131960000
H	4.2425300000	-0.3202200000	2.4578700000
H	5.1475630000	0.5168910000	1.1930480000
C	0.7332190000	1.8563220000	-1.3394490000

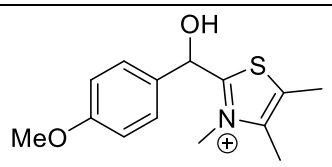
H	-0.3091280000	1.5754250000	-1.4555620000
H	1.1959100000	2.0034520000	-2.3167090000
H	0.7832140000	2.7799800000	-0.7673130000
C	-1.5325050000	-0.4748650000	-0.4775050000
C	-1.6971290000	-0.4265750000	0.9127420000
C	-2.8963530000	0.0113840000	1.4609010000
C	-3.9665740000	0.4110970000	0.6469230000
C	-3.7918220000	0.3592900000	-0.7398200000
C	-2.5930550000	-0.0788140000	-1.2976250000
H	-3.0073200000	0.0420120000	2.5394960000
H	-0.2715010000	-0.7670340000	-2.1799430000
H	-0.8949670000	-0.7406430000	1.5723800000
H	-2.4890110000	-0.1173640000	-2.3778770000
H	-4.6028560000	0.6609090000	-1.3933690000
C	-5.2725650000	0.8549720000	1.2528970000
H	-5.8576880000	1.4512130000	0.5511070000
H	-5.1120990000	1.4466620000	2.1567270000
H	-5.8784420000	-0.0124130000	1.5349720000
O	-0.1222930000	-2.4308120000	-0.9603240000
H	-0.9972530000	-2.8351340000	-0.9326830000

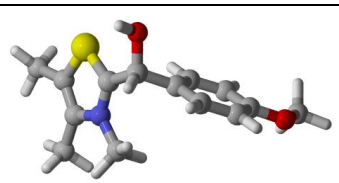
thermodynamic data

Zero-point correction= 0.291326 (Hartree/Particle)
Thermal correction to Energy= 0.309800
Thermal correction to Enthalpy= 0.310744
Thermal correction to Gibbs Free Energy= 0.242317
Sum of electronic and zero-point Energies= -1072.195113
Sum of electronic and thermal Energies= -1072.176639
Sum of electronic and thermal Enthalpies= -1072.175695
Sum of electronic and thermal Free Energies= -1072.244123

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	194.403	67.338	144.018

B3LYP/6-311+G**	





xyz-matrix

36
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3846540000	-0.4787790000	0.5089400000
N	-1.7653850000	0.7906860000	0.6371500000

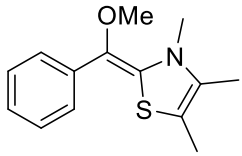
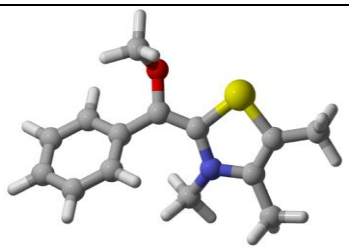
C	-2.9793810000	1.1064140000	0.0010870000
C	-3.5193770000	0.0254010000	-0.6277400000
S	-2.5059080000	-1.3806660000	-0.4026420000
C	-4.7775400000	-0.0760650000	-1.4344370000
C	-3.5226520000	2.4982480000	0.0656630000
C	-0.1463610000	-1.1228260000	1.0932080000
H	-3.6373120000	2.8414370000	1.0971480000
H	-4.5020190000	2.5377240000	-0.4069000000
H	-2.8775460000	3.2083690000	-0.4601490000
H	-5.3240430000	-0.9922990000	-1.2015630000
H	-4.5592610000	-0.0800120000	-2.5061170000
H	-5.4399340000	0.7645760000	-1.2291930000
C	-1.0092620000	1.7881580000	1.4182520000
H	0.0188990000	1.4557360000	1.5264970000
H	-1.4717010000	1.9135400000	2.3986950000
H	-1.0150880000	2.7367080000	0.8862770000
C	1.1494010000	-0.6166880000	0.4923330000
C	1.3291170000	-0.5158930000	-0.8983850000
C	2.5437320000	-0.1214670000	-1.4263900000
C	3.6226530000	0.1832560000	-0.5766870000
C	3.4571860000	0.0829330000	0.8103440000
C	2.2263050000	-0.3155340000	1.3286970000
H	2.6932490000	-0.0447150000	-2.4962490000
H	-0.1395930000	-0.9064560000	2.1709210000
O	4.7609670000	0.5566890000	-1.1909750000
C	5.9168580000	0.8635600000	-0.4051380000
H	6.6934700000	1.1249520000	-1.1197780000
H	5.7272260000	1.7139670000	0.2561150000
H	6.2348090000	-0.0043620000	0.1794270000
H	0.5177130000	-0.7601990000	-1.5758290000
H	2.1155870000	-0.3986740000	2.4057430000
H	4.2712460000	0.3039980000	1.4866680000
O	-0.3592150000	-2.5195740000	0.8959470000
H	0.4963430000	-2.9596720000	0.8322570000

thermodynamic data

Zero-point correction= 0.296467 (Hartree/Particle)
Thermal correction to Energy= 0.315632
Thermal correction to Enthalpy= 0.316576
Thermal correction to Gibbs Free Energy= 0.247923
Sum of electronic and zero-point Energies= -1147.420219
Sum of electronic and thermal Energies= -1147.401054
Sum of electronic and thermal Enthalpies= -1147.400110
Sum of electronic and thermal Free Energies= -1147.468763

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	198.062	70.547	144.494

B3LYP/6-311+G**	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

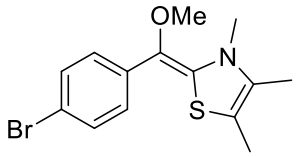
C	-0.6488500000	0.3447980000	0.1424910000
N	-1.1183930000	-0.9688900000	0.1989420000
C	-2.5160380000	-1.0784200000	0.0107830000
C	-3.1556260000	0.1015780000	-0.0987420000
S	-2.0262420000	1.4689430000	0.0488720000
C	-4.6055880000	0.3933630000	-0.3199540000
C	-3.1316650000	-2.4431770000	-0.0725230000
C	0.6262090000	0.8181270000	0.1924700000
H	-2.5791530000	-3.0823590000	-0.7679480000
H	-4.1596400000	-2.3758170000	-0.4259860000
H	-3.1536990000	-2.9512740000	0.8972550000
H	-4.7723260000	0.9246960000	-1.2631920000
H	-5.0053390000	1.0234890000	0.4820580000
H	-5.1969810000	-0.5229710000	-0.3427180000
C	-0.3522140000	-2.0062660000	0.8867520000
H	0.2439190000	-1.5484810000	1.6791340000
H	0.3304870000	-2.5341490000	0.2161290000
H	-1.0322110000	-2.7275530000	1.3358460000
C	1.8878570000	0.0839260000	0.0448420000
C	3.0170280000	0.4664760000	0.7956830000
C	4.2354920000	-0.1838900000	0.6378630000
C	4.3670610000	-1.2306670000	-0.2769250000
C	3.2647640000	-1.6070660000	-1.0434770000
C	2.0444760000	-0.9538170000	-0.8930000000
H	2.9193970000	1.2757710000	1.5098880000
H	5.0874950000	0.1233950000	1.2349670000
H	3.3603890000	-2.4003560000	-1.7773720000
H	1.2092120000	-1.2228700000	-1.5297570000
H	5.3181590000	-1.7362390000	-0.3989640000
O	0.7171070000	2.1910570000	0.4379870000
C	1.2602590000	2.9601510000	-0.6408430000
H	0.6526760000	2.8445450000	-1.5447720000
H	1.2377830000	4.0008260000	-0.3163770000
H	2.2926050000	2.6693350000	-0.8591490000

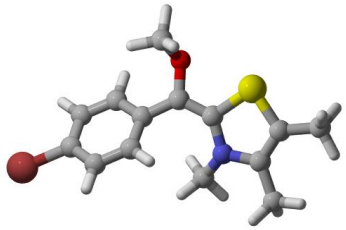
thermodynamic data

Zero-point correction= 0.278658 (Hartree/Particle)
Thermal correction to Energy= 0.296434
Thermal correction to Enthalpy= 0.297379
Thermal correction to Gibbs Free Energy= 0.233026
Sum of electronic and zero-point Energies= -1071.771819
Sum of electronic and thermal Energies= -1071.754042
Sum of electronic and thermal Enthalpies= -1071.753098
Sum of electronic and thermal Free Energies= -1071.817451

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.015	65.944	135.442

B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0214870000	0.3600660000	0.1466130000
N	-2.2002250000	-1.0196610000	0.2439260000
C	-3.5312800000	-1.4361560000	0.0052800000
C	-4.4029950000	-0.4265130000	-0.1791210000
S	-3.5999690000	1.1557380000	-0.0496820000
C	-5.8707010000	-0.4628380000	-0.4640730000
C	-3.8325160000	-2.9041560000	-0.0424170000
C	-0.8797880000	1.0995660000	0.2227450000
H	-3.1204280000	-3.4311400000	-0.6846620000
H	-4.8313120000	-3.0749530000	-0.4415980000
H	-3.7936600000	-3.3715030000	0.9470330000
H	-6.1065320000	-0.0108860000	-1.4334140000
H	-6.4311730000	0.0906490000	0.2970890000
H	-6.2490250000	-1.4859010000	-0.4709090000
C	-1.2686570000	-1.8453330000	1.0108810000
H	-0.7677270000	-1.2231800000	1.7542900000
H	-0.5003960000	-2.3047120000	0.3831920000
H	-1.8151230000	-2.6315040000	1.5291000000
C	0.5121910000	0.6506310000	0.1485380000
C	1.5070570000	1.3146710000	0.8931700000
C	2.8444900000	0.9465120000	0.8085360000
C	3.2139050000	-0.0985440000	-0.0351650000
C	2.2623550000	-0.7622660000	-0.8032730000

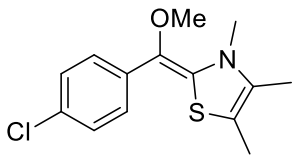
C	0.9270000000	-0.3806780000	-0.7149800000
H	1.2166270000	2.1237900000	1.5527490000
H	3.5914910000	1.4629990000	1.3980790000
Br	5.0588480000	-0.6157510000	-0.1542840000
H	2.5607300000	-1.5533280000	-1.4797270000
H	0.1989050000	-0.8677360000	-1.3532160000
O	-1.0940500000	2.4656990000	0.4209740000
C	-0.6993800000	3.3038450000	-0.6721390000
H	-1.2410810000	3.0340480000	-1.5847810000
H	-0.9559280000	4.3232480000	-0.3832100000
H	0.3772440000	3.2387610000	-0.8580370000

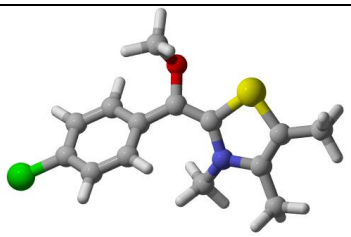
thermodynamic data

Zero-point correction= 0.268484 (Hartree/Particle)
Thermal correction to Energy= 0.287783
Thermal correction to Enthalpy= 0.288727
Thermal correction to Gibbs Free Energy= 0.219610
Sum of electronic and zero-point Energies= -3645.325324
Sum of electronic and thermal Energies= -3645.306026
Sum of electronic and thermal Enthalpies= -3645.305082
Sum of electronic and thermal Free Energies= -3645.374199

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.586	70.231	145.469

B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3676430000	0.3630290000	0.1471230000
N	-1.6272230000	-1.0048950000	0.2322280000
C	-2.9840750000	-1.3379660000	0.0065900000
C	-3.7957900000	-0.2759580000	-0.1560550000
S	-2.8981230000	1.2542460000	-0.0188930000
C	-5.2660120000	-0.2201960000	-0.4241410000
C	-3.3739310000	-2.7844660000	-0.0539830000
C	-0.1829010000	1.0313920000	0.2152970000
H	-2.7029740000	-3.3454660000	-0.7115490000
H	-4.3860960000	-2.8896560000	-0.4420050000

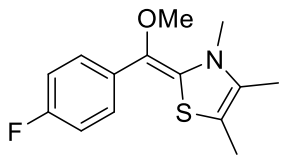
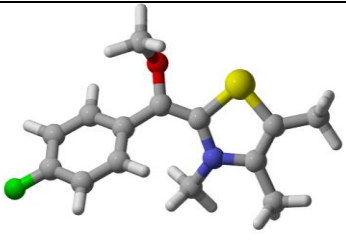
H	-3.3512130000	-3.2653660000	0.9295160000
H	-5.4846680000	0.2649300000	-1.3813790000
H	-5.7849250000	0.3495820000	0.3543430000
H	-5.7045030000	-1.2187330000	-0.4474640000
C	-0.7378290000	-1.8910660000	0.9814290000
H	-0.2143540000	-1.3127110000	1.7450270000
H	0.0134370000	-2.3663450000	0.3453160000
H	-1.3220210000	-2.6663640000	1.4736140000
C	1.1787920000	0.4996420000	0.1195780000
C	2.2192470000	1.0890270000	0.8646120000
C	3.5301360000	0.6408260000	0.7599280000
C	3.8267530000	-0.4102880000	-0.1042710000
C	2.8291780000	-1.0018280000	-0.8722850000
C	1.5208710000	-0.5408400000	-0.7643590000
H	1.9847610000	1.9032770000	1.5399020000
H	4.3165460000	1.0973600000	1.3480240000
Cl	5.4862830000	-0.9857160000	-0.2392740000
H	3.0767540000	-1.7984290000	-1.5628820000
H	0.7575870000	-0.9713340000	-1.4019850000
O	-0.3111110000	2.4062460000	0.4274100000
C	0.1214500000	3.2279810000	-0.6636220000
H	-0.4488800000	3.0021060000	-1.5707830000
H	-0.0654430000	4.2589060000	-0.3623290000
H	1.1891130000	3.0960470000	-0.8653450000

thermodynamic data

Zero-point correction= 0.269206 (Hartree/Particle)
Thermal correction to Energy= 0.288194
Thermal correction to Enthalpy= 0.289139
Thermal correction to Gibbs Free Energy= 0.221476
Sum of electronic and zero-point Energies= -1531.404826
Sum of electronic and thermal Energies= -1531.385837
Sum of electronic and thermal Enthalpies= -1531.384893
Sum of electronic and thermal Free Energies= -1531.452555

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.845	69.739	142.407

B3LYP/6-311+G**	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

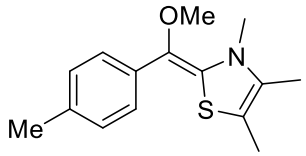
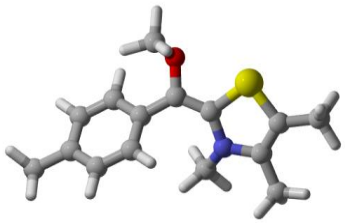
C	-1.0049230000	0.3638750000	0.1479610000
N	-1.3507910000	-0.9873330000	0.2158020000
C	-2.7298960000	-1.2282180000	0.0079120000
C	-3.4739000000	-0.1142320000	-0.1269870000
S	-2.4786170000	1.3540900000	0.0200600000
C	-4.9407320000	0.0396040000	-0.3745460000
C	-3.2137350000	-2.6453020000	-0.0693390000
C	0.2199740000	0.9532190000	0.2050530000
H	-2.5912720000	-3.2369140000	-0.7475470000
H	-4.2367160000	-2.6776150000	-0.4415270000
H	-3.2062250000	-3.1436090000	0.9057320000
H	-5.1397710000	0.5468900000	-1.3246350000
H	-5.4109920000	0.6350650000	0.4155900000
H	-5.4440100000	-0.9278910000	-0.3996650000
C	-0.5086650000	-1.9369480000	0.9411320000
H	0.0345220000	-1.4095970000	1.7281530000
H	0.2253910000	-2.4236950000	0.2937730000
H	-1.1308750000	-2.7017960000	1.4017100000
C	1.5457520000	0.3348520000	0.0870750000
C	2.6232830000	0.8309000000	0.8470540000
C	3.9018300000	0.2989390000	0.7241060000
C	4.1092220000	-0.7395610000	-0.1718050000
C	3.0859620000	-1.2471060000	-0.9556290000
C	1.8119330000	-0.6991750000	-0.8293410000
H	2.4428200000	1.6391750000	1.5454880000
H	4.7296900000	0.6731030000	1.3141330000
F	5.3565810000	-1.2654760000	-0.2941650000
H	3.2938380000	-2.0391000000	-1.6648800000
H	1.0169480000	-1.0566230000	-1.4731690000
O	0.1850940000	2.3321970000	0.4284870000
C	0.6597010000	3.1309740000	-0.6615840000
H	0.0664130000	2.9491800000	-1.5639750000
H	0.5444900000	4.1700440000	-0.3522950000
H	1.7143380000	2.9300630000	-0.8752510000

thermodynamic data

Zero-point correction= 0.270564 (Hartree/Particle)
Thermal correction to Energy= 0.289126
Thermal correction to Enthalpy= 0.290071
Thermal correction to Gibbs Free Energy= 0.223810
Sum of electronic and zero-point Energies= -1171.048517
Sum of electronic and thermal Energies= -1171.029955
Sum of electronic and thermal Enthalpies= -1171.029010
Sum of electronic and thermal Free Energies= -1171.095271

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	181.430	68.869	139.458

B3LYP/6-311+G**	

xyz-matrix

37
XYZ file generated by gabedit : coordinates in Angstrom

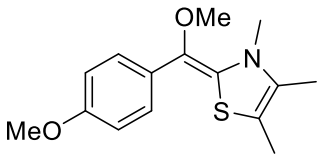
C	1.0326010000	0.3625060000	-0.1469900000
N	1.3623300000	-0.9935040000	-0.2171260000
C	2.7372490000	-1.2510720000	-0.0061190000
C	3.4951960000	-0.1468150000	0.1324380000
S	2.5192540000	1.3347570000	-0.0158680000
C	4.9629830000	-0.0123070000	0.3853040000
C	3.2033770000	-2.6741930000	0.0713690000
C	-0.1848920000	0.9656160000	-0.2051770000
H	2.5711670000	-3.2583560000	0.7470660000
H	4.2248210000	-2.7198430000	0.4465370000
H	3.1923400000	-3.1717250000	-0.9041070000
H	5.1654140000	0.4930220000	1.3358300000
H	5.4441140000	0.5766130000	-0.4033370000
H	5.4536700000	-0.9862660000	0.4129430000
C	0.5113500000	-1.9291370000	-0.9503020000
H	-0.0200630000	-1.3914940000	-1.7384970000
H	-0.2341400000	-2.4055970000	-0.3085720000
H	1.1256590000	-2.7013820000	-1.4094690000
C	-1.5177490000	0.3620900000	-0.0901980000
C	-2.5915190000	0.8667980000	-0.8501690000
C	-3.8700340000	0.3413940000	-0.7231430000
C	-4.1460340000	-0.7056880000	0.1678800000
C	-3.0866730000	-1.1944450000	0.9365810000
C	-1.8015970000	-0.6686130000	0.8208420000
H	-2.4036040000	1.6737220000	-1.5491330000
H	-4.6726890000	0.7480180000	-1.3316310000
H	-3.2714040000	-1.9881150000	1.6543380000
H	-1.0133980000	-1.0392770000	1.4666270000
O	-0.1307070000	2.3451120000	-0.4244240000
C	-0.6113950000	3.1459290000	0.6605910000
H	-0.0320480000	2.9562470000	1.5706140000
H	-0.4812220000	4.1845710000	0.3553520000
H	-1.6706390000	2.9551230000	0.8598290000
C	-5.5407580000	-1.2689090000	0.2948590000
H	-5.5782900000	-2.0732050000	1.0326630000
H	-5.8954970000	-1.6740490000	-0.6584790000
H	-6.2555460000	-0.4994050000	0.6039860000

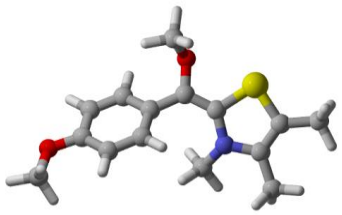
thermodynamic data

Zero-point correction= 0.305877 (Hartree/Particle)
Thermal correction to Energy= 0.325565
Thermal correction to Enthalpy= 0.326509
Thermal correction to Gibbs Free Energy= 0.255850
Sum of electronic and zero-point Energies= -1111.071845
Sum of electronic and thermal Energies= -1111.052157
Sum of electronic and thermal Enthalpies= -1111.051213
Sum of electronic and thermal Free Energies= -1111.121872

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.295	71.958	148.715

B3LYP/6-311+G**	





xyz-matrix

38
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3783520000	0.3722590000	0.1369160000
N	-1.5896100000	-1.0045090000	0.2676470000
C	-2.9289850000	-1.3935200000	0.0319970000
C	-3.7756940000	-0.3704850000	-0.1898070000
S	-2.9400910000	1.1993980000	-0.0934290000
C	-5.2396000000	-0.3817310000	-0.4949430000
C	-3.2666840000	-2.8545590000	0.0197040000
C	-0.2218090000	1.0820970000	0.2011910000
H	-2.5619000000	-3.4158230000	-0.6014820000
H	-4.2659590000	-3.0112430000	-0.3842880000
H	-3.2487670000	-3.2966680000	1.0214540000
H	-5.4523660000	0.0558210000	-1.4764240000
H	-5.7990800000	0.1992170000	0.2465750000
H	-5.6405850000	-1.3962840000	-0.4873380000
C	-0.6854550000	-1.8183480000	1.0777260000
H	-0.2463930000	-1.1990530000	1.8631380000
H	0.1322130000	-2.2432040000	0.4896050000
H	-1.2400620000	-2.6301260000	1.5445610000
C	1.1634320000	0.5938000000	0.1661910000
C	2.1521890000	1.2091830000	0.9624760000
C	3.4742460000	0.8025520000	0.9160530000
C	3.8654340000	-0.2394010000	0.0643510000

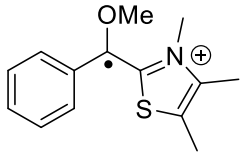
C	2.9098510000	-0.8536930000	-0.7469000000
C	1.5807580000	-0.4277180000	-0.6972270000
H	1.8621010000	2.0141590000	1.6278020000
H	4.2271010000	1.2747580000	1.5363710000
H	3.1845190000	-1.6434760000	-1.4338600000
H	0.8603730000	-0.8850300000	-1.3663570000
O	5.1920650000	-0.5701460000	0.0945960000
C	5.6497820000	-1.6100460000	-0.7563380000
H	6.7172990000	-1.7054690000	-0.5636630000
H	5.1547060000	-2.5610770000	-0.5295660000
H	5.4937060000	-1.3623190000	-1.8122980000
O	-0.4007790000	2.4614480000	0.3421380000
C	0.0596480000	3.2454090000	-0.7635090000
H	-0.4631430000	2.9651750000	-1.6844140000
H	-0.1662330000	4.2833980000	-0.5176540000
H	1.1383460000	3.1332220000	-0.9119790000

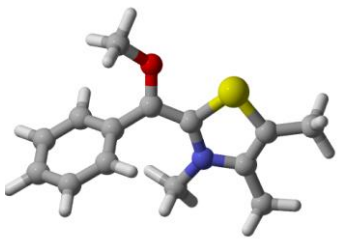
thermodynamic data

Zero-point correction= 0.310874 (Hartree/Particle)
Thermal correction to Energy= 0.331356
Thermal correction to Enthalpy= 0.332300
Thermal correction to Gibbs Free Energy= 0.261546
Sum of electronic and zero-point Energies= -1186.295065
Sum of electronic and thermal Energies= -1186.274583
Sum of electronic and thermal Enthalpies= -1186.273639
Sum of electronic and thermal Free Energies= -1186.344392

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	207.929	75.207	148.913

(u)B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.6957510000	0.3740560000	0.1115390000
N	-1.1517310000	-0.9089340000	0.2667130000
C	-2.5291760000	-1.0492460000	0.0995150000
C	-3.1673180000	0.1384150000	-0.1278470000

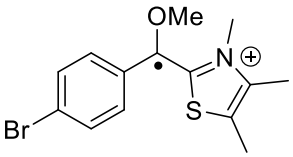
S	-2.0320210000	1.4631900000	-0.1527450000
C	-4.6241800000	0.4116620000	-0.3312310000
C	-3.1636080000	-2.4019640000	0.1897470000
C	0.6138930000	0.8740990000	0.1461810000
H	-2.6505660000	-3.1279020000	-0.4455540000
H	-4.2002430000	-2.3533140000	-0.1363990000
H	-3.1595080000	-2.7853500000	1.2147500000
H	-4.8126490000	0.8381500000	-1.3204130000
H	-4.9958250000	1.1222630000	0.4121340000
H	-5.2128530000	-0.5000540000	-0.2404330000
C	-0.3086140000	-2.0379300000	0.6947240000
H	0.5244530000	-1.6648520000	1.2824690000
H	0.0779220000	-2.5849500000	-0.1663160000
H	-0.9045570000	-2.7045420000	1.3125880000
C	1.8553430000	0.0992300000	0.0001740000
C	2.8719710000	0.1982710000	0.9666910000
C	4.0533040000	-0.5179830000	0.8127140000
C	4.2425460000	-1.3261960000	-0.3095540000
C	3.2446530000	-1.4204080000	-1.2791370000
C	2.0547220000	-0.7149850000	-1.1268680000
H	2.7230320000	0.8134910000	1.8468710000
H	4.8266530000	-0.4482870000	1.5683500000
H	5.1676320000	-1.8774290000	-0.4293510000
H	3.3975650000	-2.0347820000	-2.1584550000
H	1.2902230000	-0.7708500000	-1.8940570000
O	0.6398410000	2.2108300000	0.3004070000
C	1.7694160000	2.9955380000	-0.1586460000
H	2.1020420000	2.6493350000	-1.1375060000
H	1.3923470000	4.0132520000	-0.2219530000
H	2.5868620000	2.9453270000	0.5589250000

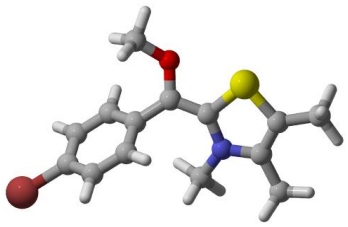
thermodynamic data

Zero-point correction= 0.280008 (Hartree/Particle)
Thermal correction to Energy= 0.297897
Thermal correction to Enthalpy= 0.298842
Thermal correction to Gibbs Free Energy= 0.232410
Sum of electronic and zero-point Energies= -1071.561836
Sum of electronic and thermal Energies= -1071.543947
Sum of electronic and thermal Enthalpies= -1071.543003
Sum of electronic and thermal Free Energies= -1071.609434

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.933	65.575	139.816

(u)B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0505240000	0.3785770000	0.1119210000
N	-2.2015590000	-0.9672160000	0.3201640000
C	-3.4970790000	-1.4366240000	0.1045150000
C	-4.3824600000	-0.4447340000	-0.2141470000
S	-3.5887590000	1.1080760000	-0.2658880000
C	-5.8489950000	-0.5354410000	-0.4967360000
C	-3.8001590000	-2.8956330000	0.2446050000
C	-0.8982800000	1.1768790000	0.1738560000
H	-3.0949830000	-3.5066930000	-0.3238240000
H	-4.7984840000	-3.1098960000	-0.1306600000
H	-3.7644950000	-3.2198160000	1.2892010000
H	-6.0685140000	-0.2745590000	-1.5360140000
H	-6.4130860000	0.1487560000	0.1426090000
H	-6.2235820000	-1.5418210000	-0.3150640000
C	-1.1478440000	-1.8433940000	0.8595640000
H	-0.4388840000	-1.2484680000	1.4264790000
H	-0.6204890000	-2.3608490000	0.0568130000
H	-1.6055070000	-2.5733450000	1.5226970000
C	0.4932340000	0.7159990000	0.1051310000
C	1.4295090000	1.1237600000	1.0726420000
C	2.7510670000	0.7048710000	0.9999490000
C	3.1553080000	-0.1153380000	-0.0558480000
C	2.2469270000	-0.5197460000	-1.0348390000
C	0.9228360000	-0.1067090000	-0.9498380000
H	1.1157870000	1.7459870000	1.9029510000
H	3.4623240000	1.0076940000	1.7574310000
Br	4.9649380000	-0.6824570000	-0.1628390000
H	2.5747060000	-1.1393710000	-1.8594690000
H	0.2248150000	-0.4009250000	-1.7257870000
O	-1.1967690000	2.4860510000	0.2781830000
C	-0.2847050000	3.5021340000	-0.2105770000
H	-0.8968530000	4.3934750000	-0.3236490000
H	0.5082920000	3.6860460000	0.5126060000
H	0.1383290000	3.2050700000	-1.1705730000

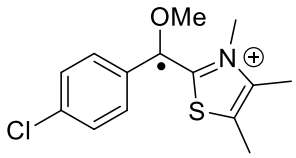
thermodynamic data

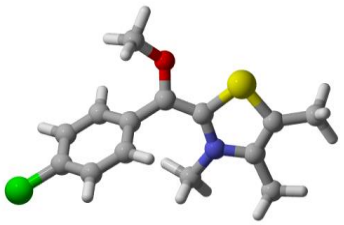
Zero-point correction= 0.269753 (Hartree/Particle)
Thermal correction to Energy= 0.289047
Thermal correction to Enthalpy= 0.289991
Thermal correction to Gibbs Free Energy= 0.219367

Sum of electronic and zero-point Energies= -3645.110759
Sum of electronic and thermal Energies= -3645.091465
Sum of electronic and thermal Enthalpies= -3645.090521
Sum of electronic and thermal Free Energies= -3645.161145

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	181.380	69.802	148.642

(u)B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4041280000	0.3867070000	0.1160140000
N	-1.6432730000	-0.9480540000	0.3125700000
C	-2.9694360000	-1.3268250000	0.1063810000
C	-3.7893610000	-0.2740170000	-0.1917660000
S	-2.8937060000	1.2221100000	-0.2363740000
C	-5.2607490000	-0.2648840000	-0.4641000000
C	-3.3702630000	-2.7633880000	0.2323380000
C	-0.1997030000	1.1042660000	0.1725230000
H	-2.7149020000	-3.4136190000	-0.3521060000
H	-4.3849560000	-2.9039210000	-0.1339570000
H	-3.3453560000	-3.1031730000	1.2722850000
H	-5.4663350000	-0.0656110000	-1.5200210000
H	-5.7617820000	0.5094130000	0.1222080000
H	-5.7154330000	-1.2202320000	-0.2051660000
C	-0.6447230000	-1.8974050000	0.8325000000
H	0.0964060000	-1.3587810000	1.4148160000
H	-0.1462650000	-2.4260930000	0.0187250000
H	-1.1465140000	-2.6142710000	1.4775540000
C	1.1560270000	0.5508080000	0.0784070000
C	2.1323910000	0.8832230000	1.0351130000
C	3.4200730000	0.3751110000	0.9383560000
C	3.7503530000	-0.4602350000	-0.1309310000
C	2.8026230000	-0.7914930000	-1.0996250000
C	1.5122920000	-0.2889270000	-0.9905160000
H	1.8746380000	1.5174160000	1.8755020000
H	4.1652310000	0.6180500000	1.6848900000
Cl	5.3663990000	-1.0919850000	-0.2591130000

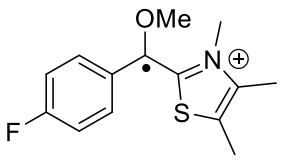
H	3.0794640000	-1.4244140000	-1.9329300000
H	0.7841450000	-0.5267060000	-1.7579670000
O	-0.4072030000	2.4291230000	0.2970650000
C	0.5613920000	3.3874580000	-0.1994620000
H	0.0087200000	4.3193790000	-0.2894430000
H	1.3799490000	3.5087700000	0.5083050000
H	0.9433240000	3.0747670000	-1.1716930000

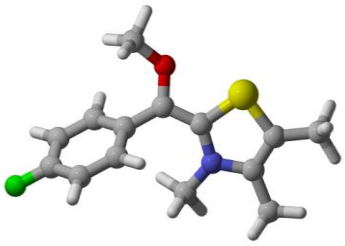
thermodynamic data

Zero-point correction= 0.270300 (Hartree/Particle)
Thermal correction to Energy= 0.289379
Thermal correction to Enthalpy= 0.290323
Thermal correction to Gibbs Free Energy= 0.220746
Sum of electronic and zero-point Energies= -1531.190520
Sum of electronic and thermal Energies= -1531.171441
Sum of electronic and thermal Enthalpies= -1531.170497
Sum of electronic and thermal Free Energies= -1531.240074

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	181.588	69.380	146.437

(u)B3LYP/6-311+G**





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.0452750000	0.3888180000	0.1155390000
N	-1.3792640000	-0.9285540000	0.2925360000
C	-2.7332720000	-1.2042410000	0.1044690000
C	-3.4778670000	-0.0882740000	-0.1601040000
S	-2.4748850000	1.3381460000	-0.1952740000
C	-4.9490810000	0.0346460000	-0.4047220000
C	-3.2383750000	-2.6090970000	0.2119440000
C	0.2090190000	1.0149690000	0.1628980000
H	-2.6466810000	-3.2948130000	-0.3992710000
H	-4.2681230000	-2.6651500000	-0.1343670000
H	-3.2179170000	-2.9711770000	1.2444590000
H	-5.1574380000	0.2710310000	-1.4524220000
H	-5.3814190000	0.8310120000	0.2061930000

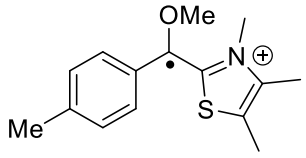
H	-5.4687620000	-0.8899570000	-0.1567230000
C	-0.4431050000	-1.9605910000	0.7685790000
H	0.3390980000	-1.4942020000	1.3595960000
H	0.0094970000	-2.4942000000	-0.0684740000
H	-0.9862120000	-2.6628540000	1.3956790000
C	1.5207580000	0.3658810000	0.0459770000
C	2.5211960000	0.6032290000	1.0071110000
C	3.7693420000	0.0077090000	0.8915400000
C	4.0163010000	-0.8154250000	-0.2016980000
C	3.0587560000	-1.0627040000	-1.1773420000
C	1.8091520000	-0.4694810000	-1.0471540000
H	2.3108220000	1.2331770000	1.8636480000
H	4.5451330000	0.1665820000	1.6298990000
F	5.2209490000	-1.3884840000	-0.3189480000
H	3.3029120000	-1.6957380000	-2.0210870000
H	1.0608020000	-0.6337350000	-1.8142040000
O	0.1010120000	2.3500950000	0.3047270000
C	1.1345340000	3.2397580000	-0.1883780000
H	0.6566540000	4.2145230000	-0.2465090000
H	1.9726580000	3.2783810000	0.5057410000
H	1.4728490000	2.9210810000	-1.1747820000

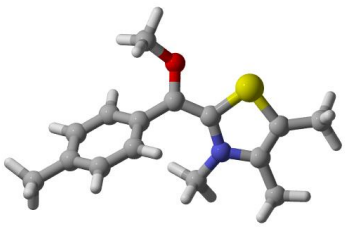
thermodynamic data

Zero-point correction= 0.271612 (Hartree/Particle)
Thermal correction to Energy= 0.290342
Thermal correction to Enthalpy= 0.291286
Thermal correction to Gibbs Free Energy= 0.222697
Sum of electronic and zero-point Energies= -1170.835187
Sum of electronic and thermal Energies= -1170.816457
Sum of electronic and thermal Enthalpies= -1170.815513
Sum of electronic and thermal Free Energies= -1170.884102

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	182.192	68.538	144.357

(u)B3LYP/6-311+G**		





xyz-matrix

37
XYZ file generated by gabedit : coordinates in Angstrom

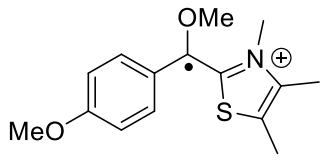
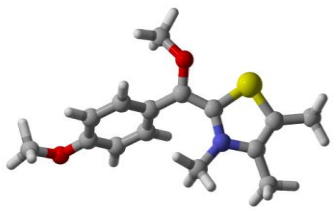
C	-1.0728830000	0.3882310000	0.1169610000
N	-1.3878010000	-0.9325220000	0.3023950000
C	-2.7363280000	-1.2306900000	0.1065830000
C	-3.4961360000	-0.1293730000	-0.1720190000
S	-2.5149390000	1.3132760000	-0.2104710000
C	-4.9673660000	-0.0303130000	-0.4271230000
C	-3.2190140000	-2.6428800000	0.2223660000
C	0.1728480000	1.0315690000	0.1672610000
H	-2.6105160000	-3.3236780000	-0.3777640000
H	-4.2448290000	-2.7195120000	-0.1316780000
H	-3.2008780000	-2.9956870000	1.2581080000
H	-5.1720700000	0.2181970000	-1.4726860000
H	-5.4196100000	0.7483590000	0.1923580000
H	-5.4716660000	-0.9681600000	-0.1977270000
C	-0.4401330000	-1.9441140000	0.7984860000
H	0.3347040000	-1.4570420000	1.3825050000
H	0.0232110000	-2.4845480000	-0.0281440000
H	-0.9765070000	-2.6426750000	1.4357210000
C	1.4905090000	0.3992720000	0.0520450000
C	2.4990790000	0.6620720000	0.9972560000
C	3.7501650000	0.0767030000	0.8692440000
C	4.0515360000	-0.7736250000	-0.2059680000
C	3.0473950000	-1.0192760000	-1.1512190000
C	1.7857990000	-0.4492790000	-1.0274400000
H	2.2909300000	1.3032240000	1.8464960000
H	4.5097120000	0.2817230000	1.6158940000
C	5.4095480000	-1.4119880000	-0.3265410000
H	3.2611660000	-1.6544800000	-2.0038300000
H	1.0356720000	-0.6354330000	-1.7885090000
H	5.6109900000	-1.7356140000	-1.3487490000
H	5.4786330000	-2.2936080000	0.3197830000
H	6.2006670000	-0.7241180000	-0.0206560000
O	0.0435500000	2.3656470000	0.3045930000
C	1.0681110000	3.2681120000	-0.1821410000
H	1.4371800000	2.9379810000	-1.1535590000
H	0.5710620000	4.2311300000	-0.2703210000
H	1.8886050000	3.3374600000	0.5302920000

thermodynamic data

Zero-point correction= 0.307070 (Hartree/Particle)
Thermal correction to Energy= 0.326866
Thermal correction to Enthalpy= 0.327810
Thermal correction to Gibbs Free Energy= 0.256371
Sum of electronic and zero-point Energies= -1110.865052
Sum of electronic and thermal Energies= -1110.845256
Sum of electronic and thermal Enthalpies= -1110.844311
Sum of electronic and thermal Free Energies= -1110.915751

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	205.112	71.696	150.356

(u)B3LYP/6-311+G**	

xyz-matrix

38
XYZ file generated by gabedit : coordinates in Angstrom

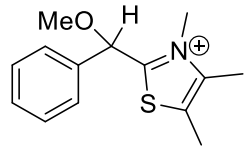
C	1.4165260000	0.3840700000	0.1284040000
N	1.6805410000	-0.9471630000	0.3182700000
C	3.0174170000	-1.2980710000	0.1232180000
C	3.8191870000	-0.2283710000	-0.1563110000
S	2.8943190000	1.2525980000	-0.1951930000
C	5.2935550000	-0.1863530000	-0.4088480000
C	3.4424980000	-2.7283950000	0.2435410000
C	0.1944020000	1.0736350000	0.1733050000
H	2.8000310000	-3.3866950000	-0.3461840000
H	3.4196750000	-3.0742420000	1.2815490000
H	4.4607530000	-2.8501690000	-0.1197390000
H	5.7770460000	0.5622440000	0.2241530000
H	5.5103070000	0.0707690000	-1.4498230000
H	5.7578000000	-1.1482040000	-0.1947200000
C	0.7019860000	-1.9132850000	0.8435220000
H	0.2294070000	-2.4731160000	0.0352550000
H	-0.0633540000	-1.3819690000	1.4009460000
H	1.2138650000	-2.6015280000	1.5119500000
C	-1.1357930000	0.4978780000	0.0150200000
C	-1.4149320000	-0.4043130000	-1.0351490000
C	-2.6797400000	-0.9289220000	-1.2039670000
C	-3.7184230000	-0.5751130000	-0.3224240000
C	-3.4587480000	0.3227530000	0.7262630000
C	-2.1861270000	0.8541950000	0.8797620000
H	-4.2370550000	0.6034830000	1.4224010000
H	-1.9971350000	1.5297130000	1.7061010000
H	-2.9045540000	-1.6035460000	-2.0207690000
O	-4.9100380000	-1.1417810000	-0.5678350000
C	-6.0327980000	-0.8270280000	0.2656390000
H	-6.8637550000	-1.3981600000	-0.1405960000
H	-5.8490740000	-1.1317210000	1.2994620000
H	-6.2642910000	0.2404440000	0.2206120000
H	-0.6352340000	-0.6629190000	-1.7431220000
O	0.3760280000	2.3996940000	0.3526900000
C	-0.5640810000	3.3590360000	-0.1906490000
H	-0.9424380000	3.0213910000	-1.1558120000
H	-1.3888070000	3.5212300000	0.5018290000
H	0.0064380000	4.2779710000	-0.3050950000

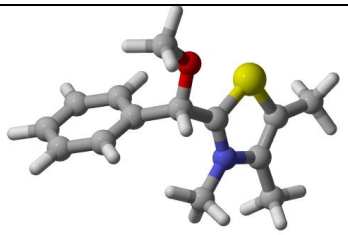
thermodynamic data

Zero-point correction= 0.312262 (Hartree/Particle)
Thermal correction to Energy= 0.332800
Thermal correction to Enthalpy= 0.333744
Thermal correction to Gibbs Free Energy= 0.261379
Sum of electronic and zero-point Energies= -1186.091088
Sum of electronic and thermal Energies= -1186.070550
Sum of electronic and thermal Enthalpies= -1186.069606
Sum of electronic and thermal Free Energies= -1186.141971

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	208.835	74.893	152.304

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.6686290000	0.3651280000	-0.3850380000
N	-1.2332220000	-0.8109790000	-0.6509840000
C	-2.5534800000	-0.9472720000	-0.1845800000
C	-2.9843980000	0.1744150000	0.4565570000
S	-1.7346570000	1.3950160000	0.4559520000
C	-4.3004740000	0.4454940000	1.1186790000
C	-3.3040750000	-2.2200000000	-0.4152050000
C	0.7252360000	0.8253510000	-0.7572710000
H	-3.3412010000	-2.4831870000	-1.4754690000
H	-4.3289730000	-2.1169960000	-0.0641940000
H	-2.8553550000	-3.0573100000	0.1274160000
H	-4.6499800000	1.4576560000	0.9050760000
H	-4.2235910000	0.3403580000	2.2045830000
H	-5.0634240000	-0.2483450000	0.7663020000
C	-0.5726890000	-1.8829850000	-1.4201110000
H	0.4967700000	-1.7022490000	-1.4497720000
H	-0.9792970000	-1.9086630000	-2.4322310000
H	-0.7515040000	-2.8368790000	-0.9284480000
C	1.8288910000	0.0049510000	-0.0978670000
C	1.8527810000	-0.1719530000	1.2902490000
C	2.8922180000	-0.8797490000	1.8863620000
C	3.9159910000	-1.4146710000	1.1029060000

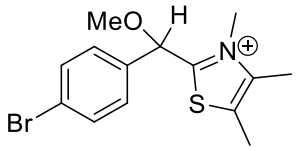
C	3.9023330000	-1.2342880000	-0.2780790000
C	2.8619920000	-0.5240380000	-0.8764450000
H	4.7020330000	-1.6366720000	-0.8884610000
H	2.8639820000	-0.3733800000	-1.9518930000
H	4.7249150000	-1.9637820000	1.5700380000
H	1.0722070000	0.2571100000	1.9092530000
H	2.9079260000	-1.0101950000	2.9619830000
H	0.8302340000	0.7405120000	-1.8510570000
O	0.7297460000	2.1897650000	-0.3784080000
C	1.8607460000	2.9460290000	-0.8259860000
H	1.6878490000	3.9667950000	-0.4917140000
H	2.7881190000	2.5683350000	-0.3881820000
H	1.9297380000	2.9268920000	-1.9193350000

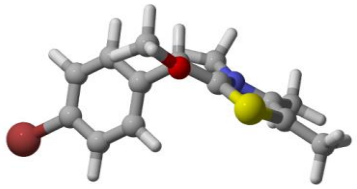
thermodynamic data

Zero-point correction= 0.292234 (Hartree/Particle)
Thermal correction to Energy= 0.310185
Thermal correction to Enthalpy= 0.311130
Thermal correction to Gibbs Free Energy= 0.244726
Sum of electronic and zero-point Energies= -1072.175522
Sum of electronic and thermal Energies= -1072.157571
Sum of electronic and thermal Enthalpies= -1072.156627
Sum of electronic and thermal Free Energies= -1072.223030

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	194.644	65.795	139.758

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	2.7334340000	0.3090730000	1.1764520000
C	3.0453460000	-0.1662310000	-0.0948070000
C	2.0925840000	-0.1581720000	-1.1149360000
C	0.8144290000	0.3214880000	-0.8517540000
C	0.4780960000	0.7927540000	0.4221860000
C	1.4492950000	0.7888540000	1.4264680000
C	-0.9047740000	1.3708750000	0.6988920000
C	-2.0330280000	0.4389290000	0.3070740000
S	-3.1379380000	0.8693970000	-0.9168020000

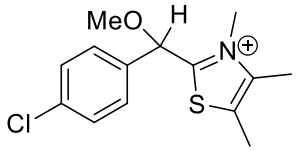
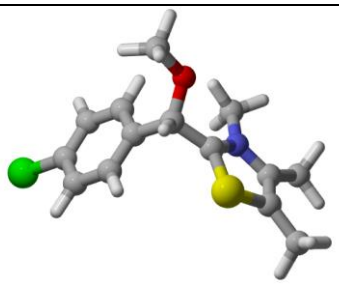
C	-4.0061670000	-0.6339860000	-0.7237120000
C	-3.4385020000	-1.3879780000	0.2584210000
N	-2.3180030000	-0.7539650000	0.8255820000
C	-3.8668800000	-2.7350550000	0.7465780000
C	-5.1892780000	-0.9365260000	-1.5913280000
C	-1.5725660000	-1.3632810000	1.9436210000
H	3.4818140000	0.3130270000	1.9581400000
Br	4.7946390000	-0.8288690000	-0.4488970000
H	2.3499490000	-0.5184230000	-2.1025350000
H	0.0852090000	0.3420300000	-1.6543330000
H	1.2147750000	1.1722480000	2.4149460000
H	-4.7892740000	-3.0335740000	0.2525020000
H	-3.1164570000	-3.5005730000	0.5282520000
H	-4.0510370000	-2.7371510000	1.8240210000
H	-5.8226500000	-0.0561520000	-1.7177950000
H	-4.8742530000	-1.2676530000	-2.5849390000
H	-5.8020970000	-1.7236910000	-1.1525530000
H	-2.1627820000	-1.2886510000	2.8580790000
H	-1.3788670000	-2.4095320000	1.7160950000
H	-0.6231660000	-0.8533360000	2.0685300000
H	-0.9909170000	1.5746900000	1.7783570000
O	-1.1830310000	2.5475070000	-0.0374910000
C	-0.3998700000	3.6932410000	0.3179320000
H	-0.7662260000	4.5086230000	-0.3020830000
H	-0.5429620000	3.9453900000	1.3745460000
H	0.6611240000	3.5265670000	0.1153030000

thermodynamic data

Zero-point correction= 0.281807 (Hartree/Particle)
Thermal correction to Energy= 0.301298
Thermal correction to Enthalpy= 0.302243
Thermal correction to Gibbs Free Energy= 0.231120
Sum of electronic and zero-point Energies= -3645.724597
Sum of electronic and thermal Energies= -3645.705106
Sum of electronic and thermal Enthalpies= -3645.704161
Sum of electronic and thermal Free Energies= -3645.775284

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.068	70.120	149.689

B3LYP/6-311+G**	

xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3762980000	0.5034170000	-0.3250440000
N	-1.8553560000	0.1511800000	0.8657210000
C	-2.9364570000	-0.7482740000	0.8240590000
C	-3.2921320000	-1.0736070000	-0.4502830000
S	-2.2594710000	-0.2371500000	-1.5817820000
C	-4.3712070000	-1.9862220000	-0.9444610000
C	-3.5591320000	-1.2352550000	2.0939600000
C	-0.1750610000	1.3847150000	-0.6370310000
H	-2.8165790000	-1.6849600000	2.7577090000
H	-4.3070390000	-1.9947390000	1.8757550000
H	-4.0567720000	-0.4265930000	2.6369440000
H	-3.9500450000	-2.8996950000	-1.3730890000
H	-4.9765120000	-1.5019400000	-1.7140710000
H	-5.0383720000	-2.2714070000	-0.1319600000
C	-1.3101740000	0.6363990000	2.1521340000
H	-2.1390510000	0.8502830000	2.8228590000
H	-0.7531730000	1.5482050000	1.9711200000
H	-0.6699300000	-0.1322520000	2.5865070000
C	1.1393770000	0.6368260000	-0.3912860000
C	1.6119820000	-0.2598530000	-1.3547390000
C	2.7954380000	-0.9625510000	-1.1565000000
C	3.5203070000	-0.7576120000	0.0161900000
C	3.0766130000	0.1461630000	0.9785340000
C	1.8853370000	0.8371120000	0.7722790000
H	3.6609880000	0.3129170000	1.8743320000
H	1.5602890000	1.5577760000	1.5120840000
Cl	5.0092510000	-1.6303390000	0.2732600000
H	1.0660450000	-0.4099160000	-2.2810670000
H	3.1608050000	-1.6514350000	-1.9070910000
H	-0.2424930000	1.5991350000	-1.7128570000
O	-0.3190200000	2.5807210000	0.0963750000
C	0.3871370000	3.7006640000	-0.4629220000
H	0.1900360000	4.5424180000	0.1976160000
H	1.4626930000	3.5099300000	-0.5069420000
H	0.0086690000	3.9268750000	-1.4651370000

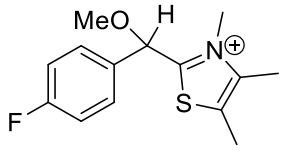
thermodynamic data

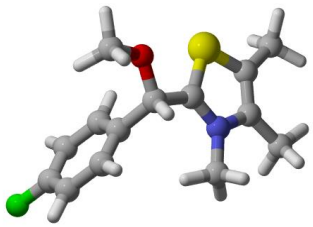
Zero-point correction= 0.282967 (Hartree/Particle)
Thermal correction to Energy= 0.302005

Thermal correction to Enthalpy= 0.302949
Thermal correction to Gibbs Free Energy= 0.233559
Sum of electronic and zero-point Energies= -1531.800603
Sum of electronic and thermal Energies= -1531.781565
Sum of electronic and thermal Enthalpies= -1531.780620
Sum of electronic and thermal Free Energies= -1531.850010

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.511	69.521	146.044

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.0244140000	0.4198050000	-0.3659850000
N	-1.4889860000	-0.7703290000	-0.7412880000
C	-2.7490200000	-1.1026560000	-0.2107550000
C	-3.2364120000	-0.1186790000	0.5953100000
S	-2.1179860000	1.2211010000	0.6665100000
C	-4.5164680000	-0.0709120000	1.3719490000
C	-3.3880800000	-2.4107070000	-0.5532720000
C	0.2846090000	1.0683820000	-0.7676290000
H	-3.4757270000	-2.5487040000	-1.6339770000
H	-4.3904670000	-2.4568560000	-0.1322330000
H	-2.8235690000	-3.2551170000	-0.1468280000
H	-4.9821600000	0.9145880000	1.3070040000
H	-4.3433220000	-0.2900150000	2.4293770000
H	-5.2311500000	-0.7996720000	0.9901480000
C	-0.7881190000	-1.6631490000	-1.6840480000
H	0.2573350000	-1.3787920000	-1.7439270000
H	-1.2544780000	-1.5933790000	-2.6679800000
H	-0.8507230000	-2.6863720000	-1.3202290000
C	1.5106920000	0.3117950000	-0.2716950000
C	1.6543660000	-0.0018720000	1.0857190000
C	2.7980670000	-0.6421490000	1.5472130000
C	3.7958360000	-0.9623660000	0.6339680000
C	3.6913160000	-0.6579360000	-0.7150040000
C	2.5394120000	-0.0139910000	-1.1607340000
H	4.4988190000	-0.9129050000	-1.3895100000

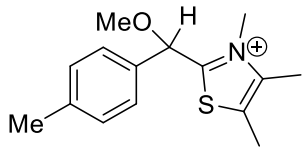
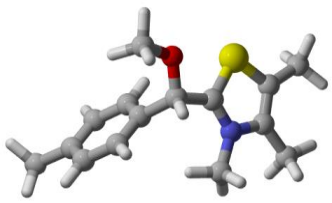
H	2.4534950000	0.2433730000	-2.2118100000
F	4.9004440000	-1.5839030000	1.0755920000
H	0.8803730000	0.2697600000	1.7949490000
H	2.9296130000	-0.8892480000	2.5931270000
H	0.3189750000	1.1102310000	-1.8682590000
O	0.1742150000	2.3773160000	-0.2388190000
C	1.1851940000	3.2986600000	-0.6642420000
H	0.9278690000	4.2536260000	-0.2111220000
H	2.1753160000	2.9858090000	-0.3232150000
H	1.1808790000	3.3996260000	-1.7552160000

thermodynamic data

Zero-point correction= 0.283857 (Hartree/Particle)
Thermal correction to Energy= 0.302682
Thermal correction to Enthalpy= 0.303626
Thermal correction to Gibbs Free Energy= 0.235215
Sum of electronic and zero-point Energies= -1171.448999
Sum of electronic and thermal Energies= -1171.430174
Sum of electronic and thermal Enthalpies= -1171.429230
Sum of electronic and thermal Free Energies= -1171.497641

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.936	68.787	143.983

B3LYP/6-311+G**		

xyz-matrix

38
XYZ file generated by gabedit : coordinates in Angstrom

C	1.0550190000	0.4254450000	0.3597750000
N	1.5029200000	-0.7654270000	0.7517830000
C	2.7513180000	-1.1294920000	0.2142280000
C	3.2467200000	-0.1695840000	-0.6150790000
S	2.1505210000	1.1882780000	-0.6997390000
C	4.5186400000	-0.1588290000	-1.4063900000
C	3.3709330000	-2.4422250000	0.5743510000
C	-0.2390930000	1.1003660000	0.7622130000
H	3.4667450000	-2.5620690000	1.6565350000
H	4.3681510000	-2.5140800000	0.1445910000
H	2.7873640000	-3.2836280000	0.1890610000

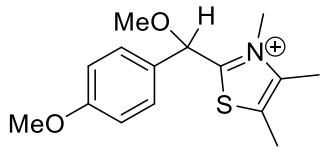
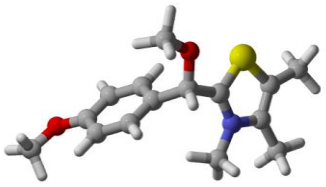
H	5.0051750000	0.8176400000	-1.3600560000
H	4.3292360000	-0.3884250000	-2.4588040000
H	5.2225170000	-0.8970140000	-1.0226560000
C	0.7935190000	-1.6272760000	1.7165760000
H	-0.2516060000	-1.3376770000	1.7600740000
H	1.2541550000	-1.5297580000	2.7009510000
H	0.8553160000	-2.6607890000	1.3835380000
C	-1.4784860000	0.3526130000	0.2891500000
C	-1.6414220000	0.0127290000	-1.0589560000
C	-2.8003840000	-0.6229180000	-1.4868530000
C	-3.8321940000	-0.9373390000	-0.5900480000
C	-3.6611820000	-0.5909500000	0.7538430000
C	-2.5022210000	0.0491570000	1.1891380000
H	-2.9106420000	-0.8776170000	-2.5355370000
H	-0.2630300000	1.1597710000	1.8624660000
H	-0.8708700000	0.2586560000	-1.7820520000
H	-2.4044170000	0.3196730000	2.2365510000
H	-4.4450680000	-0.8161680000	1.4686860000
C	-5.0972840000	-1.5998100000	-1.0713030000
H	-5.6272060000	-2.0927110000	-0.2546920000
H	-4.8889200000	-2.3430180000	-1.8439980000
H	-5.7765740000	-0.8595540000	-1.5067350000
O	-0.1113600000	2.4005860000	0.2130860000
C	-1.1184090000	3.3359120000	0.6141860000
H	-0.8516080000	4.2807940000	0.1454200000
H	-2.1083450000	3.0228170000	0.2730950000
H	-1.1211120000	3.4572220000	1.7032260000

thermodynamic data

Zero-point correction= 0.319269 (Hartree/Particle)
Thermal correction to Energy= 0.339166
Thermal correction to Enthalpy= 0.340110
Thermal correction to Gibbs Free Energy= 0.268495
Sum of electronic and zero-point Energies= -1111.478050
Sum of electronic and thermal Energies= -1111.458153
Sum of electronic and thermal Enthalpies= -1111.457209
Sum of electronic and thermal Free Energies= -1111.528824

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	212.830	71.936	150.726

B3LYP/6-311+G**	

xyz-matrix

39
XYZ file generated by gabedit : coordinates in Angstrom

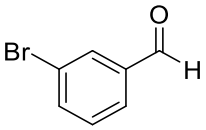
C	1.4117610000	0.4110110000	0.3610200000
N	1.7647640000	-0.8111470000	0.7537460000
C	2.9799220000	-1.2738630000	0.2148740000
C	3.5475440000	-0.3579520000	-0.6177250000
S	2.5614200000	1.0829020000	-0.7025230000
C	4.8159590000	-0.4447760000	-1.4094320000
C	3.4936300000	-2.6304670000	0.5791310000
C	0.1735870000	1.1846820000	0.7633870000
H	3.5777440000	-2.7541790000	1.6618380000
H	4.4830030000	-2.7823460000	0.1523120000
H	2.8461050000	-3.4242020000	0.1948980000
H	5.4241050000	0.4534840000	-1.2814980000
H	4.6068060000	-0.5578740000	-2.4767930000
H	5.4151720000	-1.2982660000	-1.0937420000
C	0.9891530000	-1.6102800000	1.7214600000
H	-0.0375600000	-1.2577090000	1.7373580000
H	1.4364060000	-1.5197680000	2.7127640000
H	0.9961030000	-2.6521810000	1.4102460000
C	-1.1178540000	0.5340240000	0.2973740000
C	-1.3098330000	0.1930350000	-1.0518680000
C	-2.5093910000	-0.3417980000	-1.4821140000
C	-3.5612480000	-0.5502010000	-0.5717560000
C	-3.3847780000	-0.2079740000	0.7740940000
C	-2.1684870000	0.3318640000	1.1919720000
H	-2.6684380000	-0.6025170000	-2.5211790000
H	0.1574670000	1.2494820000	1.8636170000
O	-4.6880090000	-1.0756560000	-1.0920700000
C	-5.8179150000	-1.2950880000	-0.2431670000
H	-6.5905750000	-1.7079940000	-0.8872590000
H	-5.5813370000	-2.0116330000	0.5489100000
H	-6.1693900000	-0.3556070000	0.1929390000
H	-0.5208860000	0.3652260000	-1.7763390000
H	-2.0525090000	0.6070670000	2.2362370000
H	-4.1798860000	-0.3445140000	1.4938400000
O	0.4041860000	2.4710730000	0.2107340000
C	-0.5322240000	3.4802360000	0.6013080000
H	-0.1968740000	4.3993040000	0.1251980000
H	-1.5416530000	3.2365020000	0.2607670000
H	-0.5282450000	3.6112690000	1.6893570000

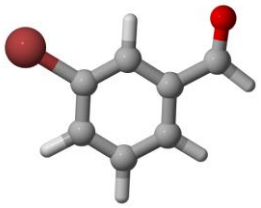
thermodynamic data

Zero-point correction= 0.324520 (Hartree/Particle)
Thermal correction to Energy= 0.344168
Thermal correction to Enthalpy= 0.345112
Thermal correction to Gibbs Free Energy= 0.275695
Sum of electronic and zero-point Energies= -1186.702876
Sum of electronic and thermal Energies= -1186.683228
Sum of electronic and thermal Enthalpies= -1186.682284
Sum of electronic and thermal Free Energies= -1186.751700

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	215.968	73.043	146.099

B3LYP/6-311+G**	***m*-Br-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.6206500000	-0.5218170000	-0.0000020000
C	-1.8979960000	0.0545200000	-0.0000020000
C	-2.0444090000	1.4445550000	-0.0000010000
C	-0.9176210000	2.2624830000	0.0000010000
C	0.3563770000	1.6984440000	0.0000010000
C	0.4889370000	0.3081330000	0.0000000000
H	-3.0385540000	1.8794320000	-0.0000010000
H	-1.0231820000	3.3411200000	0.0000020000
Br	2.2441960000	-0.4616630000	0.0000010000
H	-0.5271630000	-1.6003220000	-0.0000030000
C	-3.1033260000	-0.8099660000	-0.0000050000
H	-4.0656600000	-0.2558530000	0.0000030000
O	-3.0871180000	-2.0190670000	0.0000010000
H	1.2367850000	2.3282620000	0.0000030000

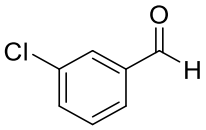
thermodynamic data

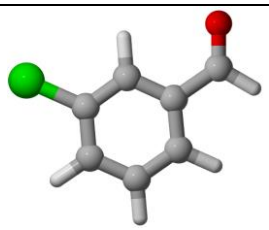
Zero-point correction= 0.099076 (Hartree/Particle)
Thermal correction to Energy= 0.106848
Thermal correction to Enthalpy= 0.107793
Thermal correction to Gibbs Free Energy= 0.065099
Sum of electronic and zero-point Energies= -2919.110971
Sum of electronic and thermal Energies= -2919.103198

Sum of electronic and thermal Enthalpies= -2919.102254
Sum of electronic and thermal Free Energies= -2919.144948

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.048	28.300	89.857

B3LYP/6-311+G**	***m*-Cl-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

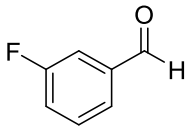
C	-0.1439210000	-0.6368930000	-0.0000020000
C	-1.2944710000	0.1618250000	-0.0000040000
C	-1.1858500000	1.5554360000	-0.0000020000
C	0.0711910000	2.1545900000	0.0000010000
C	1.2202900000	1.3680360000	0.0000020000
C	1.0986510000	-0.0233210000	0.0000000000
H	-2.0841230000	2.1640780000	-0.0000020000
H	0.1637670000	3.2343340000	0.0000020000
Cl	2.5528990000	-1.0080560000	0.0000010000
H	-0.2434900000	-1.7150820000	-0.0000040000
C	-2.6370820000	-0.4687690000	-0.0000080000
H	-3.4826070000	0.2511030000	0.0000070000
O	-2.8410810000	-1.6606850000	0.0000050000
H	2.2029660000	1.8225760000	0.0000040000

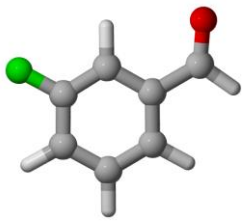
thermodynamic data

Zero-point correction= 0.099725 (Hartree/Particle)
Thermal correction to Energy= 0.107237
Thermal correction to Enthalpy= 0.108181
Thermal correction to Gibbs Free Energy= 0.066872
Sum of electronic and zero-point Energies= -805.190677
Sum of electronic and thermal Energies= -805.183165
Sum of electronic and thermal Enthalpies= -805.182221
Sum of electronic and thermal Free Energies= -805.223531

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.292	27.821	86.943

B3LYP/6-311+G**	***m*-F-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

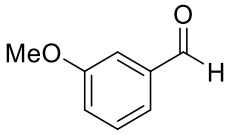
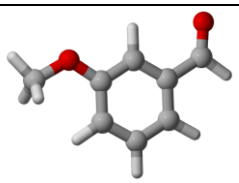
C	-0.0259730000	-0.8303500000	-0.0000250000
C	-0.8833130000	0.2775660000	-0.0000450000
C	-0.3619490000	1.5748820000	-0.0000240000
C	1.0174140000	1.7730460000	0.0000040000
C	1.8789400000	0.6790190000	0.0000200000
C	1.3351260000	-0.6015610000	0.0000050000
H	-1.0366450000	2.4243400000	-0.0000370000
H	1.4259120000	2.7764880000	0.0000150000
F	2.1802280000	-1.6580700000	0.0000190000
H	-0.4279220000	-1.8358750000	-0.0000400000
C	-2.3536110000	0.0798350000	-0.0000970000
H	-2.9448690000	1.0191960000	0.0001000000
O	-2.9041830000	-0.9971450000	0.0000900000
H	2.9551290000	0.8010380000	0.0000430000

thermodynamic data

Zero-point correction= 0.101032 (Hartree/Particle)
Thermal correction to Energy= 0.108177
Thermal correction to Enthalpy= 0.109122
Thermal correction to Gibbs Free Energy= 0.069113
Sum of electronic and zero-point Energies= -444.835506
Sum of electronic and thermal Energies= -444.828360
Sum of electronic and thermal Enthalpies= -444.827416
Sum of electronic and thermal Free Energies= -444.867425

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.882	26.976	84.206

B3LYP/6-311+G**	***m*-OMe-PhCHO**

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

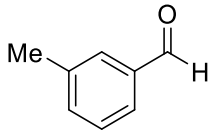
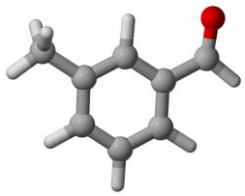
C	0.2953250000	-0.7123220000	-0.0002390000
C	1.3732840000	0.1717170000	-0.0002580000
C	1.1571360000	1.5566740000	-0.0000370000
C	-0.1436500000	2.0426690000	0.0001300000
C	-1.2299420000	1.1656300000	0.0001260000
C	-1.0101470000	-0.2189200000	-0.0000610000
H	2.0019600000	2.2369600000	-0.0000370000
H	-0.3270260000	3.1110010000	0.0002750000
H	0.4695310000	-1.7813040000	-0.0004030000
C	2.7633440000	-0.3441960000	-0.0005690000
H	3.5449440000	0.4449400000	0.0007680000
O	3.0720280000	-1.5146310000	0.0005320000
H	-2.2344070000	1.5671510000	0.0002700000
O	-2.0007100000	-1.1535020000	-0.0000830000
C	-3.3549090000	-0.7188550000	0.0000950000
H	-3.9565210000	-1.6259350000	0.0000410000
H	-3.5857510000	-0.1311810000	0.8950980000
H	-3.5859170000	-0.1309640000	-0.8947230000

thermodynamic data

Zero-point correction= 0.141483 (Hartree/Particle)
Thermal correction to Energy= 0.150434
Thermal correction to Enthalpy= 0.151378
Thermal correction to Gibbs Free Energy= 0.107253
Sum of electronic and zero-point Energies= -460.083439
Sum of electronic and thermal Energies= -460.074488
Sum of electronic and thermal Enthalpies= -460.073544
Sum of electronic and thermal Free Energies= -460.117669

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	94.399	33.311	92.869

B3LYP/6-311+G**	***m*-Me-PhCHO**

xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

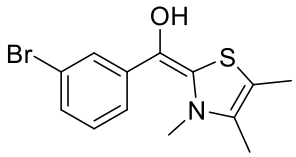
C	0.0172940000	-0.7789470000	0.0000020000
C	-0.9344310000	0.2467000000	0.0000030000
C	-0.5218050000	1.5842280000	0.0000010000
C	0.8358180000	1.8844370000	-0.0000020000
C	1.7749380000	0.8534390000	-0.0000020000
C	1.3824680000	-0.4924590000	0.0000000000
H	-1.2631490000	2.3771070000	0.0000010000
H	1.1674740000	2.9165440000	-0.0000030000
C	2.4036460000	-1.6051400000	0.0000000000
H	-0.3347260000	-1.8054930000	0.0000040000
C	-2.3807870000	-0.0670260000	0.0000070000
H	-3.0444760000	0.8239990000	-0.0000090000
O	-2.8530620000	-1.1824180000	-0.0000060000
H	2.8326700000	1.0967050000	-0.0000040000
H	3.4222610000	-1.2123520000	-0.0000100000
H	2.2907900000	-2.2442850000	-0.8808130000
H	2.2908030000	-2.2442730000	0.8808240000

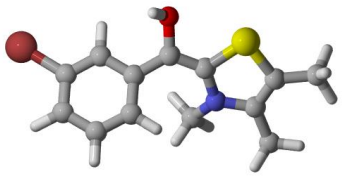
thermodynamic data

Zero-point correction= 0.136433 (Hartree/Particle)
Thermal correction to Energy= 0.143774
Thermal correction to Enthalpy= 0.144718
Thermal correction to Gibbs Free Energy= 0.104421
Sum of electronic and zero-point Energies= -384.860555
Sum of electronic and thermal Energies= -384.853214
Sum of electronic and thermal Enthalpies= -384.852270
Sum of electronic and thermal Free Energies= -384.892567

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.219	28.080	84.812

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

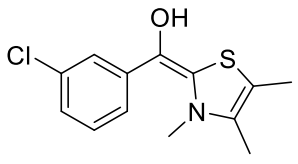
C	-1.8254570000	-0.4855790000	0.0236360000
N	-2.3592340000	0.7514770000	-0.3310640000
C	-3.7723220000	0.7937430000	-0.2722880000
C	-4.3488240000	-0.3893170000	0.0144120000
S	-3.1341610000	-1.6696900000	0.2351030000
C	-5.7941700000	-0.7413770000	0.1690430000
C	-4.4657060000	2.1031220000	-0.5013720000
C	-0.5219600000	-0.8528900000	0.1746560000
H	-4.0189700000	2.8950790000	0.1074590000
H	-5.5182820000	2.0288230000	-0.2319000000
H	-4.4189000000	2.4245590000	-1.5468820000
H	-6.0191410000	-1.0936680000	1.1812350000
H	-6.0777870000	-1.5411250000	-0.5235470000
H	-6.4365550000	0.1155280000	-0.0380770000
C	-1.6043700000	1.6851170000	-1.1656380000
H	-0.8305520000	1.1345150000	-1.7025360000
H	-1.1157750000	2.4699280000	-0.5817550000
H	-2.2686680000	2.1492680000	-1.8932970000
C	0.6547450000	-0.0109820000	0.3603380000
C	1.9197750000	-0.4819720000	-0.0544190000
C	3.0548170000	0.2788460000	0.1823790000
C	3.0001820000	1.5096960000	0.8299850000
C	1.7524060000	1.9692200000	1.2556100000
C	0.5998850000	1.2258230000	1.0362800000
Br	4.7584230000	-0.3864420000	-0.4136280000
H	1.6894350000	2.9123250000	1.7875980000
H	-0.3478620000	1.5784320000	1.4240420000
O	-0.3178170000	-2.2372130000	0.1719260000
H	0.2341130000	-2.4741830000	0.9276770000
H	3.8993990000	2.0835200000	1.0092000000
H	1.9944880000	-1.4258070000	-0.5776000000

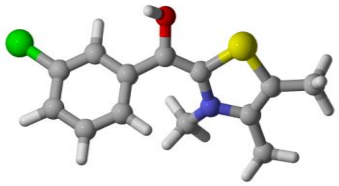
thermodynamic data

Zero-point correction= 0.240576 (Hartree/Particle)
Thermal correction to Energy= 0.258331
Thermal correction to Enthalpy= 0.259275
Thermal correction to Gibbs Free Energy= 0.193862
Sum of electronic and zero-point Energies= -3606.045228
Sum of electronic and thermal Energies= -3606.027473
Sum of electronic and thermal Enthalpies= -3606.026529
Sum of electronic and thermal Free Energies= -3606.091941

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.105	65.604	137.673

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

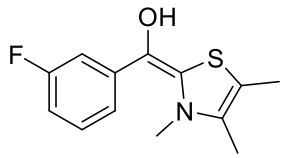
C	-1.2160910000	-0.4963700000	-0.0098730000
N	-1.7156540000	0.7686470000	-0.3127880000
C	-3.1238650000	0.8586940000	-0.2048700000
C	-3.7327490000	-0.3104630000	0.0716630000
S	-2.5590910000	-1.6388060000	0.2162330000
C	-5.1839280000	-0.6149820000	0.2676120000
C	-3.7789860000	2.1962850000	-0.3773100000
C	0.0774660000	-0.9145590000	0.0825820000
H	-3.2768490000	2.9597550000	0.2245410000
H	-4.8200450000	2.1534600000	-0.0603810000
H	-3.7693220000	2.5366260000	-1.4179710000
H	-5.3860340000	-0.9916200000	1.2758380000
H	-5.5214850000	-1.3810260000	-0.4387800000
H	-5.8008420000	0.2708230000	0.1109600000
C	-0.9543810000	1.6927880000	-1.1519590000
H	-0.2752850000	1.1208230000	-1.7876430000
H	-0.3551510000	2.3945510000	-0.5660220000
H	-1.6344100000	2.2569430000	-1.7876190000
C	1.2899530000	-0.1218770000	0.2532170000
C	2.5222610000	-0.6239360000	-0.2172320000
C	3.6918110000	0.0873820000	0.0048120000
C	3.7021820000	1.2979110000	0.6916600000
C	2.4875730000	1.7877290000	1.1733650000
C	1.3018190000	1.0933260000	0.9695740000
Cl	5.2129270000	-0.5592710000	-0.6119400000
H	2.4765280000	2.7144570000	1.7366590000
H	0.3810400000	1.4651710000	1.4017510000
O	0.2298590000	-2.3047860000	0.0344890000
H	0.8000780000	-2.5829350000	0.7620920000
H	4.6296640000	1.8299640000	0.8561670000
H	2.5501290000	-1.5522830000	-0.7721790000

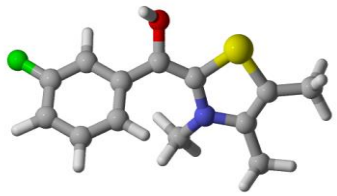
thermodynamic data

Zero-point correction= 0.241147 (Hartree/Particle)
Thermal correction to Energy= 0.258660
Thermal correction to Enthalpy= 0.259604
Thermal correction to Gibbs Free Energy= 0.195428
Sum of electronic and zero-point Energies= -1492.124942
Sum of electronic and thermal Energies= -1492.107430
Sum of electronic and thermal Enthalpies= -1492.106486
Sum of electronic and thermal Free Energies= -1492.170662

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.311	65.178	135.070

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8954400000	-0.5095240000	-0.0469450000
N	-1.3586600000	0.7809410000	-0.2956440000
C	-2.7575240000	0.9185690000	-0.1331990000
C	-3.3999200000	-0.2360720000	0.1278240000
S	-2.2717260000	-1.6100620000	0.1899700000
C	-4.8535960000	-0.4937150000	0.3675220000
C	-3.3638450000	2.2858970000	-0.2361610000
C	0.3843650000	-0.9748250000	-0.0047680000
H	-2.8258180000	3.0014010000	0.3933580000
H	-4.4022760000	2.2681280000	0.0913970000
H	-3.3511530000	2.6737010000	-1.2598760000
H	-5.0348030000	-0.8866610000	1.3735220000
H	-5.2423600000	-1.2305090000	-0.3436140000
H	-5.4429470000	0.4168720000	0.2523120000
C	-0.6010990000	1.7041770000	-1.1403250000
H	0.1166090000	1.1348700000	-1.7318580000
H	-0.0460570000	2.4453700000	-0.5589750000
H	-1.2770190000	2.2219260000	-1.8201880000
C	1.6294180000	-0.2301270000	0.1444620000
C	2.8288580000	-0.7692510000	-0.3670970000
C	4.0188160000	-0.0967810000	-0.1611300000
C	4.1051360000	1.0964850000	0.5395270000

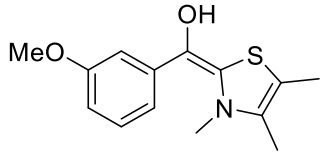
C	2.9213170000	1.6215250000	1.0616120000
C	1.7060880000	0.9733490000	0.8785830000
F	5.1573710000	-0.6299020000	-0.6777430000
H	2.9570510000	2.5386550000	1.6391150000
H	0.8114780000	1.3728760000	1.3392370000
O	0.4855770000	-2.3674990000	-0.0956090000
H	1.0700830000	-2.6849300000	0.6040850000
H	5.0633010000	1.5801740000	0.6782940000
H	2.8257590000	-1.6866020000	-0.9417030000

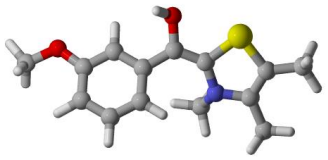
thermodynamic data

Zero-point correction= 0.242164 (Hartree/Particle)
Thermal correction to Energy= 0.258607
Thermal correction to Enthalpy= 0.259551
Thermal correction to Gibbs Free Energy= 0.198141
Sum of electronic and zero-point Energies= -1131.769893
Sum of electronic and thermal Energies= -1131.753451
Sum of electronic and thermal Enthalpies= -1131.752506
Sum of electronic and thermal Free Energies= -1131.813916

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.278	62.384	129.247

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2623630000	-0.5006330000	-0.0500460000
N	-1.7294120000	0.8097880000	-0.2538200000
C	-3.1387140000	0.9059190000	-0.0945140000
C	-3.7658670000	-0.2644540000	0.1180060000
S	-2.6266870000	-1.6348410000	0.1231660000
C	-5.2136850000	-0.5473340000	0.3653380000
C	-3.7646200000	2.2675570000	-0.1453620000
C	0.0162540000	-0.9504650000	0.0282190000
H	-3.2515340000	2.9558270000	0.5341080000
H	-4.8110690000	2.2212160000	0.1531280000
H	-3.7284240000	2.7050100000	-1.1483280000
H	-5.3793050000	-0.9590640000	1.3666230000
H	-5.5944110000	-1.2809920000	-0.3533150000

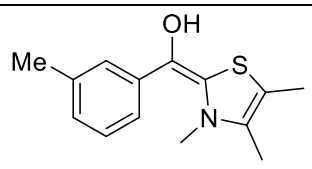
H	-5.8189520000	0.3548610000	0.2682620000
C	-1.1210950000	1.6139890000	-1.3247260000
H	-0.0399640000	1.5191100000	-1.2935210000
H	-1.3678710000	2.6657290000	-1.1792800000
H	-1.4795330000	1.2930630000	-2.3112270000
C	1.2556800000	-0.1887020000	0.1815940000
C	2.4711420000	-0.7521230000	-0.2335760000
C	3.6832260000	-0.0848970000	-0.0314830000
C	3.7051880000	1.1625880000	0.5954070000
C	2.4935200000	1.7210900000	1.0183950000
C	1.2871110000	1.0694600000	0.8251260000
H	2.5066040000	2.6810950000	1.5233620000
H	0.3676930000	1.5089430000	1.1901220000
O	0.1328440000	-2.3400920000	-0.0404910000
H	0.7637640000	-2.6321940000	0.6288970000
H	4.6309430000	1.6949750000	0.7641990000
H	2.4923060000	-1.7057190000	-0.7460860000
O	4.7933090000	-0.7368920000	-0.4911060000
C	6.0609660000	-0.1173270000	-0.3276600000
H	6.7859240000	-0.8041700000	-0.7616960000
H	6.1095950000	0.8414480000	-0.8554950000
H	6.2974220000	0.0376590000	0.7308060000

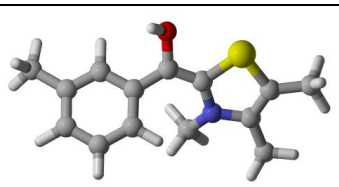
thermodynamic data

Zero-point correction= 0.283057 (Hartree/Particle)
Thermal correction to Energy= 0.301944
Thermal correction to Enthalpy= 0.302888
Thermal correction to Gibbs Free Energy= 0.236001
Sum of electronic and zero-point Energies= -1147.015969
Sum of electronic and thermal Energies= -1146.997083
Sum of electronic and thermal Enthalpies= -1146.996139
Sum of electronic and thermal Free Energies= -1147.063025

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.472	70.525	140.775

B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

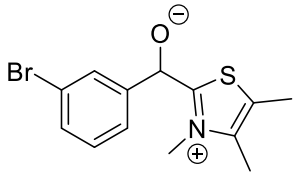
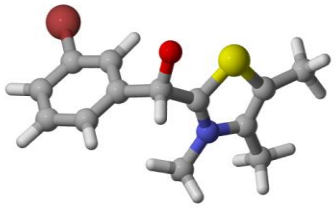
C	0.9116600000	-0.5070880000	0.0302560000
N	1.3800920000	0.7815790000	0.2943070000
C	2.7822360000	0.9082400000	0.1575520000
C	3.4211920000	-0.2482990000	-0.1033800000
S	2.2864300000	-1.6164290000	-0.1919700000
C	4.8763530000	-0.5128800000	-0.3255220000
C	3.4008150000	2.2686250000	0.2817850000
C	-0.3687650000	-0.9622080000	-0.0286150000
H	2.8664190000	2.9997920000	-0.3324670000
H	4.4376190000	2.2473310000	-0.0510350000
H	3.3974120000	2.6383150000	1.3125030000
H	5.0681660000	-0.9057920000	-1.3297440000
H	5.2529050000	-1.2527880000	0.3892360000
H	5.4694020000	0.3943080000	-0.2019370000
C	0.6090310000	1.6955550000	1.1350700000
H	-0.0265390000	1.1136280000	1.8062380000
H	-0.0373960000	2.3562320000	0.5513190000
H	1.2846500000	2.3035290000	1.7342560000
C	-1.6112850000	-0.2078090000	-0.1824310000
C	-2.8151220000	-0.7172950000	0.3488320000
C	-4.0363550000	-0.0685190000	0.1703890000
C	-4.0633690000	1.1244090000	-0.5637940000
C	-2.8895480000	1.6351980000	-1.1144860000
C	-1.6763390000	0.9789910000	-0.9374350000
H	-2.9242130000	2.5452420000	-1.7043480000
H	-0.7809580000	1.3601670000	-1.4136940000
O	-0.4791020000	-2.3565720000	0.0382960000
H	-1.0896140000	-2.6509820000	-0.6487170000
H	-5.0033380000	1.6459490000	-0.7127670000
H	-2.7795790000	-1.6299240000	0.9339740000
C	-5.3088500000	-0.6435100000	0.7471050000
H	-5.9086430000	0.1293890000	1.2357180000
H	-5.0969160000	-1.4223500000	1.4824630000
H	-5.9300180000	-1.0880970000	-0.0379440000

thermodynamic data

Zero-point correction= 0.277999 (Hartree/Particle)
Thermal correction to Energy= 0.296121
Thermal correction to Enthalpy= 0.297065
Thermal correction to Gibbs Free Energy= 0.231668
Sum of electronic and zero-point Energies= -1071.791952
Sum of electronic and thermal Energies= -1071.773830
Sum of electronic and thermal Enthalpies= -1071.772886
Sum of electronic and thermal Free Energies= -1071.838283

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	185.819	67.372	137.640

B3LYP/6-311+G**	

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.6876960000	0.6649170000	0.4746110000
N	-2.1790950000	0.6678770000	-0.7650360000
C	-3.1981890000	-0.2790110000	-0.9900720000
C	-3.4617480000	-1.0009350000	0.1321440000
S	-2.4407180000	-0.4851730000	1.4799470000
C	-4.4537860000	-2.1083920000	0.3171510000
C	-3.8256370000	-0.3848450000	-2.3459660000
C	-0.6292820000	1.4708600000	1.2690380000
H	-4.2530740000	0.5677560000	-2.6731680000
H	-4.6296660000	-1.1188710000	-2.3295920000
H	-3.1041080000	-0.7051370000	-3.1043370000
H	-5.0748410000	-1.9356800000	1.2001410000
H	-3.9511580000	-3.0706550000	0.4539190000
H	-5.1185390000	-2.1993460000	-0.5429000000
C	-1.7128940000	1.5991950000	-1.7986410000
H	-0.8150390000	2.0970670000	-1.4440560000
H	-2.4862480000	2.3401440000	-2.0105490000
H	-1.4743960000	1.0499260000	-2.7090130000
C	0.7435730000	1.3826980000	0.5655190000
C	1.3891770000	0.1435240000	0.4868040000
C	2.6459450000	0.0653600000	-0.0936780000
C	3.3028300000	1.1940710000	-0.5834120000
C	2.6663960000	2.4274230000	-0.4786450000
C	1.3938900000	2.5208370000	0.0889000000
H	3.1720630000	3.3195440000	-0.8320870000
H	0.9142900000	3.4903870000	0.1842310000
O	-0.6545610000	0.9755660000	2.5024380000
H	0.9150920000	-0.7329790000	0.9107820000
Br	3.5165590000	-1.6469620000	-0.2244920000
H	-0.9574030000	2.5395210000	1.1676610000
H	4.2896380000	1.1108950000	-1.0197460000

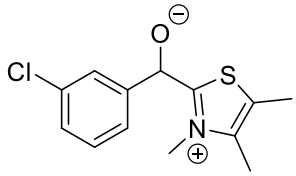
thermodynamic data

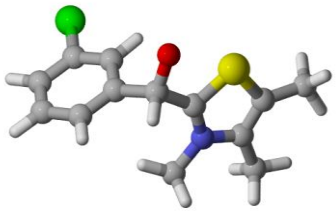
Zero-point correction= 0.239432 (Hartree/Particle)
Thermal correction to Energy= 0.257153
Thermal correction to Enthalpy= 0.258097
Thermal correction to Gibbs Free Energy= 0.190869
Sum of electronic and zero-point Energies= -3606.014481
Sum of electronic and thermal Energies= -3605.996760

Sum of electronic and thermal Enthalpies= -3605.995816
Sum of electronic and thermal Free Energies= -3606.063045

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.366	64.259	141.494

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.1289250000	0.4902540000	0.6075920000
N	-1.6306840000	0.8800720000	-0.5649010000
C	-2.8022220000	0.1996270000	-0.9521770000
C	-3.1698800000	-0.7241250000	-0.0239810000
S	-2.0537760000	-0.7340940000	1.3468440000
C	-4.3344810000	-1.6662440000	-0.0570210000
C	-3.4599470000	0.5368920000	-2.2548310000
C	0.0616710000	0.8930080000	1.5134270000
H	-3.7129620000	1.5993000000	-2.3209300000
H	-4.3831630000	-0.0298090000	-2.3645030000
H	-2.8208610000	0.2916910000	-3.1091330000
H	-4.8844640000	-1.6437780000	0.8874260000
H	-4.0046430000	-2.6969600000	-0.2191770000
H	-5.0343200000	-1.4111250000	-0.8539790000
C	-1.0266580000	1.9505940000	-1.3664320000
H	-0.0409690000	2.1738020000	-0.9681330000
H	-1.6516000000	2.8450810000	-1.3278880000
H	-0.9226410000	1.6226040000	-2.4002200000
C	1.3897070000	0.7743940000	0.7337620000
C	1.8186970000	-0.4862360000	0.3054360000
C	3.0370080000	-0.6077940000	-0.3455320000
C	3.8647020000	0.4923200000	-0.5680260000
C	3.4442870000	1.7399240000	-0.1180310000
C	2.2133430000	1.8810240000	0.5262330000
H	4.0857590000	2.6025740000	-0.2616550000
H	1.9025610000	2.8548750000	0.8922510000
O	-0.0255580000	0.1126960000	2.5863700000
H	1.2144060000	-1.3602930000	0.5151720000
Cl	3.5623750000	-2.1978530000	-0.9051970000
H	-0.0885380000	1.9902830000	1.6975230000

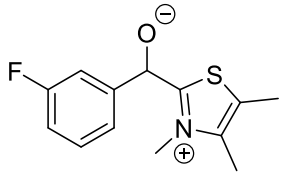
H	4.8169220000	0.3668630000	-1.0670850000

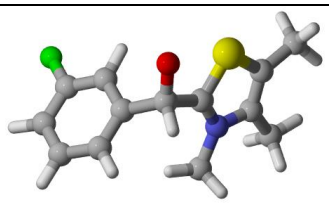
thermodynamic data

Zero-point correction= 0.240140 (Hartree/Particle)
Thermal correction to Energy= 0.257529
Thermal correction to Enthalpy= 0.258473
Thermal correction to Gibbs Free Energy= 0.193098
Sum of electronic and zero-point Energies= -1492.094066
Sum of electronic and thermal Energies= -1492.076678
Sum of electronic and thermal Enthalpies= -1492.075734
Sum of electronic and thermal Free Energies= -1492.141109

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.602	63.786	137.593

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8426350000	-0.1398330000	-0.7016870000
N	1.3592420000	1.0092720000	-0.2641700000
C	2.6076020000	0.8798240000	0.3772720000
C	3.0167760000	-0.4167980000	0.4100530000
S	1.8451270000	-1.4788980000	-0.3805080000
C	4.2642940000	-0.9854200000	1.0143330000
C	3.2922120000	2.0955780000	0.9215090000
C	-0.4211000000	-0.5886350000	-1.4799560000
H	3.4368840000	2.8605150000	0.1527420000
H	4.2739920000	1.8289500000	1.3099610000
H	2.7268680000	2.5492070000	1.7419090000
H	4.7503570000	-1.6829930000	0.3273380000
H	4.0428990000	-1.5340440000	1.9350330000
H	4.9855810000	-0.2038710000	1.2576650000
C	0.6968780000	2.3030770000	-0.4651420000
H	-0.3257820000	2.1287810000	-0.7871320000
H	1.2286710000	2.8825850000	-1.2224910000
H	0.6802450000	2.8575380000	0.4726290000
C	-1.6929380000	-0.1383630000	-0.7271020000
C	-2.0084690000	-0.7451480000	0.4925560000
C	-3.1715890000	-0.3758780000	1.1408010000

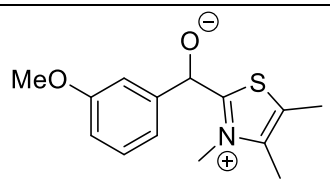
C	-4.0579060000	0.5618830000	0.6252680000
C	-3.7493820000	1.1446140000	-0.6004680000
C	-2.5738340000	0.7983670000	-1.2712640000
H	-4.4348870000	1.8610830000	-1.0395890000
H	-2.3548960000	1.2388700000	-2.2392950000
O	-0.2943830000	-1.9040690000	-1.6293190000
H	-1.3730380000	-1.5215150000	0.9015610000
F	-3.4700620000	-0.9568750000	2.3338430000
H	-0.3953520000	0.0125770000	-2.4267440000
H	-4.9637200000	0.8045940000	1.1666620000

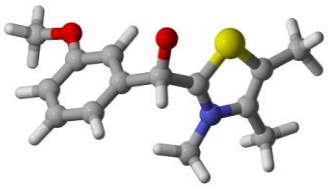
thermodynamic data

Zero-point correction= 0.241501 (Hartree/Particle)
Thermal correction to Energy= 0.258487
Thermal correction to Enthalpy= 0.259431
Thermal correction to Gibbs Free Energy= 0.195409
Sum of electronic and zero-point Energies= -1131.738469
Sum of electronic and thermal Energies= -1131.721483
Sum of electronic and thermal Enthalpies= -1131.720539
Sum of electronic and thermal Free Energies= -1131.784561

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.203	62.875	134.745

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2135110000	0.5590600000	-0.5035130000
N	1.6757800000	0.7103950000	0.7379000000
C	2.8301580000	-0.0457350000	1.0253620000
C	3.2230470000	-0.7797390000	-0.0499380000
S	2.1540460000	-0.5125680000	-1.4349800000
C	4.3802550000	-1.7245000000	-0.1617880000
C	3.4442080000	0.0301630000	2.3894530000
C	0.0584630000	1.1382990000	-1.3545770000
H	3.6863120000	1.0595260000	2.6702300000
H	4.3685120000	-0.5450050000	2.4163260000

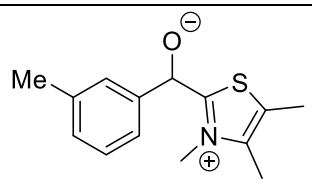
H	2.7805500000	-0.3781130000	3.1585240000
H	4.9922770000	-1.4944540000	-1.0382150000
H	4.0371270000	-2.7583850000	-0.2655420000
H	5.0264510000	-1.6756190000	0.7158520000
C	1.0488820000	1.6141410000	1.7090090000
H	0.0704220000	1.9058120000	1.3369030000
H	1.6701010000	2.5009990000	1.8505350000
H	0.9242440000	1.1003880000	2.6616610000
C	-1.2933090000	0.8988250000	-0.6459750000
C	-1.7560240000	-0.4024620000	-0.4759840000
C	-2.9972690000	-0.6446560000	0.1169550000
C	-3.7967010000	0.4260950000	0.5348200000
C	-3.3358170000	1.7294360000	0.3458030000
C	-2.0947900000	1.9709040000	-0.2369310000
H	-3.9642190000	2.5606540000	0.6480920000
H	-1.7579760000	2.9896500000	-0.4019390000
O	0.1849520000	0.5708730000	-2.5526410000
H	-1.1741000000	-1.2416620000	-0.8391090000
H	0.2252340000	2.2481840000	-1.3275490000
H	-4.7664160000	0.2615410000	0.9849070000
O	-3.3472100000	-1.9615340000	0.2472040000
C	-4.6207350000	-2.2764330000	0.7887230000
H	-4.6879160000	-3.3634370000	0.7798990000
H	-4.7208070000	-1.9172500000	1.8194800000
H	-5.4301910000	-1.8595980000	0.1793000000

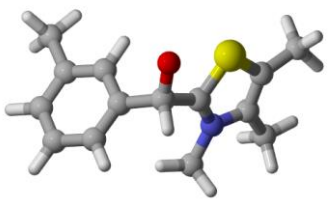
thermodynamic data

Zero-point correction= 0.281869 (Hartree/Particle)
Thermal correction to Energy= 0.300728
Thermal correction to Enthalpy= 0.301672
Thermal correction to Gibbs Free Energy= 0.233117
Sum of electronic and zero-point Energies= -1146.984109
Sum of electronic and thermal Energies= -1146.965250
Sum of electronic and thermal Enthalpies= -1146.964306
Sum of electronic and thermal Free Energies= -1147.032861

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.710	69.187	144.287

B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

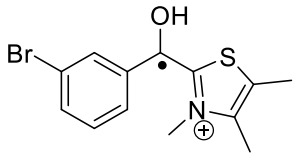
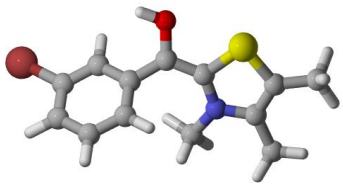
C	0.8574320000	-0.0703910000	-0.7148000000
N	1.3754860000	1.0280790000	-0.1634560000
C	2.6151420000	0.8285700000	0.4771650000
C	3.0167710000	-0.4675940000	0.3893030000
S	1.8465730000	-1.4426610000	-0.5119050000
C	4.2559300000	-1.0980820000	0.9479640000
C	3.2990760000	1.9816250000	1.1454850000
C	-0.3965850000	-0.4381270000	-1.5448400000
H	3.4669810000	2.8133820000	0.4546540000
H	4.2695330000	1.6689480000	1.5280720000
H	2.7201250000	2.3634220000	1.9925900000
H	4.7368560000	-1.7409080000	0.2060670000
H	4.0265300000	-1.7199750000	1.8189080000
H	4.9851610000	-0.3475800000	1.2570020000
C	0.7248730000	2.3402050000	-0.2500500000
H	-0.2951660000	2.2047820000	-0.5984780000
H	1.2703890000	2.9833480000	-0.9437490000
H	0.7016910000	2.8045520000	0.7352870000
C	-1.6767250000	-0.0413420000	-0.7785630000
C	-2.0310030000	-0.7433290000	0.3779680000
C	-3.2029430000	-0.4553310000	1.0775370000
C	-4.0385470000	0.5619760000	0.5921500000
C	-3.7102000000	1.2539530000	-0.5684290000
C	-2.5312790000	0.9522130000	-1.2546630000
H	-4.3774280000	2.0209890000	-0.9477640000
H	-2.2889970000	1.4752670000	-2.1757420000
O	-0.2696970000	-1.7385230000	-1.8078430000
H	-1.3884060000	-1.5545130000	0.7058840000
H	-0.3480540000	0.2404680000	-2.4372920000
H	-4.9579180000	0.7984150000	1.1191950000
C	-3.5899550000	-1.2455060000	2.3055830000
H	-4.0161160000	-0.6010310000	3.0795910000
H	-2.7297060000	-1.7662680000	2.7314130000
H	-4.3433950000	-2.0021260000	2.0609300000

thermodynamic data

Zero-point correction= 0.276896 (Hartree/Particle)
Thermal correction to Energy= 0.294953
Thermal correction to Enthalpy= 0.295897
Thermal correction to Gibbs Free Energy= 0.229130
Sum of electronic and zero-point Energies= -1071.760561
Sum of electronic and thermal Energies= -1071.742504
Sum of electronic and thermal Enthalpies= -1071.741559
Sum of electronic and thermal Free Energies= -1071.808327

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	185.086	65.982	140.523

(u)B3LYP/6-311+G**	

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.8451740000	-0.4900060000	0.0334820000
N	-2.3080550000	0.7311890000	-0.3766570000
C	-3.6978540000	0.8351380000	-0.4018370000
C	-4.3299470000	-0.3309280000	-0.0661680000
S	-3.1751790000	-1.5827320000	0.3064470000
C	-5.7940250000	-0.6298990000	0.0087950000
C	-4.3475390000	2.1261970000	-0.7897710000
C	-0.5278330000	-0.9238480000	0.2335840000
H	-4.2280380000	2.3355660000	-1.8572760000
H	-3.9302630000	2.9674080000	-0.2312330000
H	-5.4144760000	2.0883780000	-0.5809280000
H	-6.1093060000	-0.8047390000	1.0415140000
H	-6.0400070000	-1.5247430000	-0.5686280000
H	-6.3846860000	0.1935940000	-0.3900870000
C	-1.4484070000	1.7976050000	-0.9187030000
H	-1.9546120000	2.2601920000	-1.7628600000
H	-0.5134300000	1.3665710000	-1.2631140000
H	-1.2380790000	2.5534510000	-0.1610090000
C	0.6641400000	-0.1191960000	0.4941210000
C	1.8886320000	-0.4994570000	-0.0893350000
C	3.0431480000	0.2139850000	0.2108680000
C	3.0084470000	1.2938810000	1.0940330000
C	1.7969740000	1.6588750000	1.6810040000
C	0.6292830000	0.9646080000	1.3892610000
H	1.9302950000	-1.3181350000	-0.7976770000
Br	4.6890800000	-0.2889900000	-0.6021840000
H	3.9159810000	1.8364360000	1.3251130000
H	1.7745060000	2.4815020000	2.3857480000
H	-0.2964090000	1.2286680000	1.8864800000
O	-0.4151680000	-2.2722030000	0.2321330000
H	0.4122600000	-2.5482100000	0.6507700000

thermodynamic data

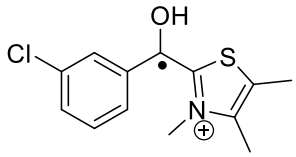
Zero-point correction= 0.241926 (Hartree/Particle)

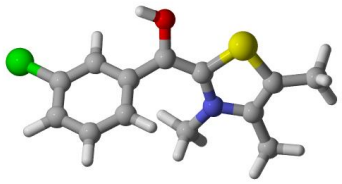
Thermal correction to Energy= 0.259533
Thermal correction to Enthalpy= 0.260477
Thermal correction to Gibbs Free Energy= 0.193684
Sum of electronic and zero-point Energies= -3605.828784
Sum of electronic and thermal Energies= -3605.811177
Sum of electronic and thermal Enthalpies= -3605.810232
Sum of electronic and thermal Free Energies= -3605.877025

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.859	64.749	140.577

Alpha-HOMO (6311) Spin-density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2402670000	-0.4988420000	-0.0113700000
N	-1.6898510000	0.7481560000	-0.3535520000
C	-3.0756850000	0.8874240000	-0.3054920000
C	-3.7215940000	-0.2746240000	0.0177840000
S	-2.5842550000	-1.5676560000	0.2867320000
C	-5.1881240000	-0.5364340000	0.1586350000
C	-3.7101610000	2.2077750000	-0.6114900000
C	0.0730960000	-0.9728730000	0.1064280000
H	-3.6399490000	2.4548270000	-1.6753020000
H	-3.2429240000	3.0164860000	-0.0445780000
H	-4.7655490000	2.1877260000	-0.3482970000
H	-5.4667770000	-0.6679000000	1.2083980000
H	-5.4763040000	-1.4445110000	-0.3764980000
H	-5.7752910000	0.2862790000	-0.2473470000
C	-0.8289150000	1.8127210000	-0.8973690000
H	-1.3675770000	2.3281380000	-1.6891040000
H	0.0706530000	1.3705760000	-1.3146570000
H	-0.5514470000	2.5264590000	-0.1207630000
C	1.2976770000	-0.2088930000	0.3365960000
C	2.4814230000	-0.5982590000	-0.3189370000

C	3.6674630000	0.0742310000	-0.0492950000
C	3.7054490000	1.1204890000	0.8730390000
C	2.5345140000	1.4934180000	1.5313020000
C	1.3353900000	0.8408030000	1.2713930000
H	2.4720920000	-1.3897170000	-1.0588330000
Cl	5.1239840000	-0.3949340000	-0.8845150000
H	4.6400490000	1.6276370000	1.0755370000
H	2.5679910000	2.2889480000	2.2659510000
H	0.4421220000	1.1093930000	1.8224900000
O	0.1491990000	-2.3226660000	0.0500270000
H	0.9870150000	-2.6353440000	0.4193460000

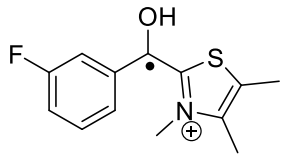
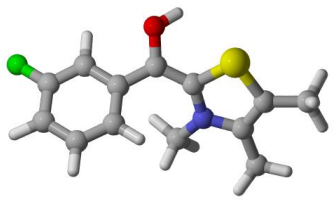
thermodynamic data

Zero-point correction= 0.242458 (Hartree/Particle)
Thermal correction to Energy= 0.259851
Thermal correction to Enthalpy= 0.260795
Thermal correction to Gibbs Free Energy= 0.194672
Sum of electronic and zero-point Energies= -1491.908421
Sum of electronic and thermal Energies= -1491.891029
Sum of electronic and thermal Enthalpies= -1491.890085
Sum of electronic and thermal Free Energies= -1491.956208

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.059	64.336	139.168

Alpha-HOMO (6311) Spin-density (6311)

(u)B3LYP/6-311+G**		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9054480000	-0.5250380000	-0.1064780000
N	-1.3628190000	0.7265340000	-0.4121500000
C	-2.7338490000	0.9051120000	-0.2157870000
C	-3.3735010000	-0.2294170000	0.1947300000
S	-2.2364070000	-1.5426300000	0.3865260000
C	-4.8213100000	-0.4597260000	0.4918850000

C	-3.3592190000	2.2388300000	-0.4809170000
C	0.4141030000	-1.0196920000	-0.1469120000
H	-3.3955730000	2.4634800000	-1.5511950000
H	-2.8093380000	3.0419520000	0.0151850000
H	-4.3806190000	2.2577550000	-0.1071510000
H	-4.9733950000	-0.7286740000	1.5408310000
H	-5.2228330000	-1.2705910000	-0.1217810000
H	-5.4085480000	0.4339080000	0.2854340000
C	-0.5486800000	1.7516430000	-1.0906510000
H	-1.1507460000	2.2178490000	-1.8675410000
H	0.3163290000	1.2793390000	-1.5461170000
H	-0.2098340000	2.5100790000	-0.3845920000
C	1.6334060000	-0.2776180000	0.1164890000
C	2.8412620000	-0.7229000000	-0.4560410000
C	4.0068890000	-0.0445950000	-0.1553040000
C	4.0363410000	1.0463700000	0.7065920000
C	2.8416630000	1.4665400000	1.2913130000
C	1.6480040000	0.8173820000	1.0044370000
H	2.8688390000	-1.5738930000	-1.1229630000
H	4.9781000000	1.5374390000	0.9172310000
H	2.8522850000	2.2942290000	1.9898520000
H	0.7387170000	1.1210530000	1.5083850000
F	5.1542700000	-0.4567450000	-0.7165030000
O	0.5994770000	-2.3481360000	-0.3195250000
H	-0.1433390000	-2.7731350000	-0.7703730000

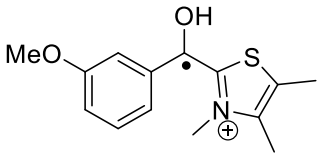
thermodynamic data

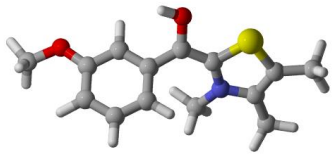
Zero-point correction= 0.243673 (Hartree/Particle)
Thermal correction to Energy= 0.260683
Thermal correction to Enthalpy= 0.261627
Thermal correction to Gibbs Free Energy= 0.196938
Sum of electronic and zero-point Energies= -1131.547471
Sum of electronic and thermal Energies= -1131.530460
Sum of electronic and thermal Enthalpies= -1131.529516
Sum of electronic and thermal Free Energies= -1131.594205

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.581	63.589	136.149

Alpha-HOMO (6311) Spin-density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2987120000	-0.5067720000	-0.0479590000
N	-1.7221730000	0.7620870000	-0.3393960000
C	-3.1032790000	0.9352960000	-0.2570480000
C	-3.7729680000	-0.2186820000	0.0417670000
S	-2.6643560000	-1.5506950000	0.2425090000
C	-5.2428210000	-0.4518300000	0.1960190000
C	-3.7051570000	2.2824380000	-0.5078750000
C	0.0044860000	-1.0150100000	0.0302380000
H	-3.6524440000	2.5597430000	-1.5651760000
H	-3.2002890000	3.0592720000	0.0711540000
H	-4.7544240000	2.2858960000	-0.2206370000
H	-5.4907340000	-0.7543100000	1.2173250000
H	-5.5854670000	-1.2429770000	-0.4762850000
H	-5.8103250000	0.4482990000	-0.0360000000
C	-0.8464560000	1.8193630000	-0.8734480000
H	-1.3820850000	2.3561440000	-1.6533470000
H	0.0423600000	1.3674090000	-1.3027660000
H	-0.5492640000	2.5148610000	-0.0878600000
C	1.2497550000	-0.2889050000	0.2679130000
C	2.4136370000	-0.6972530000	-0.3978080000
C	3.6401210000	-0.0769630000	-0.1284730000
C	3.6988030000	0.9491130000	0.8248800000
C	2.5379840000	1.3397990000	1.4946350000
C	1.3159440000	0.7389600000	1.2294420000
H	2.3894030000	-1.4659510000	-1.1619610000
H	4.6353230000	1.4378660000	1.0553940000
H	2.6017640000	2.1158490000	2.2482810000
H	0.4348450000	1.0196530000	1.7930040000
O	4.6904420000	-0.5333300000	-0.8394310000
C	5.9847570000	0.0444090000	-0.6327360000
H	6.6496130000	-0.4844210000	-1.3112110000
H	5.9825890000	1.1098210000	-0.8795650000
H	6.3203310000	-0.1038570000	0.3973740000
O	0.0471230000	-2.3632040000	-0.0704550000
H	0.8966140000	-2.6982960000	0.2497140000

thermodynamic data

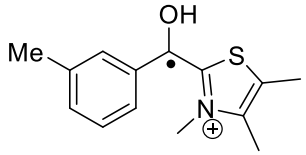
Zero-point correction= 0.284497 (Hartree/Particle)
Thermal correction to Energy= 0.303268
Thermal correction to Enthalpy= 0.304212
Thermal correction to Gibbs Free Energy= 0.235818
Sum of electronic and zero-point Energies= -1146.808034

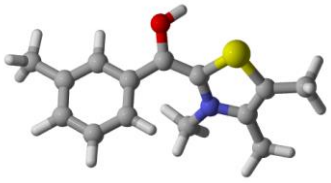
Sum of electronic and thermal Energies= -1146.789263
Sum of electronic and thermal Enthalpies= -1146.788319
Sum of electronic and thermal Free Energies= -1146.856712

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.304	69.793	143.947

Alpha-HOMO (6311) Spin-density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9202300000	-0.5242030000	0.1005760000
N	1.3856520000	0.7233360000	0.4148460000
C	2.7600030000	0.8913750000	0.2299870000
C	3.3945460000	-0.2457690000	-0.1780130000
S	2.2490550000	-1.5512360000	-0.3836700000
C	4.8427930000	-0.4857070000	-0.4655590000
C	3.3926180000	2.2202420000	0.5032060000
C	-0.4032980000	-1.0076880000	0.1253980000
H	3.4200350000	2.4437650000	1.5739470000
H	2.8532010000	3.0278530000	0.0028230000
H	4.4176800000	2.2323180000	0.1392490000
H	5.0019840000	-0.7416060000	-1.5167830000
H	5.2313140000	-1.3088020000	0.1401560000
H	5.4368210000	0.3991960000	-0.2413090000
C	0.5761250000	1.7498100000	1.0955790000
H	1.1740980000	2.1996810000	1.8853840000
H	-0.3005260000	1.2826320000	1.5335500000
H	0.2541220000	2.5204870000	0.3948570000
C	-1.6120370000	-0.2548570000	-0.1416210000
C	-2.8361790000	-0.6916770000	0.4089890000
C	-4.0289910000	-0.0300090000	0.1340340000
C	-3.9887360000	1.0797440000	-0.7258070000
C	-2.7923030000	1.5086760000	-1.2993180000
C	-1.6044700000	0.8505530000	-1.0149530000
H	-2.8392890000	-1.5553960000	1.0622280000
C	-5.3350050000	-0.4880890000	0.7318010000
H	-4.9088860000	1.6048210000	-0.9592540000

H	-2.7942250000	2.3462920000	-1.9867140000
H	-0.6879360000	1.1534730000	-1.5071490000
H	-5.1997830000	-1.3631390000	1.3686120000
H	-6.0509000000	-0.7490660000	-0.0525600000
H	-5.7890180000	0.3031340000	1.3349510000
O	-0.5947270000	-2.3385190000	0.2866620000
H	0.1429150000	-2.7654860000	0.7437190000

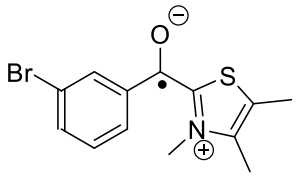
thermodynamic data

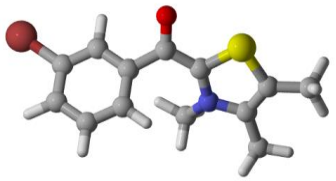
Zero-point correction= 0.281964 (Hartree/Particle)
Thermal correction to Energy= 0.299717
Thermal correction to Enthalpy= 0.300661
Thermal correction to Gibbs Free Energy= 0.235319
Sum of electronic and zero-point Energies= -1071.374745
Sum of electronic and thermal Energies= -1071.356992
Sum of electronic and thermal Enthalpies= -1071.356048
Sum of electronic and thermal Free Energies= -1071.421390

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.075	66.212	137.522

Alpha-HOMO (6311) Spin-density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	1.8356090000	-0.5329010000	0.0066400000
N	2.3129150000	0.7215230000	0.3509860000
C	3.7154520000	0.8159670000	0.3139270000
C	4.3323130000	-0.3486580000	0.0025720000
S	3.1633460000	-1.6477420000	-0.2540310000
C	5.7915770000	-0.6431710000	-0.1496730000
C	4.3602910000	2.1383260000	0.5997540000

C	0.5097640000	-1.0325090000	-0.1890660000
H	4.1572890000	2.4830800000	1.6180840000
H	4.0018160000	2.9105910000	-0.0881860000
H	5.4406100000	2.0680510000	0.4857140000
H	6.0394440000	-0.9189190000	-1.1796920000
H	6.0899650000	-1.4783850000	0.4916800000
H	6.4033030000	0.2176390000	0.1224790000
C	1.5430650000	1.6658650000	1.1703550000
H	1.9432190000	1.6909600000	2.1884970000
H	0.5066770000	1.3515300000	1.2124760000
H	1.5821370000	2.6693880000	0.7435180000
O	0.3380280000	-2.2712470000	-0.2281740000
C	-0.6617700000	-0.1249460000	-0.4216490000
C	-1.9137950000	-0.5389510000	0.0548460000
C	-3.0352640000	0.2342190000	-0.2088710000
C	-2.9583450000	1.4033870000	-0.9626660000
C	-1.7159280000	1.7957050000	-1.4584500000
C	-0.5754880000	1.0436910000	-1.1891320000
H	-1.9854230000	-1.4641020000	0.6109520000
Br	-4.7411540000	-0.3236890000	0.4756660000
H	-3.8472070000	1.9861410000	-1.1661990000
H	-1.6448680000	2.6895510000	-2.0682230000
H	0.3803580000	1.3506250000	-1.5979390000

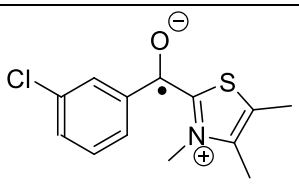
thermodynamic data

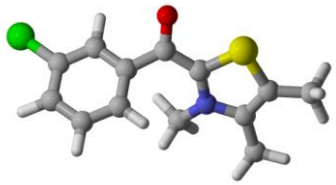
Zero-point correction= 0.228765 (Hartree/Particle)
Thermal correction to Energy= 0.246325
Thermal correction to Enthalpy= 0.247270
Thermal correction to Gibbs Free Energy= 0.180175
Sum of electronic and zero-point Energies= -3605.450900
Sum of electronic and thermal Energies= -3605.433340
Sum of electronic and thermal Enthalpies= -3605.432396
Sum of electronic and thermal Free Energies= -3605.499490

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	154.572	63.550	141.212

Alpha-HOMO (6311) spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

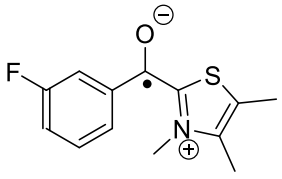
C	1.2288620000	-0.5445280000	0.0174260000
N	1.6626310000	0.7276260000	0.3440900000
C	3.0559410000	0.8851880000	0.2762580000
C	3.7156790000	-0.2584180000	-0.0304020000
S	2.5974390000	-1.6069980000	-0.2452760000
C	5.1845550000	-0.4964460000	-0.1893820000
C	3.6580970000	2.2325180000	0.5403220000
C	-0.0805370000	-1.1042220000	-0.1127800000
H	3.5875860000	2.5172870000	1.5951120000
H	3.1648990000	3.0117960000	-0.0476250000
H	4.7134430000	2.2338390000	0.2727510000
H	5.4280240000	-0.8361190000	-1.2010780000
H	5.5344130000	-1.2664550000	0.5056910000
H	5.7589750000	0.4095850000	0.0064010000
C	0.8090470000	1.7171470000	1.0057540000
H	1.3734650000	2.2159670000	1.7929880000
H	-0.0416550000	1.2117510000	1.4565630000
H	0.4319720000	2.4652330000	0.3047770000
O	-0.2023200000	-2.3504840000	-0.1083840000
C	-1.2943190000	-0.2511120000	-0.3285880000
C	-2.4969970000	-0.6522640000	0.2691890000
C	-3.6563590000	0.0687380000	0.0240180000
C	-3.6667530000	1.1702230000	-0.8293620000
C	-2.4758600000	1.5459790000	-1.4469490000
C	-1.2971480000	0.8465100000	-1.1985500000
H	-2.5087080000	-1.5272640000	0.9056440000
Cl	-5.1576660000	-0.4230760000	0.8040280000
H	-4.5873100000	1.7087320000	-1.0139310000
H	-2.4749970000	2.3833230000	-2.1359070000
H	-0.3839300000	1.1311870000	-1.7087300000

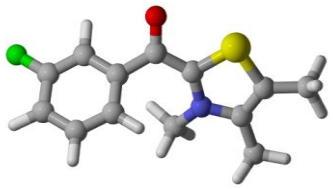
thermodynamic data

Zero-point correction= 0.229470 (Hartree/Particle)
Thermal correction to Energy= 0.246655
Thermal correction to Enthalpy= 0.247600
Thermal correction to Gibbs Free Energy= 0.182666
Sum of electronic and zero-point Energies= -1491.530620
Sum of electronic and thermal Energies= -1491.513434
Sum of electronic and thermal Enthalpies= -1491.512490
Sum of electronic and thermal Free Energies= -1491.577423

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	154.779	63.099	136.664

(u)B3LYP/6-311+G**	





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9065720000	-0.5509100000	0.0634250000
N	1.3240470000	0.7406970000	0.3293480000
C	2.7083250000	0.9281590000	0.1889800000
C	3.3807570000	-0.2089620000	-0.1135210000
S	2.2871580000	-1.5894670000	-0.2314510000
C	4.8458030000	-0.4175260000	-0.3364370000
C	3.2875370000	2.2976700000	0.3802710000
C	-0.3931190000	-1.1452730000	0.0103840000
H	3.2567100000	2.6173490000	1.4269020000
H	2.7487380000	3.0440580000	-0.2103900000
H	4.3294590000	2.3151030000	0.0649340000
H	5.0490860000	-0.7827670000	-1.3481000000
H	5.2473960000	-1.1571650000	0.3636390000
H	5.4063590000	0.5073190000	-0.1960790000
C	0.4838460000	1.7285340000	1.0108420000
H	1.0681320000	2.2354570000	1.7787070000
H	-0.3498040000	1.2204050000	1.4887190000
H	0.0818220000	2.4701330000	0.3168850000
O	-0.4814500000	-2.3935340000	0.0610990000
C	-1.6370840000	-0.3307340000	-0.1778470000
C	-2.8069230000	-0.7567800000	0.4658600000
C	-3.9836120000	-0.0681310000	0.2390000000
C	-4.0667010000	1.0159110000	-0.6241970000
C	-2.9066960000	1.4158890000	-1.2851140000
C	-1.7009540000	0.7535090000	-1.0638690000
H	-2.7885470000	-1.6205770000	1.1179190000
H	-5.0160800000	1.5133730000	-0.7774790000
H	-2.9501650000	2.2415760000	-1.9864190000

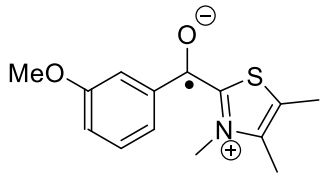
H	-0.8138600000	1.0557560000	-1.6083510000
F	-5.1096690000	-0.4703660000	0.8812720000

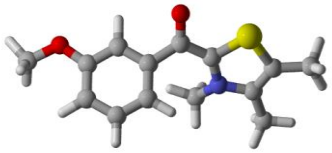
thermodynamic data

Zero-point correction= 0.230805 (Hartree/Particle)
Thermal correction to Energy= 0.247604
Thermal correction to Enthalpy= 0.248548
Thermal correction to Gibbs Free Energy= 0.184888
Sum of electronic and zero-point Energies= -1131.175265
Sum of electronic and thermal Energies= -1131.158466
Sum of electronic and thermal Enthalpies= -1131.157521
Sum of electronic and thermal Free Energies= -1131.221181

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	155.374	62.212	133.983

(u)B3LYP/6-311+G**		





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2817100000	-0.5525550000	0.0588690000
N	1.6806780000	0.7554610000	0.2950530000
C	3.0718600000	0.9384990000	0.2018730000
C	3.7580410000	-0.2000190000	-0.0549200000
S	2.6756180000	-1.5911430000	-0.1794600000
C	5.2284160000	-0.4040770000	-0.2444740000
C	3.6343230000	2.3166320000	0.3793190000
C	-0.0118850000	-1.1546110000	-0.0465100000
H	3.4402270000	2.7127360000	1.3806750000
H	3.2022740000	3.0169330000	-0.3426740000
H	4.7128120000	2.3104380000	0.2309920000
H	5.4589730000	-0.7389460000	-1.2610170000
H	5.6084970000	-1.1664480000	0.4429570000
H	5.7864490000	0.5147720000	-0.0609420000
C	0.8836860000	1.6869340000	1.1033840000
H	1.2581640000	1.7100650000	2.1324830000

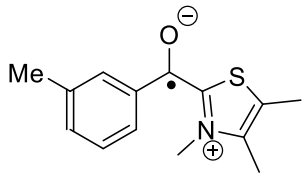
H	-0.1522950000	1.3688280000	1.1136550000
H	0.9294120000	2.6911580000	0.6805110000
O	-0.0923370000	-2.4019070000	-0.0068620000
C	-1.2536710000	-0.3416070000	-0.2703550000
C	-2.4355080000	-0.7654210000	0.3340360000
C	-3.6370290000	-0.0913000000	0.0975600000
C	-3.6650970000	1.0031480000	-0.7725030000
C	-2.4816750000	1.4084610000	-1.3953770000
C	-1.2821110000	0.7536730000	-1.1500770000
H	-2.4313510000	-1.6332690000	0.9814340000
H	-4.5855440000	1.5320310000	-0.9795820000
H	-2.5100300000	2.2426250000	-2.0880920000
H	-0.3762360000	1.0685580000	-1.6546040000
O	-4.7280150000	-0.5784220000	0.7587600000
C	-5.9882980000	0.0402800000	0.5437010000
H	-6.6985010000	-0.5114790000	1.1574830000
H	-5.9791450000	1.0901970000	0.8573020000
H	-6.2921020000	-0.0237220000	-0.5069220000

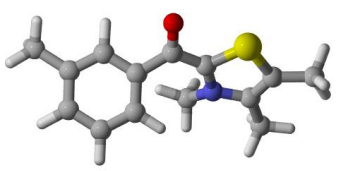
thermodynamic data

Zero-point correction= 0.271252 (Hartree/Particle)
Thermal correction to Energy= 0.289885
Thermal correction to Enthalpy= 0.290829
Thermal correction to Gibbs Free Energy= 0.222879
Sum of electronic and zero-point Energies= -1146.421657
Sum of electronic and thermal Energies= -1146.403024
Sum of electronic and thermal Enthalpies= -1146.402080
Sum of electronic and thermal Free Energies= -1146.470030

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	181.905	68.522	143.013

(u)B3LYP/6-311+G**





xyz-matrix

33
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9157650000	-0.5463420000	-0.0665900000
N	-1.3433780000	0.7521670000	-0.3051100000
C	-2.7347230000	0.9126590000	-0.1782560000
C	-3.3945730000	-0.2350690000	0.1050310000
S	-2.2854830000	-1.6064350000	0.2140010000
C	-4.8560400000	-0.4625470000	0.3328390000
C	-3.3245230000	2.2798540000	-0.3515000000
C	0.3902480000	-1.1259120000	0.0168350000
H	-3.1637590000	2.6715390000	-1.3605240000
H	-2.8855110000	2.9929080000	0.3536080000
H	-4.3985010000	2.2570330000	-0.1747690000
H	-5.0553790000	-0.7937230000	1.3571420000
H	-5.2400970000	-1.2363010000	-0.3395120000
H	-5.4341500000	0.4453260000	0.1569880000
C	-0.5831180000	1.6897150000	-1.1412240000
H	-0.9979130000	1.7135000000	-2.1545460000
H	0.4527190000	1.3753480000	-1.1937230000
H	-0.6158410000	2.6932530000	-0.7150610000
O	0.4879000000	-2.3729110000	-0.0167790000
C	1.6244480000	-0.2962040000	0.2093400000
C	2.8160290000	-0.7334370000	-0.3821790000
C	4.0217730000	-0.0582100000	-0.1851690000
C	4.0261670000	1.0646760000	0.6517650000
C	2.8538990000	1.4969100000	1.2690620000
C	1.6545340000	0.8250750000	1.0484440000
H	2.7840230000	-1.6292410000	-0.9924990000
C	5.2863510000	-0.5201600000	-0.8695180000
H	4.9558240000	1.5952450000	0.8320280000
H	2.8794120000	2.3519770000	1.9360580000
H	0.7496630000	1.1524350000	1.5483120000
H	5.2755780000	-1.5996260000	-1.0356040000
H	6.1717740000	-0.2753260000	-0.2779840000
H	5.4020880000	-0.0393100000	-1.8472220000

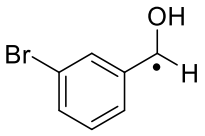
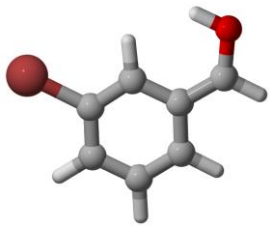
thermodynamic data

Zero-point correction= 0.266019 (Hartree/Particle)
Thermal correction to Energy= 0.283135
Thermal correction to Enthalpy= 0.284079
Thermal correction to Gibbs Free Energy= 0.219313
Sum of electronic and zero-point Energies= -1071.198709
Sum of electronic and thermal Energies= -1071.181594
Sum of electronic and thermal Enthalpies= -1071.180650
Sum of electronic and thermal Free Energies= -1071.245416

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	177.670	63.379	136.312

Alpha-HOMO (6311) spin density (6311)

(u)B3LYP/6-311+G**	

xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

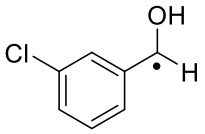
C	0.5991510000	-0.4710010000	0.0000010000
C	1.8959660000	0.1195490000	0.0000050000
C	1.9732050000	1.5427160000	0.0000070000
C	0.8292630000	2.3150680000	0.0000040000
C	-0.4446440000	1.7272160000	-0.0000010000
C	-0.5249230000	0.3345370000	-0.0000020000
H	2.9485320000	2.0161580000	0.0000120000
H	0.9111810000	3.3961360000	0.0000060000
Br	-2.2579560000	-0.4950470000	-0.0000060000
H	0.4666840000	-1.5465540000	-0.0000010000
C	3.0811620000	-0.6362560000	0.0000060000
H	4.0579450000	-0.1735920000	0.0000080000
H	-1.3402790000	2.3328400000	-0.0000040000
O	3.1565400000	-1.9883270000	0.0000070000
H	2.2769830000	-2.3826920000	0.0000060000

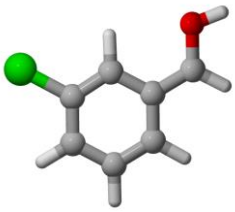
thermodynamic data

Zero-point correction= 0.108942 (Hartree/Particle)
Thermal correction to Energy= 0.117474
Thermal correction to Enthalpy= 0.118418
Thermal correction to Gibbs Free Energy= 0.073544
Sum of electronic and zero-point Energies= -2919.668963
Sum of electronic and thermal Energies= -2919.660431
Sum of electronic and thermal Enthalpies= -2919.659487
Sum of electronic and thermal Free Energies= -2919.704362

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.716	31.469	94.447

(u)B3LYP/6-311+G**	





xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.1354500000	-0.5936680000	0.0000210000
C	-1.2741500000	0.2590670000	0.0000580000
C	-1.0632100000	1.6657180000	0.0000440000
C	0.2178680000	2.1852070000	-0.0000200000
C	1.3381350000	1.3443740000	-0.0000680000
C	1.1286640000	-0.0364850000	-0.0000380000
H	-1.9192840000	2.3316270000	0.0000770000
H	0.3628290000	3.2596480000	-0.0000380000
Cl	2.5317900000	-1.1049510000	-0.0000840000
H	-0.2651320000	-1.6668550000	0.0000460000
C	-2.5802430000	-0.2581730000	0.0000900000
H	-3.4562740000	0.3789310000	0.0003100000
H	2.3424180000	1.7460320000	-0.0001250000
O	-2.7727210000	-1.6067040000	0.0000800000
H	-3.7129050000	-1.8078190000	-0.0000080000

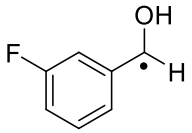
thermodynamic data

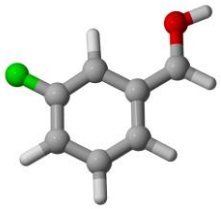
Zero-point correction= 0.109711 (Hartree/Particle)
Thermal correction to Energy= 0.117891
Thermal correction to Enthalpy= 0.118835
Thermal correction to Gibbs Free Energy= 0.075859
Sum of electronic and zero-point Energies= -805.749391
Sum of electronic and thermal Energies= -805.741211
Sum of electronic and thermal Enthalpies= -805.740267
Sum of electronic and thermal Free Energies= -805.783243

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.978	31.010	90.450

Alpha-HOMO (6311) spin density (6311)

(u)B3LYP/6-311+G**	





xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

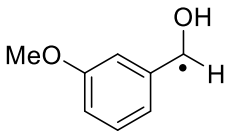
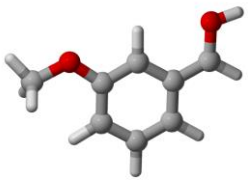
C	-0.0222790000	-0.7989240000	0.0000530000
C	-0.8457930000	0.3602140000	0.0000240000
C	-0.2154080000	1.6366040000	0.0001110000
C	1.1634910000	1.7428100000	0.0000800000
C	1.9748610000	0.6005390000	0.0000780000
C	1.3453870000	-0.6406000000	0.0001560000
H	-0.8284080000	2.5311210000	0.0001140000
H	1.6269580000	2.7227640000	0.0000630000
F	2.1247270000	-1.7533930000	-0.0001510000
H	-0.4564960000	-1.7893540000	-0.0000210000
C	-2.2472570000	0.2688920000	-0.0000160000
H	-2.8858410000	1.1437120000	-0.0000440000
H	3.0552120000	0.6608760000	0.0000190000
O	-2.8439390000	-0.9558320000	-0.0002630000
H	-3.8004750000	-0.8591370000	0.0004150000

thermodynamic data

Zero-point correction= 0.110988 (Hartree/Particle)
Thermal correction to Energy= 0.118803
Thermal correction to Enthalpy= 0.119747
Thermal correction to Gibbs Free Energy= 0.078067
Sum of electronic and zero-point Energies= -445.394207
Sum of electronic and thermal Energies= -445.386393
Sum of electronic and thermal Enthalpies= -445.385448
Sum of electronic and thermal Free Energies= -445.427128

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.550	30.172	87.723

(u)B3LYP/6-311+G**	

xyz-matrix

19
XYZ file generated by gabedit : coordinates in Angstrom

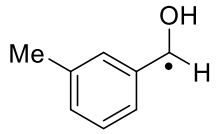
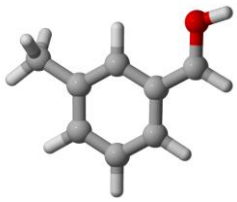
C	0.2782390000	-0.6665090000	-0.0001190000
C	1.3506180000	0.2561000000	-0.0000590000
C	1.0491430000	1.6487330000	-0.0000100000
C	-0.2638490000	2.0703310000	-0.0000350000
C	-1.3275110000	1.1536430000	-0.0001160000
C	-1.0398340000	-0.2179390000	-0.0001600000
H	1.8569810000	2.3721720000	0.0000490000
H	-0.4866450000	3.1317880000	-0.0000020000
H	0.4703930000	-1.7310960000	-0.0001410000
C	2.6931790000	-0.1643020000	-0.0000420000
H	3.5201800000	0.5352360000	-0.0000090000
H	-2.3458070000	1.5162190000	-0.0001730000
O	-1.9947020000	-1.1979280000	-0.0003120000
C	-3.3620980000	-0.8172550000	0.0006310000
H	-3.9293940000	-1.7468700000	0.0009990000
H	-3.6176240000	-0.2379680000	0.8948900000
H	-3.6188760000	-0.2379480000	-0.8932610000
O	2.9875790000	-1.4965380000	-0.0000260000
H	3.9404480000	-1.6226130000	-0.0001890000

thermodynamic data

Zero-point correction= 0.151352 (Hartree/Particle)
Thermal correction to Energy= 0.161027
Thermal correction to Enthalpy= 0.161971
Thermal correction to Gibbs Free Energy= 0.116009
Sum of electronic and zero-point Energies= -460.640084
Sum of electronic and thermal Energies= -460.630409
Sum of electronic and thermal Enthalpies= -460.629465
Sum of electronic and thermal Free Energies= -460.675427

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.046	36.570	96.735

(u)B3LYP/6-311+G**	

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

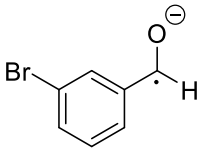
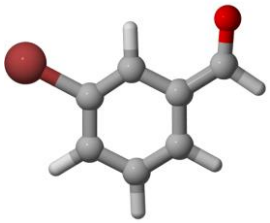
C	0.0178680000	-0.7484680000	-0.0002860000
C	-0.8972820000	0.3375600000	0.0000660000
C	-0.3685840000	1.6587300000	0.0002820000
C	0.9974460000	1.8621280000	0.0001190000
C	1.8828590000	0.7752270000	-0.0002110000
C	1.3937970000	-0.5392040000	-0.0003190000
H	-1.0475210000	2.5051900000	0.0004640000
H	1.3898200000	2.8733560000	0.0001540000
C	2.3413800000	-1.7167430000	0.0002250000
H	-0.3748370000	-1.7587490000	-0.0005590000
C	-2.2893650000	0.1427680000	0.0000800000
H	-2.9919450000	0.9674170000	0.0004360000
H	2.9531050000	0.9507100000	-0.0004420000
H	3.3829580000	-1.3893940000	-0.0087610000
H	2.1820760000	-2.3527980000	-0.8757640000
H	2.1941640000	-2.3420270000	0.8861120000
O	-2.7995540000	-1.1244100000	-0.0001480000
H	-3.7601030000	-1.0904170000	-0.0001980000

thermodynamic data

Zero-point correction= 0.146245 (Hartree/Particle)
Thermal correction to Energy= 0.154302
Thermal correction to Enthalpy= 0.155247
Thermal correction to Gibbs Free Energy= 0.113157
Sum of electronic and zero-point Energies= -385.416670
Sum of electronic and thermal Energies= -385.408613
Sum of electronic and thermal Enthalpies= -385.407668
Sum of electronic and thermal Free Energies= -385.449758

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	96.826	31.361	88.585

(u)B3LYP/6-311+G**	

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

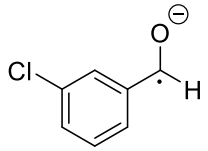
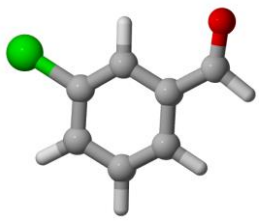
C	-0.6188400000	-0.5195590000	0.0000120000
C	-1.9449810000	0.0425530000	0.0000120000
C	-2.0408110000	1.4700220000	0.0000000000
C	-0.9207140000	2.2732060000	-0.0000090000
C	0.3859350000	1.7222110000	-0.0000090000
C	0.4652770000	0.3213750000	0.0000020000
H	-3.0295540000	1.9226470000	0.0000000000
H	-1.0325360000	3.3546900000	-0.0000160000
Br	2.2573430000	-0.4709520000	0.0000030000
H	-0.5158290000	-1.5962410000	0.0000210000
C	-3.1020210000	-0.7922930000	0.0000200000
H	-4.0654060000	-0.2332390000	-0.0000320000
H	1.2707730000	2.3427650000	-0.0000160000
O	-3.1221890000	-2.0515460000	-0.0000300000

thermodynamic data

Zero-point correction= 0.095348 (Hartree/Particle)
Thermal correction to Energy= 0.103397
Thermal correction to Enthalpy= 0.104341
Thermal correction to Gibbs Free Energy= 0.060654
Sum of electronic and zero-point Energies= -2919.145806
Sum of electronic and thermal Energies= -2919.137757
Sum of electronic and thermal Enthalpies= -2919.136812
Sum of electronic and thermal Free Energies= -2919.180500

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	64.883	29.908	91.948

(u)B3LYP/6-311+G**	

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

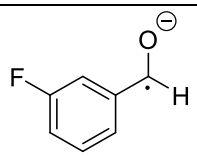
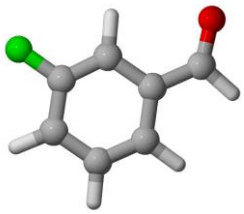
C	-0.1402190000	-0.6366460000	0.0002080000
C	-1.3398990000	0.1588010000	0.0003540000
C	-1.1715470000	1.5795520000	0.0002360000
C	0.0777110000	2.1626220000	0.0000160000
C	1.2587850000	1.3794480000	-0.0001350000
C	1.0825300000	-0.0126860000	-0.0000300000
H	-2.0599800000	2.2066480000	0.0003420000
H	0.1665940000	3.2461870000	-0.0000390000
Cl	2.5655680000	-1.0288860000	-0.0001790000
H	-0.2321280000	-1.7146600000	0.0003080000
C	-2.6315080000	-0.4471880000	0.0005490000
H	-3.4750710000	0.2801700000	-0.0003560000
H	2.2451180000	1.8223540000	-0.0003090000
O	-2.8842890000	-1.6816330000	-0.0005110000

thermodynamic data

Zero-point correction= 0.096037 (Hartree/Particle)
Thermal correction to Energy= 0.103797
Thermal correction to Enthalpy= 0.104741
Thermal correction to Gibbs Free Energy= 0.062504
Sum of electronic and zero-point Energies= -805.224310
Sum of electronic and thermal Energies= -805.216550
Sum of electronic and thermal Enthalpies= -805.215606
Sum of electronic and thermal Free Energies= -805.257843

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.134	29.379	88.896

(u)B3LYP/6-311+G**	

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

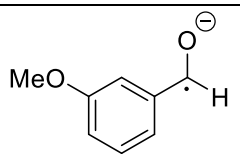
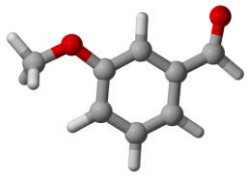
C	-0.0193130000	-0.8323570000	-0.0000240000
C	-0.9271910000	0.2844110000	0.0000010000
C	-0.3417680000	1.5901850000	0.0000830000
C	1.0250560000	1.7752470000	0.0001250000
C	1.9172570000	0.6732140000	0.0000980000
C	1.3306230000	-0.5956720000	0.0000310000
H	-1.0029390000	2.4535750000	0.0001060000
H	1.4315140000	2.7835220000	0.0001800000
F	2.1884360000	-1.6824490000	-0.0000210000
H	-0.4134610000	-1.8406030000	-0.0000850000
C	-2.3412380000	0.0971700000	-0.0000520000
H	-2.9266920000	1.0446360000	-0.0000880000
H	2.9933540000	0.7877290000	0.0001270000
O	-2.9547820000	-1.0050000000	-0.0002020000

thermodynamic data

Zero-point correction= 0.097300 (Hartree/Particle)
Thermal correction to Energy= 0.104666
Thermal correction to Enthalpy= 0.105610
Thermal correction to Gibbs Free Energy= 0.064739
Sum of electronic and zero-point Energies= -444.866611
Sum of electronic and thermal Energies= -444.859245
Sum of electronic and thermal Enthalpies= -444.858301
Sum of electronic and thermal Free Energies= -444.899172

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.679	28.494	86.020

(u)B3LYP/6-311+G**	

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

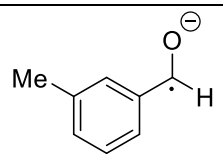
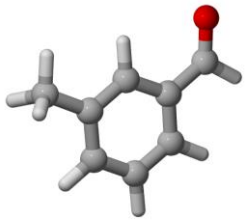
C	0.2881400000	-0.7151340000	0.0000540000
C	1.4167470000	0.1693930000	0.0001340000
C	1.1365650000	1.5722640000	0.0000620000
C	-0.1555740000	2.0455190000	-0.0000800000
C	-1.2707810000	1.1651600000	-0.0002000000
C	-1.0032220000	-0.2165600000	-0.0001400000
H	1.9706120000	2.2705110000	0.0001400000
H	-0.3365240000	3.1180290000	-0.0001120000
H	0.4555940000	-1.7850670000	0.0001400000
C	2.7598220000	-0.3155530000	0.0002500000
H	3.5329110000	0.4867530000	-0.0003340000
H	-2.2768380000	1.5610770000	-0.0003650000
O	-2.0166940000	-1.1751290000	-0.0003000000
C	-3.3522950000	-0.7320160000	0.0005970000
H	-3.9725850000	-1.6311880000	0.0007500000
H	-3.5886620000	-0.1352670000	0.8921590000
H	-3.5897630000	-0.1348620000	-0.8904050000
O	3.1277990000	-1.5234230000	-0.0004540000

thermodynamic data

Zero-point correction= 0.137314 (Hartree/Particle)
Thermal correction to Energy= 0.146610
Thermal correction to Enthalpy= 0.147554
Thermal correction to Gibbs Free Energy= 0.101636
Sum of electronic and zero-point Energies= -460.104213
Sum of electronic and thermal Energies= -460.094918
Sum of electronic and thermal Enthalpies= -460.093973
Sum of electronic and thermal Free Energies= -460.139891

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.999	34.859	96.642

(u)B3LYP/6-311+G**	

xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

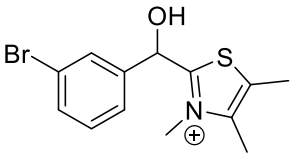
C	-0.0160230000	-0.7810180000	-0.0000090000
C	0.9747990000	0.2596940000	-0.0000040000
C	0.4859960000	1.6040950000	0.0000130000
C	-0.8678660000	1.8756780000	0.0000300000
C	-1.8239460000	0.8353220000	0.0000210000
C	-1.3713820000	-0.5072460000	0.0000090000
H	1.2042020000	2.4214510000	0.0000080000
H	-1.2056220000	2.9101840000	0.0000330000
C	-2.3824900000	-1.6327180000	0.0000130000
H	0.3391100000	-1.8067740000	-0.0000350000
C	2.3713480000	-0.0320590000	-0.0000190000
H	3.0259350000	0.8703620000	-0.0000350000
H	-2.8868990000	1.0582500000	0.0000990000
H	-3.0352380000	-1.5856140000	0.8813550000
H	-1.8885020000	-2.6080680000	-0.0000770000
H	-3.0353600000	-1.5855060000	-0.8812330000
O	2.9074690000	-1.1755970000	-0.0000550000

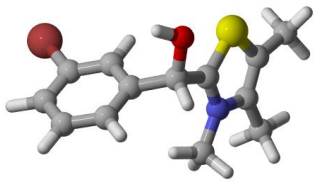
thermodynamic data

Zero-point correction= 0.132631 (Hartree/Particle)
Thermal correction to Energy= 0.140938
Thermal correction to Enthalpy= 0.141882
Thermal correction to Gibbs Free Energy= 0.098891
Sum of electronic and zero-point Energies= -384.880782
Sum of electronic and thermal Energies= -384.872474
Sum of electronic and thermal Enthalpies= -384.871530
Sum of electronic and thermal Free Energies= -384.914522

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	88.440	31.439	90.483

B3LYP/6-311+G**	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.6775090000	0.6582760000	0.5140850000
N	-2.2088580000	0.6925290000	-0.7083200000
C	-3.1840070000	-0.2925710000	-0.9526950000
C	-3.3804930000	-1.0926780000	0.1367580000
S	-2.3514170000	-0.5922530000	1.4578300000
C	-4.3047910000	-2.2611610000	0.3072380000
C	-3.8591680000	-0.3624210000	-2.2877740000
C	-0.6243090000	1.5837170000	1.0901370000
H	-4.3330980000	0.5888830000	-2.5538650000
H	-4.6378840000	-1.1258000000	-2.2740110000
H	-3.1552830000	-0.6267430000	-3.0858790000
H	-4.9161160000	-2.1543520000	1.2093320000
H	-3.7443400000	-3.1991060000	0.3912540000
H	-4.9814120000	-2.3509120000	-0.5450830000
C	-1.8464180000	1.6942100000	-1.7286760000
H	-0.9118670000	2.1758180000	-1.4505080000
H	-2.6440990000	2.4370210000	-1.8124210000
H	-1.7092490000	1.1932960000	-2.6873580000
C	0.7468510000	1.4147520000	0.4472370000
C	1.3516330000	0.1507810000	0.3993480000
C	2.6299330000	0.0239780000	-0.1381700000
C	3.3199510000	1.1377620000	-0.6243900000
C	2.7169880000	2.3931240000	-0.5650650000
C	1.4345230000	2.5367940000	-0.0306000000
H	3.2527420000	3.2635920000	-0.9309610000
H	0.9784400000	3.5224170000	0.0267890000
H	0.8416390000	-0.7272160000	0.7826570000
Br	3.4444710000	-1.6920300000	-0.2111280000
H	-0.9610800000	2.6206720000	0.9308420000
H	4.3154110000	1.0203190000	-1.0379580000
O	-0.6275150000	1.3730890000	2.0266710000
H	-0.3974340000	2.1564730000	2.5318860000

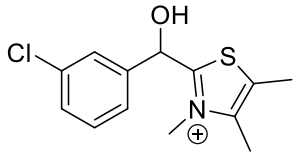
thermodynamic data

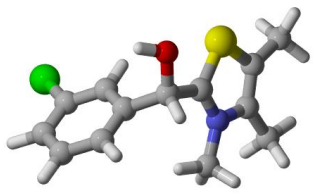
Zero-point correction= 0.253885 (Hartree/Particle)
Thermal correction to Energy= 0.271907
Thermal correction to Enthalpy= 0.272851
Thermal correction to Gibbs Free Energy= 0.205184
Sum of electronic and zero-point Energies= -3606.441352
Sum of electronic and thermal Energies= -3606.423330
Sum of electronic and thermal Enthalpies= -3606.422385

Sum of electronic and thermal Free Energies= -3606.490053

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.624	65.546	142.418

B3LYP/6-311+G**	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	1.1214940000	-0.6988560000	0.4356590000
N	1.6224120000	-0.6663210000	-0.7975430000
C	2.7673580000	0.1363590000	-0.9437090000
C	3.1305750000	0.7226920000	0.2315550000
S	2.0379690000	0.2531130000	1.5105590000
C	4.2628070000	1.6611860000	0.5165350000
C	3.4280430000	0.2679070000	-2.2786230000
C	-0.0865180000	-1.4765610000	0.9099930000
H	3.7089290000	-0.7049150000	-2.6904090000
H	4.3345480000	0.8629440000	-2.1882410000
H	2.7787980000	0.7693960000	-3.0022850000
H	4.7363470000	1.4309240000	1.4729820000
H	3.9140780000	2.6970370000	0.5562740000
H	5.0283550000	1.5924400000	-0.2560590000
C	1.0640990000	-1.4304250000	-1.9297250000
H	0.0806940000	-1.8063020000	-1.6668010000
H	1.7291860000	-2.2603010000	-2.1723550000
H	0.9667110000	-0.7731920000	-2.7918170000
C	-1.4035090000	-0.9822860000	0.3277340000
C	-1.7178070000	0.3810500000	0.3268890000
C	-2.9555690000	0.7960570000	-0.1527690000
C	-3.8895250000	-0.1249160000	-0.6272280000
C	-3.5726130000	-1.4796220000	-0.6166640000
C	-2.3345840000	-1.9123560000	-0.1430220000
H	-4.2964900000	-2.2006980000	-0.9767770000
H	-2.1014460000	-2.9720320000	-0.1327730000
H	-1.0202500000	1.1181120000	0.7055960000
Cl	-3.3403830000	2.5001380000	-0.1598780000
H	0.0527550000	-2.5254000000	0.6126260000
H	-4.8483140000	0.2179360000	-0.9944350000
O	-0.0283020000	-1.3691420000	2.3271090000

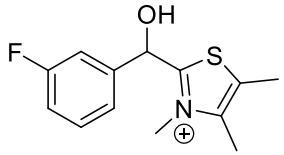
H -0.9008740000 -1.5420760000 2.6996240000

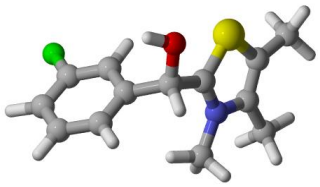
thermodynamic data

Zero-point correction= 0.254405 (Hartree/Particle)
Thermal correction to Energy= 0.272206
Thermal correction to Enthalpy= 0.273150
Thermal correction to Gibbs Free Energy= 0.206760
Sum of electronic and zero-point Energies= -1492.520978
Sum of electronic and thermal Energies= -1492.503177
Sum of electronic and thermal Enthalpies= -1492.502233
Sum of electronic and thermal Free Energies= -1492.568623

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.812	65.143	139.731

B3LYP/6-311+G**	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8459930000	-0.2434990000	-0.7094580000
N	1.3584480000	0.9464920000	-0.4021460000
C	2.5934440000	0.8972700000	0.2677140000
C	3.0122270000	-0.3841230000	0.4677310000
S	1.8589820000	-1.5136610000	-0.1982390000
C	4.2449530000	-0.8848490000	1.1561380000
C	3.2804790000	2.1613930000	0.6747120000
C	-0.4470480000	-0.5157430000	-1.4467290000
H	3.4198770000	2.8376970000	-0.1723440000
H	4.2633810000	1.9356540000	1.0835910000
H	2.7194060000	2.6942530000	1.4482110000
H	4.6596130000	-1.7546000000	0.6428820000
H	4.0276250000	-1.1769380000	2.1875170000
H	5.0170680000	-0.1158420000	1.1789210000
C	0.7217730000	2.2275170000	-0.7649790000
H	-0.3248720000	2.0597990000	-0.9986280000
H	1.2344270000	2.6600280000	-1.6255680000
H	0.7842680000	2.9094920000	0.0803540000
C	-1.6945330000	-0.1251050000	-0.6668100000
C	-1.8594850000	-0.5219180000	0.6651660000
C	-3.0417820000	-0.1993590000	1.3114910000

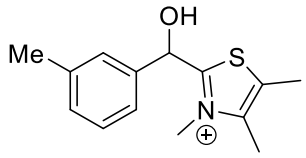
C	-4.0674610000	0.4991820000	0.6870930000
C	-3.8949550000	0.8840790000	-0.6385350000
C	-2.7146480000	0.5761490000	-1.3165600000
H	-4.6849640000	1.4231260000	-1.1470470000
H	-2.5961800000	0.8743280000	-2.3529210000
H	-1.1032300000	-1.0840580000	1.1999740000
F	-3.1958880000	-0.5779260000	2.5925350000
H	-0.4273410000	0.0625360000	-2.3810120000
H	-4.9734970000	0.7254730000	1.2350110000
O	-0.3878410000	-1.9059040000	-1.7408650000
H	-1.2764570000	-2.2352260000	-1.9198410000

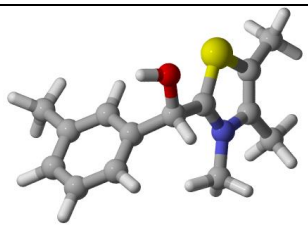
thermodynamic data

Zero-point correction= 0.255831 (Hartree/Particle)
Thermal correction to Energy= 0.273245
Thermal correction to Enthalpy= 0.274189
Thermal correction to Gibbs Free Energy= 0.208934
Sum of electronic and zero-point Energies= -1132.165581
Sum of electronic and thermal Energies= -1132.148167
Sum of electronic and thermal Enthalpies= -1132.147223
Sum of electronic and thermal Free Energies= -1132.212478

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.464	64.228	137.342

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8608840000	0.0335290000	0.7523640000
N	-1.3803180000	1.0271080000	0.0345160000
C	-2.6034190000	0.7233560000	-0.5893870000
C	-3.0060310000	-0.5509310000	-0.3245240000
S	-1.8525290000	-1.3510680000	0.7162390000
C	-4.2237590000	-1.2826750000	-0.7993800000
C	-3.2955400000	1.7510170000	-1.4268400000
C	0.4216390000	0.0641990000	1.5537120000
H	-3.4670600000	2.6769570000	-0.8719600000
H	-4.2639900000	1.3763820000	-1.7523340000

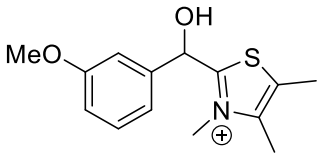
H	-2.7204220000	1.9941940000	-2.3252490000
H	-4.6628340000	-1.8810920000	0.0014610000
H	-3.9812100000	-1.9564230000	-1.6260570000
H	-4.9859910000	-0.5851120000	-1.1458740000
C	-0.7625530000	2.3630760000	-0.0720280000
H	0.2850470000	2.3011860000	0.2056500000
H	-1.2857480000	3.0612880000	0.5832670000
H	-0.8296270000	2.7061850000	-1.1020830000
C	1.6775460000	0.1700370000	0.7022240000
C	1.8949680000	-0.7005520000	-0.3742130000
C	3.0791540000	-0.6556120000	-1.1118000000
C	4.0484620000	0.2923530000	-0.7495810000
C	3.8446220000	1.1584320000	0.3181190000
C	2.6586800000	1.1004020000	1.0504680000
H	4.6100880000	1.8767100000	0.5870250000
H	2.5076440000	1.7682240000	1.8927380000
H	1.1412070000	-1.4370310000	-0.6348660000
H	0.3764240000	0.9390290000	2.2175720000
H	4.9753220000	0.3453530000	-1.3108250000
C	3.3244660000	-1.6025810000	-2.2595280000
H	3.5646930000	-1.0570550000	-3.1761160000
H	2.4540870000	-2.2304300000	-2.4568720000
H	4.1708270000	-2.2615680000	-2.0452330000
O	0.3704530000	-1.1268990000	2.3320380000
H	1.2665060000	-1.3785700000	2.5843930000

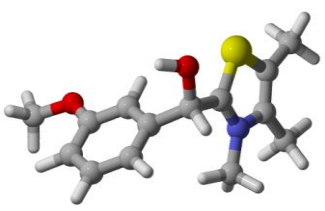
thermodynamic data

Zero-point correction= 0.291386 (Hartree/Particle)
Thermal correction to Energy= 0.309791
Thermal correction to Enthalpy= 0.310735
Thermal correction to Gibbs Free Energy= 0.243495
Sum of electronic and zero-point Energies= -1072.194427
Sum of electronic and thermal Energies= -1072.176022
Sum of electronic and thermal Enthalpies= -1072.175078
Sum of electronic and thermal Free Energies= -1072.242318

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	194.397	67.371	141.518

B3LYP/6-311+G**	





xyz-matrix

36
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2157530000	-0.6910090000	0.3675650000
N	1.7011890000	-0.5270690000	-0.8638830000
C	2.8241290000	0.3180980000	-0.9446600000
C	3.1838170000	0.8024720000	0.2817530000
S	2.1175830000	0.1827600000	1.5211700000
C	4.2980020000	1.7372710000	0.6479130000
C	3.4668130000	0.5858660000	-2.2704670000
C	0.0399160000	-1.5535720000	0.7744290000
H	3.7533070000	-0.3413560000	-2.7770720000
H	4.3702650000	1.1797750000	-2.1341670000
H	2.8029880000	1.1475990000	-2.9371180000
H	4.8796620000	1.3496080000	1.4895350000
H	3.9103610000	2.7213540000	0.9323630000
H	4.9808500000	1.8759120000	-0.1918490000
C	1.1423640000	-1.1951230000	-2.0552650000
H	0.1399790000	-1.5538860000	-1.8350130000
H	1.7871250000	-2.0287980000	-2.3444710000
H	1.0828460000	-0.4764950000	-2.8722000000
C	-1.3022360000	-1.0469240000	0.2631130000
C	-1.6647540000	0.2927970000	0.4192600000
C	-2.9332810000	0.7342650000	0.0090660000
C	-3.8360250000	-0.1789140000	-0.5603520000
C	-3.4630740000	-1.5168490000	-0.7084300000
C	-2.2038610000	-1.9619070000	-0.3038420000
H	-4.1684900000	-2.2184310000	-1.1426300000
H	-1.9323020000	-3.0081490000	-0.4144060000
H	-0.9949120000	1.0178900000	0.8712820000
H	0.2096210000	-2.5623920000	0.3678770000
H	-4.8198400000	0.1388580000	-0.8829160000
O	-3.1832670000	2.0512440000	0.2030690000
C	-4.4635150000	2.5792950000	-0.1606730000
H	-4.4268280000	3.6366350000	0.0988850000
H	-4.6426390000	2.4717620000	-1.2362530000
H	-5.2648120000	2.0907970000	0.4044090000
O	0.1187140000	-1.5962450000	2.1963470000
H	-0.7646950000	-1.7499560000	2.5604180000

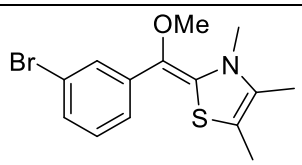
thermodynamic data

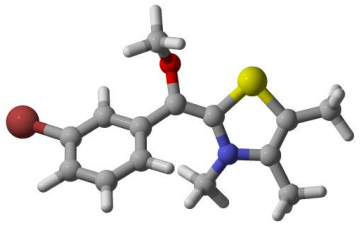
Zero-point correction= 0.296512 (Hartree/Particle)
Thermal correction to Energy= 0.315669
Thermal correction to Enthalpy= 0.316613
Thermal correction to Gibbs Free Energy= 0.247742
Sum of electronic and zero-point Energies= -1147.419455
Sum of electronic and thermal Energies= -1147.400298
Sum of electronic and thermal Enthalpies= -1147.399354
Sum of electronic and thermal Free Energies= -1147.468225

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	198.085	70.542	144.951

B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

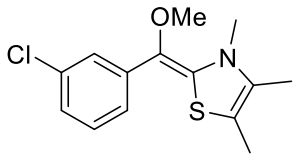
C	1.8267190000	0.3396570000	-0.0618290000
N	2.3393080000	-0.9445550000	-0.2371460000
C	3.7536130000	-0.9939660000	-0.2402730000
C	4.3495380000	0.2116790000	-0.1711350000
S	3.1513120000	1.5249630000	-0.1097930000
C	5.8019700000	0.5666880000	-0.1383690000
C	4.4313960000	-2.3302390000	-0.2927960000
C	0.5358700000	0.7519920000	0.0841930000
H	4.0037940000	-3.0170550000	0.4438930000
H	5.4934050000	-2.2265850000	-0.0749580000
H	4.3456920000	-2.8046340000	-1.2759590000
H	6.0733850000	1.0752170000	0.7928500000
H	6.0590650000	1.2402920000	-0.9629590000
H	6.4302730000	-0.3201490000	-0.2311010000
C	1.5364390000	-1.9942600000	-0.8628330000
H	0.7829980000	-1.5338960000	-1.5044160000
H	1.0183970000	-2.6185330000	-0.1301680000
H	2.1747140000	-2.6273570000	-1.4764820000
C	-0.6529540000	-0.0488150000	0.3836180000
C	-1.8975670000	0.3301060000	-0.1612050000
C	-3.0393940000	-0.3880360000	0.1574300000
C	-3.0093030000	-1.4869410000	1.0128050000
C	-1.7818130000	-1.8525490000	1.5653140000
C	-0.6227720000	-1.1441080000	1.2675660000
Br	-4.7199880000	0.1448890000	-0.6138040000
H	-1.7392330000	-2.6887990000	2.2547560000
H	0.3098250000	-1.4123630000	1.7491820000
H	-3.9144260000	-2.0294310000	1.2507670000
H	-1.9473410000	1.1760260000	-0.8337410000
O	0.3466920000	2.1225050000	-0.1032490000
C	-0.0606740000	2.8425880000	1.0671630000
H	0.6841720000	2.7423660000	1.8635890000
H	-0.1394300000	3.8883140000	0.7696820000
H	-1.0318110000	2.4951160000	1.4330280000

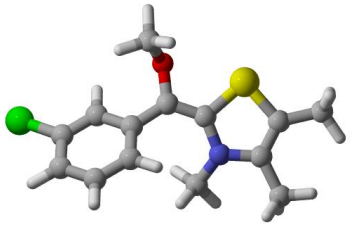
thermodynamic data

Zero-point correction= 0.268485 (Hartree/Particle)
Thermal correction to Energy= 0.287765
Thermal correction to Enthalpy= 0.288709
Thermal correction to Gibbs Free Energy= 0.219687
Sum of electronic and zero-point Energies= -3645.325493
Sum of electronic and thermal Energies= -3645.306213
Sum of electronic and thermal Enthalpies= -3645.305269
Sum of electronic and thermal Free Energies= -3645.374290

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.575	70.239	145.269

B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2476090000	0.3414180000	-0.0894290000
N	1.7477490000	-0.9527180000	-0.2225540000
C	3.1593090000	-1.0240620000	-0.1541430000
C	3.7705230000	0.1730870000	-0.0718140000
S	2.5919990000	1.5055300000	-0.0880740000
C	5.2251250000	0.5059460000	0.0280190000
C	3.8165800000	-2.3716310000	-0.1550190000
C	-0.0420050000	0.7751950000	-0.0113840000
H	3.3431630000	-3.0403650000	0.5702080000
H	4.8687130000	-2.2817880000	0.1114810000
H	3.7692370000	-2.8593600000	-1.1341810000
H	5.4580340000	1.0261720000	0.9631790000
H	5.5341550000	1.1610750000	-0.7936340000
H	5.8424580000	-0.3921580000	-0.0183220000
C	0.9611570000	-1.9997830000	-0.8729950000
H	0.2291770000	-1.5362060000	-1.5361180000
H	0.4193590000	-2.6234450000	-0.1569530000
H	1.6155990000	-2.6340630000	-1.4685560000
C	-1.2565310000	-0.0036160000	0.2395440000
C	-2.4669820000	0.3880870000	-0.3673950000

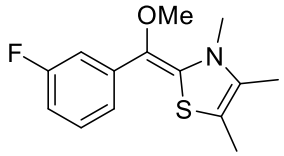
C	-3.6347860000	-0.3074740000	-0.0960720000
C	-3.6624570000	-1.3963320000	0.7718270000
C	-2.4693180000	-1.7750800000	1.3861300000
C	-1.2857960000	-1.0890180000	1.1359440000
Cl	-5.1323350000	0.1976110000	-0.8814060000
H	-2.4729350000	-2.6037700000	2.0857960000
H	-0.3813480000	-1.3671300000	1.6634870000
H	-4.5890940000	-1.9186760000	0.9696250000
H	-2.4760220000	1.2260640000	-1.0518200000
O	-0.2002000000	2.1458850000	-0.2248770000
C	-0.6504730000	2.8870910000	0.9160160000
H	0.0538410000	2.7845800000	1.7482260000
H	-0.6973840000	3.9302210000	0.6029980000
H	-1.6436190000	2.5599670000	1.2391900000

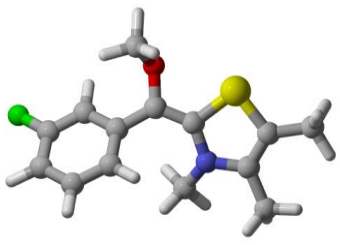
thermodynamic data

Zero-point correction= 0.269154 (Hartree/Particle)
Thermal correction to Energy= 0.288134
Thermal correction to Enthalpy= 0.289079
Thermal correction to Gibbs Free Energy= 0.221513
Sum of electronic and zero-point Energies= -1531.405139
Sum of electronic and thermal Energies= -1531.386158
Sum of electronic and thermal Enthalpies= -1531.385214
Sum of electronic and thermal Free Energies= -1531.452780

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.807	69.776	142.203

B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9427570000	0.3433520000	0.1168600000
N	-1.4263200000	-0.9606480000	0.2112230000
C	-2.8315370000	-1.0546970000	0.0751530000
C	-3.4590210000	0.1330060000	-0.0206280000
S	-2.3058420000	1.4847260000	0.0677780000
C	-4.9128120000	0.4424880000	-0.1859790000

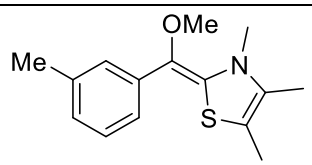
C	-3.4637940000	-2.4133390000	0.0265590000
C	0.3414170000	0.7991930000	0.1022080000
H	-2.9489680000	-3.0608110000	-0.6897960000
H	-4.5057750000	-2.3376310000	-0.2810730000
H	-3.4467810000	-2.9171860000	0.9984570000
H	-5.1103730000	0.9678790000	-1.1264010000
H	-5.2713740000	1.0843020000	0.6259980000
H	-5.5160510000	-0.4662600000	-0.1768080000
C	-0.6549980000	-2.0018800000	0.8893790000
H	0.0490630000	-1.5321110000	1.5775070000
H	-0.0831890000	-2.6207960000	0.1929110000
H	-1.3251000000	-2.6410860000	1.4621840000
C	1.5792870000	0.0445560000	-0.1031330000
C	2.7563290000	0.4525490000	0.5558650000
C	3.9357320000	-0.2270210000	0.3206240000
C	4.0304020000	-1.3052900000	-0.5475790000
C	2.8691750000	-1.6987700000	-1.2130600000
C	1.6647850000	-1.0342270000	-1.0054770000
F	5.0563070000	0.1765720000	0.9764380000
H	2.9135230000	-2.5212180000	-1.9184340000
H	0.7876960000	-1.3237060000	-1.5714100000
H	4.9807360000	-1.8000440000	-0.7009640000
H	2.7399030000	1.2822780000	1.2508100000
O	0.4662780000	2.1697250000	0.3395460000
C	0.9495050000	2.9332440000	-0.7727680000
H	0.2821350000	2.8283990000	-1.6345450000
H	0.9640170000	3.9730710000	-0.4457610000
H	1.9609730000	2.6279170000	-1.0581420000

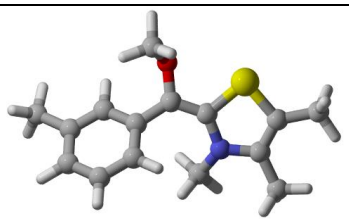
thermodynamic data

Zero-point correction= 0.270428 (Hartree/Particle)
Thermal correction to Energy= 0.289035
Thermal correction to Enthalpy= 0.289979
Thermal correction to Gibbs Free Energy= 0.223610
Sum of electronic and zero-point Energies= -1171.049799
Sum of electronic and thermal Energies= -1171.031191
Sum of electronic and thermal Enthalpies= -1171.030247
Sum of electronic and thermal Free Energies= -1171.096616

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	181.372	68.923	139.685

B3LYP/6-311+G**	





xyz-matrix

37
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9586560000	0.3443500000	0.1082940000
N	-1.4433140000	-0.9614630000	0.2062050000
C	-2.8502070000	-1.0523320000	0.0964360000
C	-3.4787300000	0.1358560000	0.0144420000
S	-2.3235370000	1.4881430000	0.0875970000
C	-4.9347900000	0.4464550000	-0.1260910000
C	-3.4863310000	-2.4096340000	0.0563850000
C	0.3240280000	0.7970030000	0.0732190000
H	-2.9837000000	-3.0580180000	-0.6678000000
H	-4.5327390000	-2.3314000000	-0.2353610000
H	-3.4559990000	-2.9140800000	1.0277790000
H	-5.1469980000	0.9793900000	-1.0592250000
H	-5.2812050000	1.0821470000	0.6961590000
H	-5.5382970000	-0.4622230000	-0.1149730000
C	-0.6566500000	-2.0056450000	0.8600760000
H	0.0384310000	-1.5425160000	1.5623920000
H	-0.0715630000	-2.5957340000	0.1495850000
H	-1.3170800000	-2.6714650000	1.4133170000
C	1.5612570000	0.0381370000	-0.1446360000
C	2.7398270000	0.4114950000	0.5322550000
C	3.9506220000	-0.2464080000	0.3261960000
C	3.9923510000	-1.3070650000	-0.5904020000
C	2.8442620000	-1.6798180000	-1.2840030000
C	1.6400440000	-1.0126840000	-1.0740420000
H	2.8913700000	-2.4848930000	-2.0099510000
H	0.7643990000	-1.2805510000	-1.6541100000
H	4.9264780000	-1.8305660000	-0.7679160000
H	2.6895850000	1.2318000000	1.2401230000
C	5.1945720000	0.1630070000	1.0797250000
H	5.5629400000	-0.6539380000	1.7084790000
H	5.0033970000	1.0218070000	1.7260790000
H	6.0032260000	0.4318070000	0.3929390000
O	0.4523840000	2.1705400000	0.2985630000
C	0.9396110000	2.9198100000	-0.8200270000
H	0.2713130000	2.8116800000	-1.6810320000
H	0.9612710000	3.9630120000	-0.5035420000
H	1.9486260000	2.6042100000	-1.1033830000

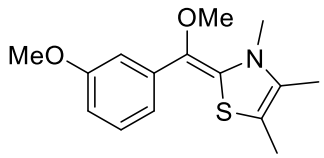
thermodynamic data

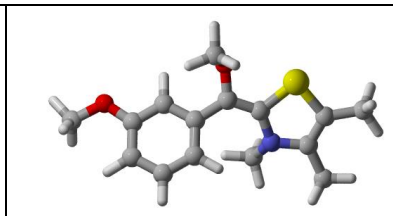
Zero-point correction= 0.305710 (Hartree/Particle)
Thermal correction to Energy= 0.325449

Thermal correction to Enthalpy= 0.326393
Thermal correction to Gibbs Free Energy= 0.256950
Sum of electronic and zero-point Energies= -1111.072221
Sum of electronic and thermal Energies= -1111.052482
Sum of electronic and thermal Enthalpies= -1111.051538
Sum of electronic and thermal Free Energies= -1111.120981

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.222	72.090	146.155

B3LYP/6-311+G**	





xyz-matrix

38
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2868780000	0.3321710000	0.1171070000
N	-1.7520550000	-0.9940650000	0.1558140000
C	-3.1677530000	-1.0717640000	0.0547960000
C	-3.8006510000	0.1143010000	0.0343890000
S	-2.6558800000	1.4734300000	0.1684850000
C	-5.2572360000	0.4251090000	-0.1026810000
C	-3.7959340000	-2.4294640000	-0.0462800000
C	-0.0147660000	0.8031660000	0.0502330000
H	-3.3244060000	-3.0175760000	-0.8402790000
H	-4.8571160000	-2.3461980000	-0.2768780000
H	-3.7054050000	-2.9979570000	0.8848290000
H	-5.4684850000	0.9698120000	-1.0291540000
H	-5.6009570000	1.0521170000	0.7270280000
H	-5.8608370000	-0.4834330000	-0.1018230000
C	-1.0899940000	-1.9501540000	1.0560020000
H	-0.0119320000	-1.8495110000	0.9796780000
H	-1.3510940000	-2.9678410000	0.7659660000
H	-1.3912170000	-1.7844980000	2.0982870000
C	1.2301600000	0.0605040000	-0.1836740000
C	2.4230230000	0.5201690000	0.3878050000
C	3.6351600000	-0.1317330000	0.1470070000
C	3.6772490000	-1.2595250000	-0.6769300000
C	2.4872730000	-1.7133640000	-1.2550960000
C	1.2803300000	-1.0717770000	-1.0243930000

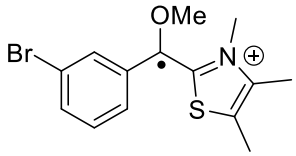
H	2.5175790000	-2.5781610000	-1.9093570000
H	0.3753970000	-1.4249410000	-1.5031460000
H	4.6046270000	-1.7772200000	-0.8798840000
H	2.4190340000	1.3879460000	1.0351320000
O	4.7264150000	0.4096550000	0.7686000000
C	5.9907970000	-0.2094490000	0.5828360000
H	6.6979300000	0.3768120000	1.1677490000
H	5.9891740000	-1.2427630000	0.9472020000
H	6.2937780000	-0.1958680000	-0.4700520000
O	0.1017410000	2.1747140000	0.2774720000
C	0.5152100000	2.9388540000	-0.8619910000
H	-0.2005550000	2.8276080000	-1.6832310000
H	0.5412890000	3.9795410000	-0.5383350000
H	1.5104570000	2.6384980000	-1.2035600000

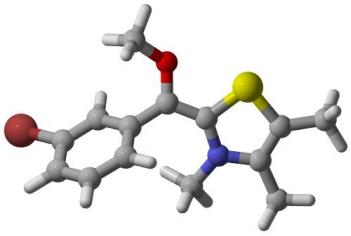
thermodynamic data

Zero-point correction= 0.310860 (Hartree/Particle)
Thermal correction to Energy= 0.331314
Thermal correction to Enthalpy= 0.332258
Thermal correction to Gibbs Free Energy= 0.261535
Sum of electronic and zero-point Energies= -1186.295924
Sum of electronic and thermal Energies= -1186.275470
Sum of electronic and thermal Enthalpies= -1186.274526
Sum of electronic and thermal Free Energies= -1186.345249

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	207.903	75.178	148.849

(u)B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.8521630000	0.3773360000	-0.0425300000
N	2.2113350000	-0.9360670000	-0.1950450000
C	3.5869910000	-1.1447740000	-0.2864540000
C	4.3096780000	0.0161570000	-0.2651570000
S	3.2613390000	1.4019980000	-0.1115730000
C	5.7888130000	0.2173450000	-0.3655480000

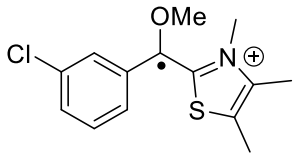
C	4.1296900000	-2.5341940000	-0.4097620000
C	0.5846190000	0.9483480000	0.1402670000
H	3.9112170000	-2.9689080000	-1.3900130000
H	3.7147290000	-3.1953820000	0.3546390000
H	5.2107550000	-2.5279820000	-0.2889950000
H	6.1823300000	0.7118030000	0.5268410000
H	6.0406230000	0.8406970000	-1.2280160000
H	6.3089710000	-0.7325130000	-0.4802930000
C	1.2514570000	-2.0389060000	-0.3736680000
H	1.6834720000	-2.7722840000	-1.0496110000
H	0.3358210000	-1.6540680000	-0.8119320000
H	1.0206360000	-2.5136340000	0.5810230000
C	-0.6388190000	0.2516190000	0.5720170000
C	-1.8054360000	0.3397080000	-0.2063750000
C	-2.9640100000	-0.2983570000	0.2218250000
C	-2.9893070000	-1.0127850000	1.4205370000
C	-1.8327690000	-1.0889510000	2.1937480000
C	-0.6598580000	-0.4654230000	1.7777940000
H	-1.7990660000	0.8772860000	-1.1463500000
Br	-4.5364500000	-0.1957670000	-0.8490280000
H	-3.9006770000	-1.4979180000	1.7452700000
H	-1.8537210000	-1.6305750000	3.1319470000
H	0.2278850000	-0.5099020000	2.3981460000
O	0.5856320000	2.2729020000	-0.0929860000
C	-0.4066870000	3.1422590000	0.5101760000
H	0.0051050000	4.1431370000	0.4088370000
H	-1.3527420000	3.0727610000	-0.0243840000
H	-0.5445500000	2.8903380000	1.5620110000

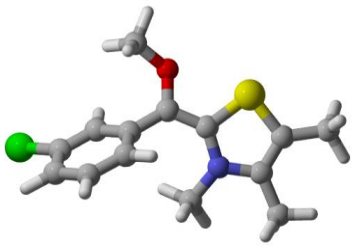
thermodynamic data

Zero-point correction= 0.269572 (Hartree/Particle)
Thermal correction to Energy= 0.288957
Thermal correction to Enthalpy= 0.289901
Thermal correction to Gibbs Free Energy= 0.218941
Sum of electronic and zero-point Energies= -3645.110193
Sum of electronic and thermal Energies= -3645.090809
Sum of electronic and thermal Enthalpies= -3645.089864
Sum of electronic and thermal Free Energies= -3645.160824

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	181.323	69.905	149.348

(u)B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2866520000	0.3769180000	-0.0554580000
N	1.6760170000	-0.9280780000	-0.2090880000
C	3.0575160000	-1.1139840000	-0.2159610000
C	3.7585330000	0.0571490000	-0.1286060000
S	2.6810240000	1.4235230000	-0.0152440000
C	5.2385310000	0.2779820000	-0.1167460000
C	3.6324390000	-2.4916060000	-0.3250190000
C	0.0011690000	0.9258870000	0.0517220000
H	3.4793630000	-2.9180860000	-1.3211820000
H	3.1866270000	-3.1700160000	0.4063150000
H	4.7041740000	-2.4667250000	-0.1401560000
H	5.5862340000	0.5716570000	0.8781890000
H	5.5209300000	1.0712140000	-0.8132880000
H	5.7740590000	-0.6240620000	-0.4099810000
C	0.7473640000	-2.0414210000	-0.4683710000
H	1.2370920000	-2.7606690000	-1.1195750000
H	-0.1398650000	-1.6638450000	-0.9672570000
H	0.4554270000	-2.5306910000	0.4619170000
C	-1.2391280000	0.2028330000	0.3815300000
C	-2.3457610000	0.2856550000	-0.4792670000
C	-3.5215230000	-0.3773250000	-0.1467490000
C	-3.6238130000	-1.1107860000	1.0360420000
C	-2.5271250000	-1.1808170000	1.8913770000
C	-1.3370170000	-0.5326740000	1.5722430000
H	-2.2836920000	0.8374280000	-1.4090100000
Cl	-4.8869000000	-0.2903350000	-1.2301330000
H	-4.5507040000	-1.6135300000	1.2807290000
H	-2.6081340000	-1.7372200000	2.8174820000
H	-0.4968780000	-0.5727430000	2.2558460000
O	-0.0026260000	2.2552520000	-0.1524900000
C	-1.0500370000	3.0960440000	0.3954410000
H	-0.6488190000	4.1050260000	0.3448760000
H	-1.9539530000	3.0238220000	-0.2074050000
H	-1.2588710000	2.8191640000	1.4291320000

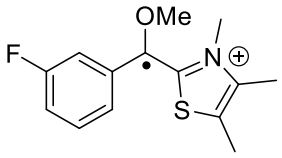
thermodynamic data

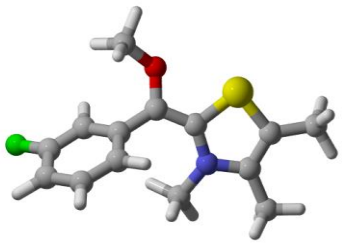
Zero-point correction= 0.270141 (Hartree/Particle)
Thermal correction to Energy= 0.289316
Thermal correction to Enthalpy= 0.290261
Thermal correction to Gibbs Free Energy= 0.220196

Sum of electronic and zero-point Energies= -1531.189840
Sum of electronic and thermal Energies= -1531.170664
Sum of electronic and thermal Enthalpies= -1531.169720
Sum of electronic and thermal Free Energies= -1531.239785

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	181.549	69.478	147.464

(u)B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9883730000	0.3768090000	-0.0763950000
N	1.4057120000	-0.9190520000	-0.2311870000
C	2.7875310000	-1.0870160000	-0.1502550000
C	3.4640610000	0.0910740000	0.0090520000
S	2.3611740000	1.4405660000	0.0785070000
C	4.9364520000	0.3353340000	0.1126770000
C	3.3866060000	-2.4548400000	-0.2521950000
C	-0.3094200000	0.9064630000	-0.0418950000
H	3.3055780000	-2.8592280000	-1.2658750000
H	2.9029060000	-3.1557850000	0.4322710000
H	4.4436690000	-2.4220570000	0.0024320000
H	5.1986920000	0.7662260000	1.0830010000
H	5.2722150000	1.0314500000	-0.6607420000
H	5.4988770000	-0.5893580000	-0.0078390000
C	0.5117760000	-2.0377960000	-0.5752180000
H	1.0545790000	-2.7382340000	-1.2043120000
H	-0.3432480000	-1.6606690000	-1.1279310000
H	0.1617920000	-2.5482590000	0.3230430000
C	-1.5571460000	0.1607060000	0.1955240000
C	-2.6138550000	0.2524660000	-0.7254950000
C	-3.7860310000	-0.4358620000	-0.4613820000
C	-3.9600580000	-1.2006830000	0.6857520000
C	-2.9115640000	-1.2766690000	1.5990290000
C	-1.7140440000	-0.6053490000	1.3610100000
H	-2.5245650000	0.8217010000	-1.6426080000
H	-4.8990270000	-1.7144180000	0.8497190000

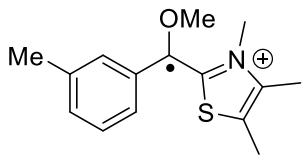
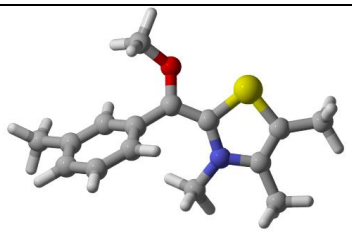
H	-3.0344270000	-1.8556240000	2.5062980000
H	-0.9136460000	-0.6506380000	2.0901750000
F	-4.7880550000	-0.3615920000	-1.3525530000
O	-0.3193600000	2.2393460000	-0.2206550000
C	-1.4098170000	3.0564010000	0.2770590000
H	-1.6959920000	2.7404290000	1.2805030000
H	-1.0118040000	4.0677990000	0.2948030000
H	-2.2641850000	3.0043040000	-0.3961300000

thermodynamic data

Zero-point correction= 0.271540 (Hartree/Particle)
Thermal correction to Energy= 0.290349
Thermal correction to Enthalpy= 0.291294
Thermal correction to Gibbs Free Energy= 0.221941
Sum of electronic and zero-point Energies= -1170.834303
Sum of electronic and thermal Energies= -1170.815494
Sum of electronic and thermal Enthalpies= -1170.814550
Sum of electronic and thermal Free Energies= -1170.883903

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	182.197	68.584	145.965

(u)B3LYP/6-311+G**		

xyz-matrix

37
XYZ file generated by gabedit : coordinates in Angstrom

C	1.0029230000	0.3766650000	-0.0770510000
N	1.4204150000	-0.9190590000	-0.2360530000
C	2.8034850000	-1.0853600000	-0.1692310000
C	3.4806770000	0.0925130000	-0.0181980000
S	2.3770980000	1.4421670000	0.0611040000
C	4.9539400000	0.3378460000	0.0702280000
C	3.4014210000	-2.4534590000	-0.2759820000
C	-0.2956200000	0.9031320000	-0.0256130000
H	3.3101610000	-2.8590650000	-1.2882890000
H	2.9238280000	-3.1535940000	0.4136250000
H	4.4609400000	-2.4209150000	-0.0315980000
H	5.2259510000	0.7703400000	1.0371680000
H	5.2816420000	1.0329950000	-0.7075560000

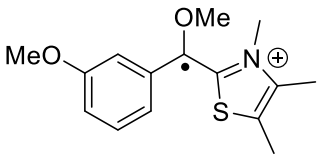
H	5.5157700000	-0.5867100000	-0.0545910000
C	0.5257140000	-2.0387390000	-0.5738600000
H	1.0566970000	-2.7250020000	-1.2286430000
H	-0.3475780000	-1.6587450000	-1.0948100000
H	0.2033020000	-2.5656770000	0.3252650000
C	-1.5359120000	0.1569350000	0.2321460000
C	-2.6187420000	0.2542850000	-0.6610670000
C	-3.8127570000	-0.4268600000	-0.4270570000
C	-3.9136540000	-1.2034000000	0.7381500000
C	-2.8551210000	-1.2986720000	1.6362370000
C	-1.6619950000	-0.6245230000	1.3893640000
H	-2.5132140000	0.8484300000	-1.5627190000
C	-4.9684810000	-0.3366260000	-1.3914140000
H	-4.8365710000	-1.7355300000	0.9429660000
H	-2.9625460000	-1.8919210000	2.5367310000
H	-0.8463740000	-0.6792520000	2.1015790000
H	-4.7250640000	0.2832510000	-2.2555490000
H	-5.8483610000	0.0936240000	-0.9046660000
H	-5.2535860000	-1.3273360000	-1.7558500000
O	-0.3071540000	2.2367150000	-0.2091140000
C	-1.3848350000	3.0528500000	0.3141850000
H	-1.6494910000	2.7343170000	1.3227350000
H	-0.9863370000	4.0643250000	0.3256450000
H	-2.2546590000	3.0019670000	-0.3388430000

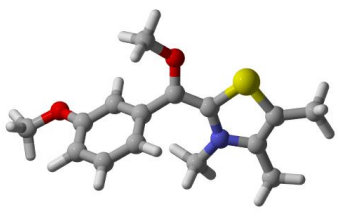
thermodynamic data

Zero-point correction= 0.307038 (Hartree/Particle)
Thermal correction to Energy= 0.326894
Thermal correction to Enthalpy= 0.327838
Thermal correction to Gibbs Free Energy= 0.256085
Sum of electronic and zero-point Energies= -1110.864319
Sum of electronic and thermal Energies= -1110.844463
Sum of electronic and thermal Enthalpies= -1110.843519
Sum of electronic and thermal Free Energies= -1110.915272

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	205.129	71.739	151.016

(u)B3LYP/6-311+G**	





xyz-matrix

38
XYZ file generated by gabedit : coordinates in Angstrom

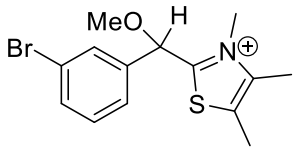
C	1.3416930000	0.3760080000	-0.0787070000
N	1.6904400000	-0.9432600000	-0.2059740000
C	3.0654120000	-1.1745640000	-0.1846360000
C	3.8032090000	-0.0268530000	-0.1002400000
S	2.7691760000	1.3771950000	-0.0275560000
C	5.2888190000	0.1487340000	-0.0727900000
C	3.5936440000	-2.5728240000	-0.2654860000
C	0.0725290000	0.9653080000	0.0004960000
H	3.4431470000	-3.0068000000	-1.2587650000
H	3.1112130000	-3.2255870000	0.4659220000
H	4.6623370000	-2.5834830000	-0.0626070000
H	5.6193050000	0.5761250000	0.8781860000
H	5.6175730000	0.8209180000	-0.8699570000
H	5.8010590000	-0.8024760000	-0.2104870000
C	0.7299620000	-2.0290660000	-0.4656320000
H	1.2031620000	-2.7677690000	-1.1074800000
H	-0.1411150000	-1.6268930000	-0.9736160000
H	0.4139740000	-2.5005270000	0.4658360000
C	-1.1924670000	0.2823890000	0.3217670000
C	-2.2782200000	0.3789570000	-0.5528270000
C	-3.4952920000	-0.2407880000	-0.2409450000
C	-3.6211000000	-0.9490020000	0.9623790000
C	-2.5353030000	-1.0309690000	1.8338180000
C	-1.3209430000	-0.4282580000	1.5283790000
H	-2.1985620000	0.9085950000	-1.4947280000
H	-4.5531550000	-1.4288440000	1.2275570000
H	-2.6488060000	-1.5674970000	2.7685280000
H	-0.4930140000	-0.4778370000	2.2253910000
O	-4.4737030000	-0.0975280000	-1.1598070000
C	-5.7526400000	-0.6950350000	-0.9210000000
H	-6.3573190000	-0.4438810000	-1.7890530000
H	-5.6685190000	-1.7822660000	-0.8363160000
H	-6.2164280000	-0.2823310000	-0.0206830000
O	0.1157610000	2.2921510000	-0.2143870000
C	-0.9287420000	3.1662980000	0.2818310000
H	-0.4916900000	4.1613800000	0.2560360000
H	-1.8016010000	3.1239280000	-0.3676510000
H	-1.2012840000	2.8939610000	1.3017170000

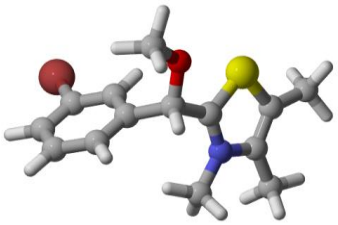
thermodynamic data

Zero-point correction= 0.312126 (Hartree/Particle)
Thermal correction to Energy= 0.332723
Thermal correction to Enthalpy= 0.333667
Thermal correction to Gibbs Free Energy= 0.260950
Sum of electronic and zero-point Energies= -1186.088769
Sum of electronic and thermal Energies= -1186.068172
Sum of electronic and thermal Enthalpies= -1186.067228
Sum of electronic and thermal Free Energies= -1186.139945

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	208.787	74.943	153.046

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	1.6797190000	0.6740870000	-0.0268400000
N	2.1278860000	0.0481920000	1.0595270000
C	3.1153690000	-0.9227120000	0.8121070000
C	3.4092560000	-1.0218290000	-0.5144350000
S	2.4548560000	0.1135970000	-1.4368860000
C	4.3696940000	-1.9360950000	-1.2110620000
C	3.7010070000	-1.7041630000	1.9445650000
C	0.6287680000	1.7627980000	-0.0978420000
H	4.1126020000	-1.0516640000	2.7187950000
H	4.5091110000	-2.3364800000	1.5822190000
H	2.9576280000	-2.3580680000	2.4101690000
H	4.9241360000	-1.4089660000	-1.9901980000
H	3.8443240000	-2.7721060000	-1.6813830000
H	5.0953770000	-2.3467950000	-0.5093680000
C	1.6838400000	0.3630730000	2.4308950000
H	0.7661260000	0.9404930000	2.3923110000
H	2.4624090000	0.9288310000	2.9446170000
H	1.4900550000	-0.5644460000	2.9658610000
C	-0.7509030000	1.3000450000	0.3628770000
C	-1.3249900000	0.1524110000	-0.1939630000
C	-2.6024500000	-0.2325370000	0.1985500000
C	-3.3227500000	0.5110130000	1.1337270000
C	-2.7490650000	1.6575350000	1.6757230000
C	-1.4678130000	2.0545240000	1.2940640000
H	-3.3075890000	2.2460910000	2.3937760000
H	-1.0361770000	2.9571380000	1.7145330000
H	-0.7936060000	-0.4280830000	-0.9381230000
Br	-3.3775550000	-1.8036170000	-0.5567960000
H	0.9527420000	2.5941230000	0.5487190000
H	-4.3170570000	0.2008500000	1.4277630000
O	0.6631660000	2.1637820000	-1.4540100000
C	-0.0686660000	3.3567930000	-1.7608660000

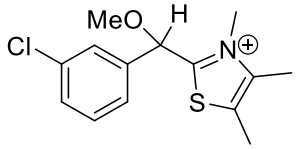
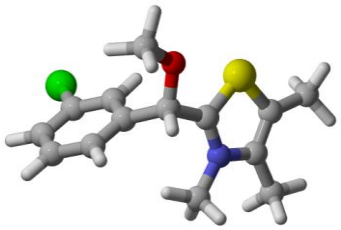
H	0.0956720000	3.5426250000	-2.8200370000
H	-1.1371830000	3.2251150000	-1.5730480000
H	0.3115320000	4.2031360000	-1.1781830000

thermodynamic data

Zero-point correction= 0.281808 (Hartree/Particle)
Thermal correction to Energy= 0.301269
Thermal correction to Enthalpy= 0.302213
Thermal correction to Gibbs Free Energy= 0.231292
Sum of electronic and zero-point Energies= -3645.724783
Sum of electronic and thermal Energies= -3645.705323
Sum of electronic and thermal Enthalpies= -3645.704379
Sum of electronic and thermal Free Energies= -3645.775300

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.049	70.155	149.266

B3LYP/6-311+G**		

xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	1.1550160000	0.6641610000	0.1809880000
N	1.6709090000	-0.1892410000	1.0633770000
C	2.8378030000	-0.8449600000	0.6321910000
C	3.2021490000	-0.4615690000	-0.6231520000
S	2.0851420000	0.7267520000	-1.2458200000
C	4.3540280000	-0.9260030000	-1.4611120000
C	3.5179750000	-1.8351280000	1.5226400000
C	-0.0875420000	1.5163680000	0.3373710000
H	3.7858630000	-1.3975050000	2.4878720000
H	4.4341990000	-2.1883990000	1.0535720000
H	2.8879050000	-2.7096900000	1.7091430000
H	4.7671350000	-0.1080390000	-2.0543160000
H	4.0441450000	-1.7160190000	-2.1512030000
H	5.1568970000	-1.3181570000	-0.8366850000
C	1.1155890000	-0.4201290000	2.4105510000
H	0.1391530000	0.0455800000	2.4886270000
H	1.7905990000	-0.0005620000	3.1574080000

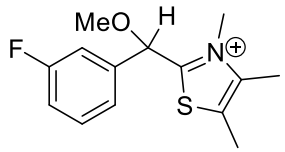
H	1.0057590000	-1.4908380000	2.5737580000
C	-1.3660110000	0.6944770000	0.4797140000
C	-1.6766590000	-0.2827910000	-0.4709340000
C	-2.8679810000	-0.9910990000	-0.3582960000
C	-3.7603320000	-0.7393720000	0.6838340000
C	-3.4489940000	0.2412950000	1.6202960000
C	-2.2566910000	0.9586450000	1.5222410000
H	-4.1427170000	0.4508620000	2.4256330000
H	-2.0315960000	1.7306700000	2.2509710000
H	-1.0135290000	-0.4834090000	-1.3035400000
Cl	-3.2488020000	-2.2169280000	-1.5448260000
H	0.0329960000	2.1361470000	1.2401760000
H	-4.6836960000	-1.2999870000	0.7527470000
O	-0.0711770000	2.3344280000	-0.8163250000
C	-1.0074080000	3.4192250000	-0.8135090000
H	-0.8364460000	3.9624960000	-1.7403310000
H	-2.0371280000	3.0539010000	-0.7872130000
H	-0.8247580000	4.0832270000	0.0385660000

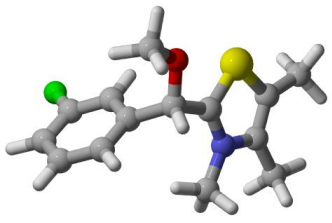
thermodynamic data

Zero-point correction= 0.282288 (Hartree/Particle)
Thermal correction to Energy= 0.301614
Thermal correction to Enthalpy= 0.302558
Thermal correction to Gibbs Free Energy= 0.232031
Sum of electronic and zero-point Energies= -1531.804507
Sum of electronic and thermal Energies= -1531.785181
Sum of electronic and thermal Enthalpies= -1531.784236
Sum of electronic and thermal Free Energies= -1531.854763

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.266	69.750	148.436

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8977970000	0.4886590000	-0.3939800000
N	-1.4425350000	-0.6320070000	-0.8631030000
C	-2.7014060000	-0.9449890000	-0.3187730000

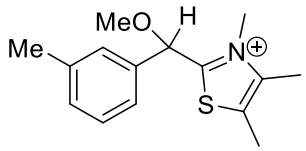
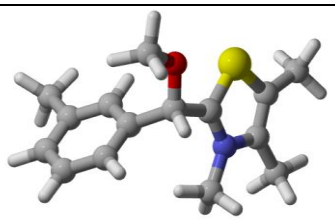
C	-3.1047640000	-0.0183260000	0.5946210000
S	-1.9083670000	1.2445480000	0.7510250000
C	-4.3538060000	0.0240850000	1.4202640000
C	-3.4237160000	-2.1783580000	-0.7586730000
C	0.4352330000	1.0986010000	-0.7761620000
H	-3.5571370000	-2.2051270000	-1.8431700000
H	-4.4115600000	-2.2140640000	-0.3037220000
H	-2.8921260000	-3.0861370000	-0.4584240000
H	-4.7767730000	1.0304750000	1.4466900000
H	-4.1540000000	-0.2822490000	2.4509400000
H	-5.1128910000	-0.6429850000	1.0124150000
C	-0.8258740000	-1.4705210000	-1.9090170000
H	0.2191540000	-1.2017010000	-2.0222840000
H	-1.3552990000	-1.3242750000	-2.8515880000
H	-0.8871010000	-2.5154850000	-1.6116400000
C	1.6268950000	0.2201820000	-0.4049450000
C	1.7732300000	-0.2420040000	0.9071430000
C	2.8906860000	-0.9964820000	1.2246630000
C	3.8715950000	-1.3073960000	0.2914460000
C	3.7205350000	-0.8350850000	-1.0082330000
C	2.6042010000	-0.0736200000	-1.3587530000
H	4.4789880000	-1.0553780000	-1.7495990000
H	2.5062730000	0.3001410000	-2.3726560000
H	1.0534340000	-0.0113720000	1.6834030000
F	3.0262730000	-1.4430840000	2.4866400000
H	0.4410950000	1.2543120000	-1.8667070000
H	4.7284380000	-1.8982920000	0.5896930000
O	0.4277430000	2.3459000000	-0.1093380000
C	1.4717920000	3.2518190000	-0.4874370000
H	1.2953220000	4.1627780000	0.0803390000
H	2.4562570000	2.8485430000	-0.2372570000
H	1.4203170000	3.4732640000	-1.5591400000

thermodynamic data

Zero-point correction= 0.283882 (Hartree/Particle)
Thermal correction to Energy= 0.302701
Thermal correction to Enthalpy= 0.303645
Thermal correction to Gibbs Free Energy= 0.234530
Sum of electronic and zero-point Energies= -1171.449009
Sum of electronic and thermal Energies= -1171.430191
Sum of electronic and thermal Enthalpies= -1171.429246
Sum of electronic and thermal Free Energies= -1171.498361

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.948	68.777	145.465

B3LYP/6-311+G**	

xyz-matrix

38
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9111130000	0.5040110000	-0.3727300000
N	-1.4560970000	-0.5976580000	-0.8844570000
C	-2.7072570000	-0.9411660000	-0.3403880000
C	-3.1043610000	-0.0589470000	0.6179430000
S	-1.9125200000	1.2027460000	0.8164760000
C	-4.3441870000	-0.0615650000	1.4586970000
C	-3.4296040000	-2.1570010000	-0.8268450000
C	0.4107980000	1.1401000000	-0.7481770000
H	-3.5723170000	-2.1375650000	-1.9103100000
H	-4.4132960000	-2.2158890000	-0.3651410000
H	-2.8924780000	-3.0751380000	-0.5711010000
H	-4.7529620000	0.9454210000	1.5641870000
H	-4.1384690000	-0.4456700000	2.4618710000
H	-5.1170170000	-0.6862530000	1.0111810000
C	-0.8465220000	-1.3847400000	-1.9734920000
H	0.2010780000	-1.1193470000	-2.0709400000
H	-1.3745130000	-1.1846960000	-2.9070600000
H	-0.9171320000	-2.4431140000	-1.7312510000
C	1.6149230000	0.2554450000	-0.4432100000
C	1.8103400000	-0.2549240000	0.8460740000
C	2.9318680000	-1.0254820000	1.1570460000
C	3.8622030000	-1.2809400000	0.1379260000
C	3.6824040000	-0.7728760000	-1.1430270000
C	2.5587080000	0.0000260000	-1.4383240000
H	4.4194250000	-0.9703320000	-1.9125660000
H	2.4297450000	0.4088890000	-2.4357750000
H	1.0906010000	-0.0332370000	1.6279170000
H	0.3920510000	1.3464260000	-1.8305610000
H	4.7406210000	-1.8788380000	0.3568680000
C	3.1532360000	-1.5615370000	2.5492010000
H	3.2989040000	-2.6450630000	2.5359390000
H	2.3090460000	-1.3406660000	3.2044510000
H	4.0486470000	-1.1213010000	2.9976790000
O	0.4022240000	2.3584110000	-0.0263550000
C	1.4421600000	3.2806430000	-0.3714060000
H	1.2717480000	4.1646140000	0.2394930000
H	2.4289050000	2.8657970000	-0.1509590000
H	1.3810600000	3.5520610000	-1.4312220000

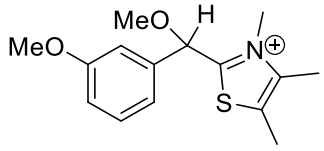
thermodynamic data

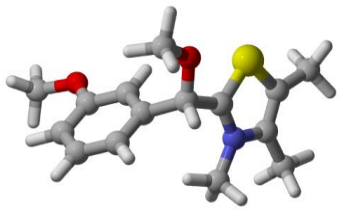
Zero-point correction= 0.319475 (Hartree/Particle)

Thermal correction to Energy= 0.339231
Thermal correction to Enthalpy= 0.340175
Thermal correction to Gibbs Free Energy= 0.269731
Sum of electronic and zero-point Energies= -1111.477329
Sum of electronic and thermal Energies= -1111.457573
Sum of electronic and thermal Enthalpies= -1111.456629
Sum of electronic and thermal Free Energies= -1111.527073

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	212.871	71.890	148.262

B3LYP/6-311+G**	





xyz-matrix

39
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2436600000	0.6169720000	0.1788440000
N	1.7189540000	-0.2938020000	1.0251690000
C	2.8573470000	-0.9822800000	0.5680050000
C	3.2400060000	-0.5657010000	-0.6707560000
S	2.1766810000	0.6956410000	-1.2452490000
C	4.3708780000	-1.0447100000	-1.5285700000
C	3.4921470000	-2.0336900000	1.4212670000
C	0.0429540000	1.5179370000	0.3735790000
H	3.7632920000	-1.6470190000	2.4070500000
H	4.4012330000	-2.3987060000	0.9474960000
H	2.8296850000	-2.8925320000	1.5634270000
H	4.8738820000	-0.2107940000	-2.0223550000
H	4.0132640000	-1.7267850000	-2.3051560000
H	5.1150160000	-1.5730890000	-0.9328440000
C	1.1477960000	-0.5509260000	2.3609540000
H	0.1625060000	-0.1011930000	2.4286900000
H	1.8057360000	-0.1334400000	3.1244580000
H	1.0511370000	-1.6250290000	2.5063980000
C	-1.2702960000	0.7494800000	0.4883120000
C	-1.6272670000	-0.1685340000	-0.4951650000
C	-2.8555100000	-0.8389820000	-0.4247160000
C	-3.7237160000	-0.5815940000	0.6448270000
C	-3.3580770000	0.3427070000	1.6212190000
C	-2.1391970000	1.0121740000	1.5539100000
H	-4.0395950000	0.5454950000	2.4390150000

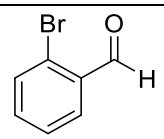
H	-1.8766700000	1.7420290000	2.3123590000
H	-0.9859930000	-0.3703370000	-1.3453750000
H	0.1945630000	2.0928400000	1.3012250000
H	-4.6772550000	-1.0858920000	0.7193830000
O	-3.1040690000	-1.7088250000	-1.4302220000
C	-4.3514770000	-2.4082730000	-1.4553440000
H	-4.3234660000	-3.0228890000	-2.3520900000
H	-4.4613440000	-3.0501820000	-0.5763400000
H	-5.1917930000	-1.7109280000	-1.5169860000
O	0.0999760000	2.3842190000	-0.7445100000
C	-0.8049150000	3.4935040000	-0.7057980000
H	-0.6103950000	4.0684610000	-1.6086960000
H	-1.8445320000	3.1566560000	-0.7010190000
H	-0.6120990000	4.1180320000	0.1736160000

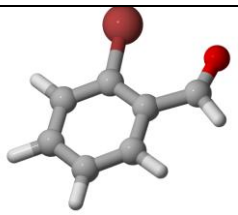
thermodynamic data

Zero-point correction= 0.324374 (Hartree/Particle)
Thermal correction to Energy= 0.345002
Thermal correction to Enthalpy= 0.345946
Thermal correction to Gibbs Free Energy= 0.273621
Sum of electronic and zero-point Energies= -1186.702539
Sum of electronic and thermal Energies= -1186.681912
Sum of electronic and thermal Enthalpies= -1186.680968
Sum of electronic and thermal Free Energies= -1186.753293

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	216.492	75.169	152.221

B3LYP/6-311+G**	***o*-Br-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	0.1879300000	-0.3829760000	-0.0000020000
C	0.7946270000	0.8865020000	-0.0000110000
C	2.1979710000	0.9456480000	-0.0000080000
C	2.9814210000	-0.1996990000	0.0000010000

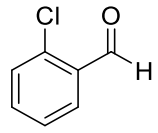
C	2.3578960000	-1.4456190000	0.0000090000
C	0.9676990000	-1.5370130000	0.0000070000
H	2.6677880000	1.9243940000	-0.0000140000
H	4.0620330000	-0.1244170000	0.0000030000
Br	-1.7060610000	-0.6274480000	-0.0000030000
C	0.0958110000	2.1994320000	-0.0000280000
H	0.8060010000	3.0544460000	0.0000370000
O	-1.0946490000	2.3960170000	0.0000280000
H	2.9491770000	-2.3542660000	0.0000170000
H	0.4842070000	-2.5052610000	0.0000130000

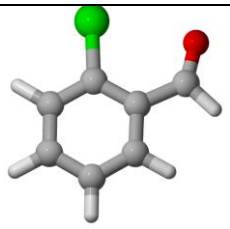
thermodynamic data

Zero-point correction= 0.098995 (Hartree/Particle)
Thermal correction to Energy= 0.106796
Thermal correction to Enthalpy= 0.107741
Thermal correction to Gibbs Free Energy= 0.065008
Sum of electronic and zero-point Energies= -2919.103378
Sum of electronic and thermal Energies= -2919.095577
Sum of electronic and thermal Enthalpies= -2919.094633
Sum of electronic and thermal Free Energies= -2919.137365

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.016	28.290	89.938

B3LYP/6-311+G**	***o*-Cl-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	0.0341110000	-0.6116730000	0.0000000000
C	-0.0193700000	0.7946500000	0.0000020000
C	-1.2841340000	1.4044710000	0.0000010000
C	-2.4570520000	0.6625640000	0.0000000000
C	-2.3780340000	-0.7287400000	-0.0000010000
C	-1.1382910000	-1.3632080000	-0.0000010000
H	-1.3280500000	2.4891920000	0.0000020000
H	-3.4196300000	1.1592850000	-0.0000010000
Cl	1.5467650000	-1.4855480000	0.0000010000
C	1.1476270000	1.7158950000	0.0000040000
H	0.8397470000	2.7842350000	-0.0000060000

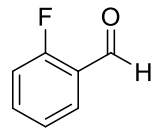
O	2.3171270000	1.4187380000	-0.0000040000
H	-3.2811320000	-1.3283440000	-0.0000030000
H	-1.0721030000	-2.4437190000	-0.0000020000

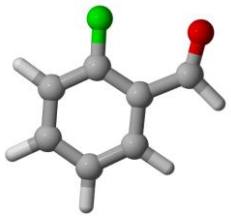
thermodynamic data

Zero-point correction= 0.099682 (Hartree/Particle)
Thermal correction to Energy= 0.107217
Thermal correction to Enthalpy= 0.108161
Thermal correction to Gibbs Free Energy= 0.066798
Sum of electronic and zero-point Energies= -805.183456
Sum of electronic and thermal Energies= -805.175921
Sum of electronic and thermal Enthalpies= -805.174977
Sum of electronic and thermal Free Energies= -805.216339

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.280	27.797	87.055

B3LYP/6-311+G**	***o*-F-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	0.0061770000	0.8458220000	-0.0000060000
C	-0.3899670000	-0.4985740000	-0.0000150000
C	0.6218440000	-1.4705840000	-0.0000070000
C	1.9662680000	-1.1216670000	0.0000050000
C	2.3222840000	0.2272290000	0.0000110000
C	1.3415940000	1.2170880000	0.0000060000
H	0.3302670000	-2.5161560000	-0.0000120000
H	2.7305330000	-1.8890240000	0.0000090000
F	-0.9158920000	1.8197870000	-0.0000110000
C	-1.7998660000	-0.9596760000	-0.0000350000
H	-1.8871070000	-2.0682890000	0.0000480000
O	-2.7878790000	-0.2658450000	0.0000340000
H	3.3674630000	0.5143230000	0.0000210000
H	1.5949050000	2.2699950000	0.0000110000

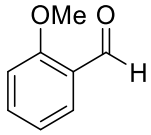
thermodynamic data

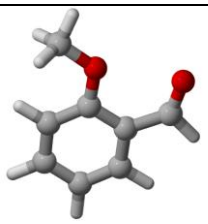
Zero-point correction= 0.101085 (Hartree/Particle)
Thermal correction to Energy= 0.108271

Thermal correction to Enthalpy= 0.109215
Thermal correction to Gibbs Free Energy= 0.069121
Sum of electronic and zero-point Energies= -444.829711
Sum of electronic and thermal Energies= -444.822525
Sum of electronic and thermal Enthalpies= -444.821581
Sum of electronic and thermal Free Energies= -444.861676

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.941	26.922	84.386

B3LYP/6-311+G**	***o*-OMe-PhCHO**





xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.2152770000	-0.4586420000	0.0000530000
C	0.2109980000	0.8947700000	0.0001490000
C	1.5844850000	1.1671460000	0.0000750000
C	2.5367480000	0.1557080000	-0.0000380000
C	2.1036720000	-1.1677330000	-0.0001110000
C	0.7450640000	-1.4782200000	-0.0000660000
H	1.8983200000	2.2066070000	0.0001360000
H	3.5936720000	0.3915220000	-0.0000730000
C	-0.6970970000	2.0637200000	0.0003520000
H	-0.1380500000	3.0267240000	-0.0004860000
O	-1.9063660000	2.0666240000	-0.0003300000
H	2.8270170000	-1.9757590000	-0.0002080000
H	0.4407890000	-2.5156920000	-0.0001300000
O	-1.5428480000	-0.6864170000	0.0000920000
C	-2.0227460000	-2.0264280000	0.0000250000
H	-3.1077770000	-1.9444840000	0.0000910000
H	-1.6977170000	-2.5661890000	-0.8953460000
H	-1.6976170000	-2.5663110000	0.8952870000

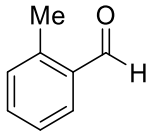
thermodynamic data

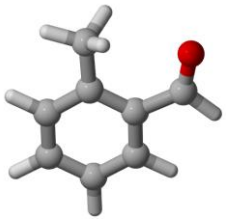
Zero-point correction= 0.141580 (Hartree/Particle)
Thermal correction to Energy= 0.150525
Thermal correction to Enthalpy= 0.151469
Thermal correction to Gibbs Free Energy= 0.107400
Sum of electronic and zero-point Energies= -460.078085

Sum of electronic and thermal Energies= -460.069140
Sum of electronic and thermal Enthalpies= -460.068196
Sum of electronic and thermal Free Energies= -460.112265

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	94.456	33.222	92.751

B3LYP/6-311+G**	***o*-Me-PhCHO**





xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

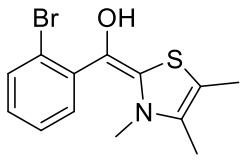
C	0.0533280000	0.8505900000	-0.0000010000
C	0.3135670000	-0.5417810000	-0.0000020000
C	-0.7498870000	-1.4565000000	-0.0000010000
C	-2.0709140000	-1.0287080000	0.0000010000
C	-2.3334000000	0.3393140000	0.0000020000
C	-1.2835390000	1.2570660000	0.0000010000
H	-0.5239530000	-2.5185110000	-0.0000020000
H	-2.8824550000	-1.7466460000	0.0000010000
C	1.1468880000	1.8870180000	-0.0000020000
C	1.6743590000	-1.1210120000	-0.0000050000
H	1.6798540000	-2.2327620000	0.0000060000
O	2.7221880000	-0.5108330000	0.0000050000
H	-3.3573600000	0.6965960000	0.0000030000
H	-1.5062820000	2.3188440000	0.0000020000
H	0.7160310000	2.8902540000	-0.0000020000
H	1.7971200000	1.7814820000	-0.8713380000
H	1.7971210000	1.7814830000	0.8713340000

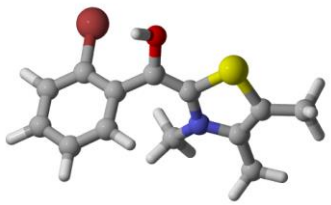
thermodynamic data

Zero-point correction= 0.136967 (Hartree/Particle)
Thermal correction to Energy= 0.144831
Thermal correction to Enthalpy= 0.145775
Thermal correction to Gibbs Free Energy= 0.104603
Sum of electronic and zero-point Energies= -384.858024
Sum of electronic and thermal Energies= -384.850160
Sum of electronic and thermal Enthalpies= -384.849216
Sum of electronic and thermal Free Energies= -384.890388

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.883	29.851	86.655

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

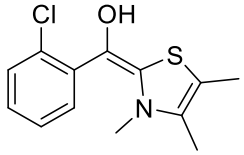
C	1.2282620000	-0.2422370000	-0.3362150000
N	1.7948680000	0.7367060000	0.4794460000
C	3.2029920000	0.6620270000	0.5637200000
C	3.7424300000	-0.3780630000	-0.1012270000
S	2.4908910000	-1.3627960000	-0.8943730000
C	5.1731380000	-0.7863410000	-0.2525360000
C	3.9433070000	1.7110610000	1.3374630000
C	-0.0729280000	-0.4404300000	-0.6763690000
H	3.6271130000	2.7167870000	1.0440700000
H	5.0137560000	1.6320440000	1.1539480000
H	3.7903020000	1.6175330000	2.4177970000
H	5.4884710000	-0.7741230000	-1.3014380000
H	5.3333610000	-1.8031840000	0.1222990000
H	5.8374480000	-0.1233730000	0.3034930000
C	0.9877450000	1.4705930000	1.4474200000
H	0.1944710000	0.8190280000	1.8224310000
H	0.5195800000	2.3580770000	1.0121360000
H	1.6092080000	1.7794370000	2.2852990000
C	-1.1791290000	0.5208750000	-0.5825740000
C	-2.4582470000	0.2151770000	-0.0703100000
C	-3.4976960000	1.1402620000	-0.0856680000
C	-3.2888670000	2.4171430000	-0.6028520000
C	-2.0343210000	2.7595350000	-1.1040790000
C	-1.0090910000	1.8217870000	-1.1028480000
Br	-2.8067200000	-1.4754070000	0.7724210000
H	-4.4617760000	0.8656630000	0.3230340000
H	-1.8610430000	3.7468610000	-1.5170800000
H	-0.0472760000	2.0723290000	-1.5359580000
O	-0.3327030000	-1.6793270000	-1.2697340000
H	-0.8883700000	-1.5469580000	-2.0464130000
H	-4.1023340000	3.1332240000	-0.6101810000

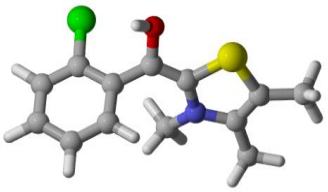
thermodynamic data

Zero-point correction= 0.240302 (Hartree/Particle)
Thermal correction to Energy= 0.258228
Thermal correction to Enthalpy= 0.259173
Thermal correction to Gibbs Free Energy= 0.193273
Sum of electronic and zero-point Energies= -3606.039022
Sum of electronic and thermal Energies= -3606.021095
Sum of electronic and thermal Enthalpies= -3606.020151
Sum of electronic and thermal Free Energies= -3606.086050

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.041	65.755	138.697

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8967250000	-0.3888720000	-0.1977480000
N	1.3868850000	0.7794460000	0.3851030000
C	2.7965820000	0.8691760000	0.3806370000
C	3.4181430000	-0.2173170000	-0.1176660000
S	2.2501260000	-1.4599570000	-0.6246290000
C	4.8767490000	-0.4971030000	-0.2929340000
C	3.4486450000	2.1188550000	0.8908940000
C	-0.3887350000	-0.7792660000	-0.4074140000
H	3.0078060000	3.0104810000	0.4343980000
H	4.5116550000	2.1151100000	0.6546110000
H	3.3569300000	2.2232750000	1.9771550000
H	5.1343170000	-0.6565890000	-1.3455310000
H	5.1719030000	-1.3996960000	0.2533230000
H	5.4879800000	0.3262300000	0.0791640000
C	0.5502240000	1.5924020000	1.2603220000
H	-0.1586410000	0.9445360000	1.7814550000
H	-0.0216260000	2.3450210000	0.7096890000
H	1.1701340000	2.0948240000	2.0000590000
C	-1.5895340000	0.0648690000	-0.4150450000
C	-2.8010740000	-0.2825990000	0.2202640000
C	-3.9397250000	0.5101380000	0.1179120000
C	-3.9032930000	1.6931930000	-0.6162980000
C	-2.7202790000	2.0747710000	-1.2472180000
C	-1.5939640000	1.2664020000	-1.1546140000

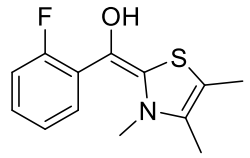
Cl	-2.8966870000	-1.7085940000	1.2468880000
H	-4.8439850000	0.2048430000	0.6292960000
H	-2.6815280000	2.9880560000	-1.8301070000
H	-0.6878060000	1.5402190000	-1.6829480000
O	-0.5348740000	-2.1292610000	-0.7390610000
H	-1.1442540000	-2.2078100000	-1.4819160000
H	-4.7932320000	2.3069870000	-0.6914730000

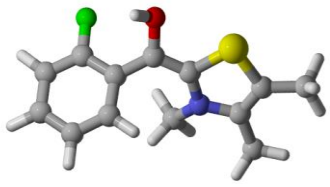
thermodynamic data

Zero-point correction= 0.240930 (Hartree/Particle)
Thermal correction to Energy= 0.258576
Thermal correction to Enthalpy= 0.259520
Thermal correction to Gibbs Free Energy= 0.194978
Sum of electronic and zero-point Energies= -1492.119280
Sum of electronic and thermal Energies= -1492.101634
Sum of electronic and thermal Enthalpies= -1492.100690
Sum of electronic and thermal Free Energies= -1492.165232

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.259	65.313	135.841

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7463960000	-0.4687830000	-0.0497720000
N	1.1986640000	0.8013000000	0.3087230000
C	2.5999940000	0.9531740000	0.2060160000
C	3.2543720000	-0.1716240000	-0.1421810000
S	2.1339510000	-1.5352240000	-0.3660030000
C	4.7156490000	-0.4065830000	-0.3574840000
C	3.2062370000	2.2997840000	0.4642240000
C	-0.5251390000	-0.9461410000	-0.1280210000
H	2.6833230000	3.0823540000	-0.0940170000
H	4.2502920000	2.3112780000	0.1547680000
H	3.1780860000	2.5737910000	1.5240980000
H	4.9278400000	-0.7220890000	-1.3846760000
H	5.0884350000	-1.1938460000	0.3068460000
H	5.2975600000	0.4942160000	-0.1577190000
C	0.3762870000	1.6882590000	1.1242670000

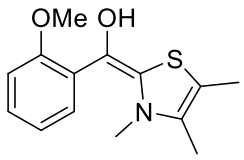
H	-0.2470120000	1.0881690000	1.7920900000
H	-0.2848310000	2.3165610000	0.5206730000
H	1.0145340000	2.3310380000	1.7270250000
C	-1.7668930000	-0.1761600000	-0.2190310000
C	-2.9469140000	-0.5581360000	0.4429020000
C	-4.1457950000	0.1214960000	0.3147860000
C	-4.2075540000	1.2477440000	-0.5048110000
C	-3.0635490000	1.6657340000	-1.1840650000
C	-1.8733910000	0.9587670000	-1.0505010000
F	-2.9177510000	-1.6257330000	1.2782180000
H	-5.0084420000	-0.2301430000	0.8677970000
H	-3.1037260000	2.5304640000	-1.8365260000
H	-0.9994920000	1.2616900000	-1.6156870000
O	-0.6086460000	-2.3385040000	-0.2056170000
H	-1.2784100000	-2.5812540000	-0.8545390000
H	-5.1412990000	1.7867030000	-0.6121400000

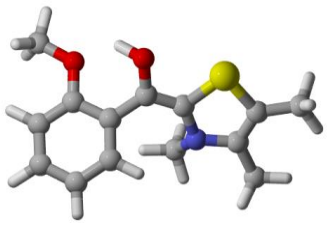
thermodynamic data

Zero-point correction= 0.242400 (Hartree/Particle)
Thermal correction to Energy= 0.259633
Thermal correction to Enthalpy= 0.260577
Thermal correction to Gibbs Free Energy= 0.197361
Sum of electronic and zero-point Energies= -1131.764994
Sum of electronic and thermal Energies= -1131.747761
Sum of electronic and thermal Enthalpies= -1131.746817
Sum of electronic and thermal Free Energies= -1131.810033

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.922	64.400	133.049

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9390100000	-0.4024770000	-0.1127160000
N	1.5059200000	0.8182920000	0.3132050000
C	2.9276120000	0.7877420000	0.2760000000
C	3.4627640000	-0.3886690000	-0.0931890000
S	2.2113520000	-1.6097440000	-0.4342510000

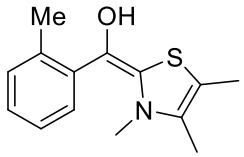
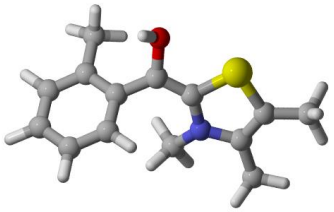
C	4.8950780000	-0.7713720000	-0.2924930000
C	3.6699320000	2.0476900000	0.6083230000
C	-0.3603970000	-0.7188970000	-0.3382770000
H	3.2785600000	2.8919310000	0.0313290000
H	4.7283660000	1.9438750000	0.3730750000
H	3.5937800000	2.3081210000	1.6689790000
H	5.1014710000	-1.0301220000	-1.3367040000
H	5.1524370000	-1.6463010000	0.3141670000
H	5.5685560000	0.0379620000	-0.0072680000
C	0.8909610000	1.4958030000	1.4645030000
H	1.0947850000	0.9559440000	2.3988910000
H	-0.1836630000	1.5667550000	1.3269410000
H	1.2838700000	2.5090370000	1.5442620000
C	-1.5101670000	0.1987910000	-0.3751260000
C	-2.7922800000	-0.2057650000	0.0700680000
C	-3.8881410000	0.6507470000	-0.0124420000
C	-3.7330530000	1.9345580000	-0.5377060000
C	-2.4854010000	2.3554390000	-0.9863910000
C	-1.3972400000	1.4908330000	-0.9095540000
H	-4.8621760000	0.3327760000	0.3339620000
H	-2.3602200000	3.3454710000	-1.4093700000
H	-0.4287480000	1.8087470000	-1.2769960000
O	-0.5789940000	-2.0390190000	-0.7250230000
H	-1.4019760000	-2.3306950000	-0.3093250000
H	-4.5913640000	2.5938760000	-0.5958760000
O	-2.8713760000	-1.4780820000	0.5929470000
C	-4.1200970000	-1.9501920000	1.0879460000
H	-3.9329590000	-2.9589110000	1.4524460000
H	-4.4767130000	-1.3266010000	1.9134740000
H	-4.8755840000	-1.9825920000	0.2965300000

thermodynamic data

Zero-point correction= 0.283536 (Hartree/Particle)
Thermal correction to Energy= 0.302255
Thermal correction to Enthalpy= 0.303199
Thermal correction to Gibbs Free Energy= 0.236696
Sum of electronic and zero-point Energies= -1147.014102
Sum of electronic and thermal Energies= -1146.995383
Sum of electronic and thermal Enthalpies= -1146.994438
Sum of electronic and thermal Free Energies= -1147.060941

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.668	70.130	139.966

B3LYP/6-311+G**	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7400970000	-0.4500290000	-0.0953470000
N	1.1943760000	0.8072220000	0.3069620000
C	2.5978340000	0.9523720000	0.2500020000
C	3.2561980000	-0.1632410000	-0.1194260000
S	2.1326460000	-1.5098150000	-0.4231820000
C	4.7210100000	-0.4020090000	-0.3031330000
C	3.2064640000	2.2841340000	0.5710840000
C	-0.5293760000	-0.9188540000	-0.2129470000
H	2.7199050000	3.0878400000	0.0097810000
H	4.2638870000	2.2896190000	0.3110690000
H	3.1313940000	2.5307300000	1.6354700000
H	4.9586850000	-0.6841070000	-1.3346560000
H	5.0716510000	-1.2140200000	0.3434450000
H	5.3036390000	0.4871300000	-0.0579720000
C	0.3381480000	1.7105670000	1.0657070000
H	-0.3074730000	1.1279370000	1.7278400000
H	-0.3036840000	2.3156860000	0.4196990000
H	0.9505000000	2.3741760000	1.6725140000
C	-1.7921970000	-0.1630900000	-0.2622950000
C	-2.9183120000	-0.5453190000	0.5113190000
C	-4.1058690000	0.1761250000	0.3668360000
C	-4.2113480000	1.2557190000	-0.5096290000
C	-3.1064690000	1.6335900000	-1.2680980000
C	-1.9161830000	0.9228310000	-1.1480790000
H	-4.9643150000	-0.1058090000	0.9686820000
H	-3.1741360000	2.4649220000	-1.9612650000
H	-1.0640830000	1.1906150000	-1.7635990000
O	-0.6175580000	-2.3105390000	-0.3823960000
H	-1.1495950000	-2.4898120000	-1.1670350000
H	-5.1481870000	1.7946620000	-0.5965950000
C	-2.8429440000	-1.6717690000	1.5129800000
H	-3.6660460000	-1.6063180000	2.2279520000
H	-1.8978260000	-1.6470690000	2.0619120000
H	-2.8891510000	-2.6515480000	1.0302650000

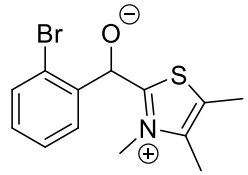
thermodynamic data

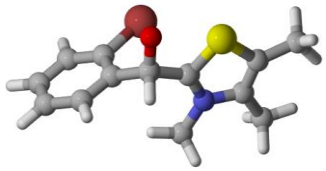
Zero-point correction= 0.278117 (Hartree/Particle)
Thermal correction to Energy= 0.296102
Thermal correction to Enthalpy= 0.297047
Thermal correction to Gibbs Free Energy= 0.232540

Sum of electronic and zero-point Energies= -1071.788981
Sum of electronic and thermal Energies= -1071.770996
Sum of electronic and thermal Enthalpies= -1071.770052
Sum of electronic and thermal Free Energies= -1071.834559

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	185.807	67.339	135.766

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8693070000	0.6807600000	0.5565330000
N	-1.3758800000	1.0493440000	-0.6195770000
C	-2.7051500000	0.6369680000	-0.8368760000
C	-3.1981220000	-0.0383430000	0.2355420000
S	-1.9939920000	-0.1600630000	1.5210100000
C	-4.5560800000	-0.6447850000	0.4158850000
C	-3.3764050000	0.9590290000	-2.1361410000
C	0.4338270000	0.9591810000	1.3380770000
H	-3.4190710000	2.0374810000	-2.3169960000
H	-4.3991180000	0.5856500000	-2.1323000000
H	-2.8601650000	0.4986980000	-2.9842440000
H	-5.0497840000	-0.2469880000	1.3070750000
H	-4.4903470000	-1.7301130000	0.5352910000
H	-5.2023060000	-0.4428100000	-0.4392210000
C	-0.6041810000	1.8034210000	-1.6134370000
H	0.3986710000	1.9677540000	-1.2294160000
H	-1.0844320000	2.7641830000	-1.8056800000
H	-0.5378320000	1.2344730000	-2.5413450000
C	1.7348230000	0.7269950000	0.5333900000
C	2.0805920000	-0.4295630000	-0.1725160000
C	3.3345320000	-0.5972850000	-0.7552660000
C	4.2935450000	0.4053770000	-0.6325550000
C	3.9864510000	1.5680900000	0.0688410000
C	2.7250340000	1.7148760000	0.6371600000
H	4.7261650000	2.3528710000	0.1801770000
H	2.4899840000	2.6123680000	1.2006750000
O	0.3596060000	0.2781590000	2.4719180000
Br	0.8340460000	-1.8843890000	-0.4131240000
H	0.3876560000	2.0800970000	1.4557630000

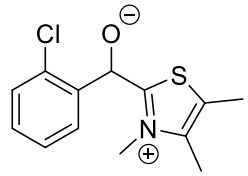
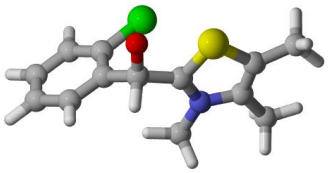
H	5.2717020000	0.2694510000	-1.0796070000
H	3.5581060000	-1.5074810000	-1.2971200000

thermodynamic data

Zero-point correction= 0.239446 (Hartree/Particle)
Thermal correction to Energy= 0.257127
Thermal correction to Enthalpy= 0.258071
Thermal correction to Gibbs Free Energy= 0.192004
Sum of electronic and zero-point Energies= -3606.009075
Sum of electronic and thermal Energies= -3605.991394
Sum of electronic and thermal Enthalpies= -3605.990450
Sum of electronic and thermal Free Energies= -3606.056518

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.350	64.193	139.051

B3LYP/6-311+G**		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7363420000	-0.2815770000	0.6473910000
N	-1.2437340000	0.9453800000	0.5356550000
C	-2.5833810000	0.9846480000	0.1019660000
C	-3.0808410000	-0.2665110000	-0.0891780000
S	-1.8679910000	-1.4980690000	0.2745330000
C	-4.4484130000	-0.6684410000	-0.5500780000
C	-3.2583420000	2.3066510000	-0.0952600000
C	0.5855850000	-0.8877640000	1.1625280000
H	-3.2670790000	2.9017540000	0.8230750000
H	-4.2928200000	2.1577570000	-0.4005240000
H	-2.7676440000	2.9002490000	-0.8729060000
H	-4.9064590000	-1.3755730000	0.1470540000
H	-4.4077970000	-1.1542620000	-1.5294670000
H	-5.1128020000	0.1926650000	-0.6330080000
C	-0.4662040000	2.1533010000	0.8323730000
H	0.5471790000	1.8631750000	1.0953420000
H	-0.9204860000	2.6922250000	1.6654730000
H	-0.4319440000	2.7984950000	-0.0459970000
C	1.8582170000	-0.2580710000	0.5496810000
C	2.1074680000	-0.0746920000	-0.8145390000

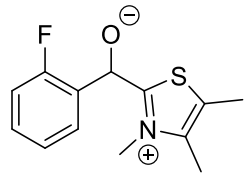
C	3.3377750000	0.3703520000	-1.2907820000
C	4.3694160000	0.6380350000	-0.3946820000
C	4.1576910000	0.4628910000	0.9704900000
C	2.9177150000	0.0222510000	1.4231710000
H	4.9547920000	0.6603530000	1.6783010000
H	2.7562000000	-0.1338120000	2.4851010000
O	0.4951280000	-2.2013490000	1.0043700000
Cl	0.8534710000	-0.3814480000	-2.0246780000
H	0.5996300000	-0.5392110000	2.2348380000
H	5.3294160000	0.9766710000	-0.7671230000
H	3.4817240000	0.4999230000	-2.3561780000

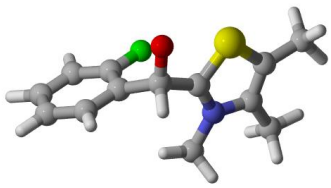
thermodynamic data

Zero-point correction= 0.240066 (Hartree/Particle)
Thermal correction to Energy= 0.257507
Thermal correction to Enthalpy= 0.258451
Thermal correction to Gibbs Free Energy= 0.193388
Sum of electronic and zero-point Energies= -1492.089814
Sum of electronic and thermal Energies= -1492.072373
Sum of electronic and thermal Enthalpies= -1492.071429
Sum of electronic and thermal Free Energies= -1492.136492

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.588	63.737	136.936

B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.6601090000	-0.3969400000	-0.5541080000
N	1.1831220000	0.8255280000	-0.6316940000
C	2.5027320000	0.9257790000	-0.1485690000
C	2.9658580000	-0.2779360000	0.2824090000
S	1.7467800000	-1.5406480000	0.0816580000
C	4.3025710000	-0.6070200000	0.8733800000
C	3.1946670000	2.2537590000	-0.1580110000
C	-0.6695700000	-1.0480130000	-0.9728290000
H	3.2773030000	2.6642440000	-1.1691780000
H	4.2030830000	2.1541710000	0.2404540000

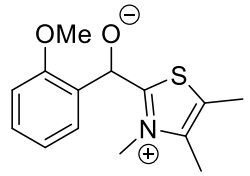
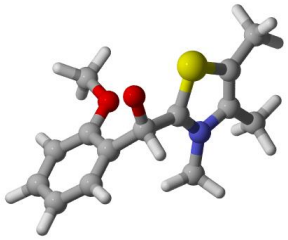
H	2.6684780000	2.9890860000	0.4586270000
H	4.7584840000	-1.4601600000	0.3636560000
H	4.2127920000	-0.8680200000	1.9321790000
H	4.9937140000	0.2332330000	0.7944060000
C	0.4359130000	1.9714780000	-1.1607250000
H	-0.5442230000	1.6332600000	-1.4852590000
H	0.9711270000	2.4048390000	-2.0067490000
H	0.3095860000	2.7256880000	-0.3828100000
C	-1.8976430000	-0.3317670000	-0.3682120000
C	-1.9795690000	0.1049580000	0.9514580000
C	-3.1369930000	0.6135290000	1.5182740000
C	-4.2886710000	0.6912230000	0.7366110000
C	-4.2534380000	0.2666030000	-0.5903160000
C	-3.0694720000	-0.2355650000	-1.1266750000
H	-5.1460110000	0.3192330000	-1.2031610000
H	-3.0452660000	-0.5855850000	-2.1537840000
O	-0.5832270000	-2.3352560000	-0.6546370000
F	-0.8623410000	0.0643260000	1.7362280000
H	-0.7317570000	-0.8321350000	-2.0768110000
H	-5.2046240000	1.0799800000	1.1663100000
H	-3.1251010000	0.9364230000	2.5523710000

thermodynamic data

Zero-point correction= 0.241426 (Hartree/Particle)
Thermal correction to Energy= 0.258535
Thermal correction to Enthalpy= 0.259479
Thermal correction to Gibbs Free Energy= 0.195012
Sum of electronic and zero-point Energies= -1131.736755
Sum of electronic and thermal Energies= -1131.719646
Sum of electronic and thermal Enthalpies= -1131.718702
Sum of electronic and thermal Free Energies= -1131.783169

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.233	62.812	135.682

B3LYP/6-311+G**		

xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

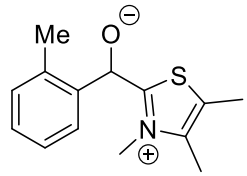
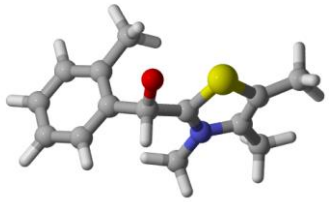
C	-0.7520150000	0.0549660000	0.7681150000
N	-1.2698530000	1.1059420000	0.1349180000
C	-2.5908930000	0.9193920000	-0.3192390000
C	-3.0596170000	-0.3137330000	0.0086540000
S	-1.8434780000	-1.2457060000	0.8945470000
C	-4.4003940000	-0.9126740000	-0.2880340000
C	-3.2783610000	2.0223370000	-1.0637240000
C	0.5559970000	-0.2394690000	1.5169780000
H	-3.3147020000	2.9472020000	-0.4799320000
H	-4.3041330000	1.7380710000	-1.2933600000
H	-2.7784830000	2.2469290000	-2.0114580000
H	-4.8837340000	-1.2687580000	0.6261500000
H	-4.3108210000	-1.7685180000	-0.9639330000
H	-5.0690870000	-0.1887890000	-0.7558840000
C	-0.5216670000	2.3509540000	-0.0650180000
H	0.5032720000	2.1993980000	0.2634020000
H	-0.9765430000	3.1586720000	0.5116420000
H	-0.5178700000	2.6152570000	-1.1226980000
C	1.8231180000	0.0773590000	0.6941780000
C	2.0032420000	-0.3493890000	-0.6353930000
C	3.2348910000	-0.1877810000	-1.2730880000
C	4.3010570000	0.4069550000	-0.5943640000
C	4.1393250000	0.8451850000	0.7139440000
C	2.9036860000	0.6744960000	1.3409180000
H	4.9646070000	1.3020130000	1.2479060000
H	2.7753080000	0.9856380000	2.3731350000
O	0.4729090000	-1.4972100000	1.9465630000
H	0.5511060000	0.5371550000	2.3340690000
H	5.2538790000	0.5223820000	-1.0991360000
H	3.3737540000	-0.5170920000	-2.2947720000
O	0.9055200000	-0.8853750000	-1.2571140000
C	1.0953000000	-1.6382630000	-2.4460110000
H	0.1324730000	-2.0977220000	-2.6670840000
H	1.3908210000	-1.0015130000	-3.2881360000
H	1.8453430000	-2.4219500000	-2.3001840000

thermodynamic data

Zero-point correction= 0.281937 (Hartree/Particle)
Thermal correction to Energy= 0.300778
Thermal correction to Enthalpy= 0.301722
Thermal correction to Gibbs Free Energy= 0.233931
Sum of electronic and zero-point Energies= -1146.981368
Sum of electronic and thermal Energies= -1146.962527
Sum of electronic and thermal Enthalpies= -1146.961583
Sum of electronic and thermal Free Energies= -1147.029373

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.741	69.074	142.677

B3LYP/6-311+G**	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

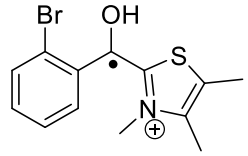
C	0.6791330000	-0.1792470000	-0.5611140000
N	1.1660360000	1.0206080000	-0.2378140000
C	2.5103790000	1.0091910000	0.1868650000
C	3.0267380000	-0.2483890000	0.1720610000
S	1.8301670000	-1.4251290000	-0.3867200000
C	4.4013900000	-0.6977450000	0.5633890000
C	3.1711760000	2.2912220000	0.5911570000
C	-0.6297710000	-0.7386640000	-1.1710400000
H	3.1362050000	3.0379260000	-0.2077840000
H	4.2184770000	2.1125340000	0.8297000000
H	2.7029110000	2.7300260000	1.4781120000
H	4.8446130000	-1.3269900000	-0.2131470000
H	4.3779040000	-1.2856120000	1.4860780000
H	5.0702880000	0.1487100000	0.7251200000
C	0.3811060000	2.2551150000	-0.3593480000
H	-0.6621880000	1.9942500000	-0.5150460000
H	0.7433390000	2.8457350000	-1.2034190000
H	0.4685950000	2.8384020000	0.5567720000
C	-1.8969320000	-0.2198370000	-0.4524230000
C	-2.2193920000	-0.5797640000	0.8735530000
C	-3.4221140000	-0.1162720000	1.4160580000
C	-4.3061530000	0.6755870000	0.6834670000
C	-3.9970240000	1.0105640000	-0.6302640000
C	-2.8006250000	0.5563310000	-1.1843580000
H	-4.6832310000	1.6042030000	-1.2245100000
H	-2.5672870000	0.7935330000	-2.2187070000
O	-0.4715800000	-2.0610230000	-1.2185090000
H	-0.6474510000	-0.2383460000	-2.1777340000
H	-5.2345940000	1.0104940000	1.1330560000
H	-3.6761390000	-0.3949130000	2.4344010000
C	-1.3176220000	-1.4628500000	1.7018280000
H	-1.8383510000	-1.8157580000	2.5947980000
H	-0.4229140000	-0.9251030000	2.0376620000
H	-0.9842130000	-2.3145500000	1.1059660000

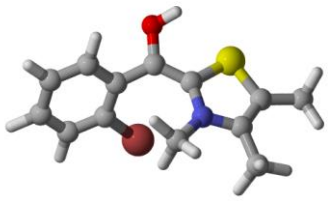
thermodynamic data

Zero-point correction= 0.277222 (Hartree/Particle)
Thermal correction to Energy= 0.294961
Thermal correction to Enthalpy= 0.295905
Thermal correction to Gibbs Free Energy= 0.231124
Sum of electronic and zero-point Energies= -1071.757750
Sum of electronic and thermal Energies= -1071.740011
Sum of electronic and thermal Enthalpies= -1071.739067
Sum of electronic and thermal Free Energies= -1071.803849

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	185.091	65.823	136.344

(u)B3LYP/6-311+G**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8966900000	0.8849520000	0.0074260000
N	1.2681350000	0.0079990000	0.9869270000
C	2.6000610000	-0.3960170000	0.9267110000
C	3.3068750000	0.2147110000	-0.0712570000
S	2.2733860000	1.2789380000	-0.9924070000
C	4.7460740000	0.0729620000	-0.4527800000
C	3.1284060000	-1.3904580000	1.9119750000
C	-0.3682570000	1.4384390000	-0.2503440000
H	2.4927790000	-2.2777080000	1.9589260000
H	3.1967520000	-0.9665800000	2.9184100000
H	4.1262130000	-1.7131460000	1.6231410000
H	5.2460170000	1.0450830000	-0.4654300000
H	4.8504460000	-0.3686020000	-1.4478740000
H	5.2764820000	-0.5626640000	0.2548790000
C	0.3872280000	-0.4022590000	2.0931160000
H	-0.0799820000	-1.3626320000	1.8719230000
H	-0.3829570000	0.3494950000	2.2365650000
H	0.9781930000	-0.4809850000	3.0023640000
C	-1.6804890000	0.8882150000	0.0863330000
C	-2.0726040000	-0.4448590000	-0.1567350000
C	-3.3519400000	-0.8822430000	0.1679060000
C	-4.2687890000	0.0042230000	0.7295010000
C	-3.9172150000	1.3362790000	0.9463290000

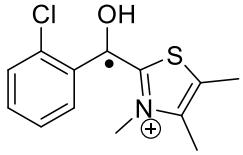
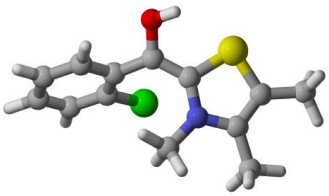
C	-2.6436530000	1.7725180000	0.6174550000
Br	-0.9273600000	-1.6934630000	-1.0573370000
H	-5.2633100000	-0.3471400000	0.9772560000
H	-4.6346350000	2.0309160000	1.3652060000
H	-2.3646310000	2.8066660000	0.7765690000
H	-3.6388830000	-1.9044130000	-0.0414460000
O	-0.4437760000	2.6019570000	-0.9354950000
H	0.3798650000	3.1094790000	-0.9035270000

thermodynamic data

Zero-point correction= 0.241849 (Hartree/Particle)
Thermal correction to Energy= 0.259406
Thermal correction to Enthalpy= 0.260350
Thermal correction to Gibbs Free Energy= 0.194491
Sum of electronic and zero-point Energies= -3605.821332
Sum of electronic and thermal Energies= -3605.803775
Sum of electronic and thermal Enthalpies= -3605.802831
Sum of electronic and thermal Free Energies= -3605.868690

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.780	64.828	138.614

(u)B3LYP/6-311+G**		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7510030000	0.6855620000	-0.1711580000
N	-1.1441740000	-0.4985630000	-0.7258660000
C	-2.4921680000	-0.8033060000	-0.5456860000
C	-3.1863720000	0.1780780000	0.1045890000
S	-2.1233010000	1.4905380000	0.5488560000
C	-4.6369790000	0.2517610000	0.4609460000
C	-3.0454280000	-2.0918310000	-1.0677150000
C	0.5331800000	1.2555770000	-0.1216970000
H	-2.4342700000	-2.9413970000	-0.7547940000
H	-3.1000970000	-2.0954720000	-2.1605730000
H	-4.0526430000	-2.2512530000	-0.6890190000

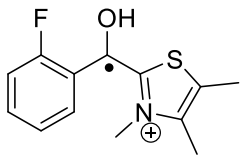
H	-5.1173700000	1.1043140000	-0.0273140000
H	-4.7757380000	0.3633770000	1.5395880000
H	-5.1616080000	-0.6494930000	0.1469900000
C	-0.2690800000	-1.3402630000	-1.5592400000
H	0.1506410000	-2.1552810000	-0.9690620000
H	0.5356400000	-0.7326910000	-1.9622610000
H	-0.8517580000	-1.7454710000	-2.3830780000
C	1.8241550000	0.5744730000	-0.1414130000
C	2.1220850000	-0.5805600000	0.6127460000
C	3.3867330000	-1.1546320000	0.5733890000
C	4.3851050000	-0.5817390000	-0.2110820000
C	4.1272020000	0.5794120000	-0.9403040000
C	2.8674000000	1.1541810000	-0.8953070000
Cl	0.9460730000	-1.2872340000	1.7111010000
H	5.3685630000	-1.0355860000	-0.2342990000
H	4.9074520000	1.0352960000	-1.5369110000
H	2.6616030000	2.0590330000	-1.4529710000
H	3.5924070000	-2.0303380000	1.1752470000
O	0.6426750000	2.5963590000	0.0234970000
H	-0.1544050000	3.0681240000	-0.2572840000

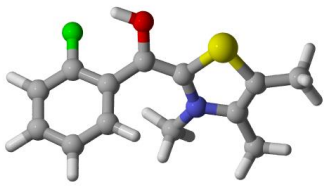
thermodynamic data

Zero-point correction= 0.242457 (Hartree/Particle)
Thermal correction to Energy= 0.259778
Thermal correction to Enthalpy= 0.260723
Thermal correction to Gibbs Free Energy= 0.196067
Sum of electronic and zero-point Energies= -1491.901969
Sum of electronic and thermal Energies= -1491.884648
Sum of electronic and thermal Enthalpies= -1491.883704
Sum of electronic and thermal Free Energies= -1491.948359

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.013	64.409	136.078

(u)B3LYP/6-311+G**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

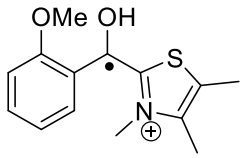
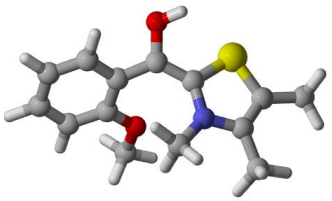
C	0.7640740000	-0.4704840000	0.0170920000
N	1.2329680000	0.7552930000	0.3973090000
C	2.6115770000	0.9127320000	0.2426590000
C	3.2323620000	-0.2187750000	-0.2066960000
S	2.0805640000	-1.5040610000	-0.4603190000
C	4.6830880000	-0.4625270000	-0.4806010000
C	3.2596200000	2.2181990000	0.5827920000
C	-0.5577840000	-0.9525980000	-0.0202260000
H	3.2820180000	2.3916970000	1.6630800000
H	2.7379830000	3.0570700000	0.1159580000
H	4.2879300000	2.2310480000	0.2279370000
H	4.8634440000	-0.6193610000	-1.5478990000
H	5.0366280000	-1.3506460000	0.0495360000
H	5.2915100000	0.3803300000	-0.1555500000
C	0.4249460000	1.7582320000	1.1131090000
H	1.0302780000	2.1931860000	1.9051260000
H	-0.4387350000	1.2730870000	1.5577130000
H	0.0873040000	2.5456350000	0.4384240000
C	-1.7714650000	-0.1604950000	-0.1822130000
C	-2.9908330000	-0.5492350000	0.3994090000
C	-4.1674440000	0.1525640000	0.2288000000
C	-4.1555380000	1.2899930000	-0.5760320000
C	-2.9738770000	1.6992940000	-1.1991730000
C	-1.8012430000	0.9843780000	-1.0077340000
F	-3.0067120000	-1.6657020000	1.1687100000
H	-5.0721290000	1.8469610000	-0.7265640000
H	-2.9760860000	2.5647520000	-1.8500170000
H	-0.8995580000	1.2799210000	-1.5305840000
H	-5.0685130000	-0.1956690000	0.7177930000
O	-0.6067620000	-2.3008630000	-0.0209950000
H	-1.5122730000	-2.6295300000	-0.0985720000

thermodynamic data

Zero-point correction= 0.243825 (Hartree/Particle)
Thermal correction to Energy= 0.260891
Thermal correction to Enthalpy= 0.261835
Thermal correction to Gibbs Free Energy= 0.197484
Sum of electronic and zero-point Energies= -1131.552720
Sum of electronic and thermal Energies= -1131.535654
Sum of electronic and thermal Enthalpies= -1131.534710
Sum of electronic and thermal Free Energies= -1131.599061

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.712	63.636	135.438

(u)B3LYP/6-311+G**	

xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7791510000	-0.7256460000	-0.0861050000
N	1.1922590000	0.3769860000	-0.7742240000
C	2.5375150000	0.7027440000	-0.5976380000
C	3.2087330000	-0.1815190000	0.1956440000
S	2.1279650000	-1.4286940000	0.7744330000
C	4.6474380000	-0.2044610000	0.6046460000
C	3.1079440000	1.9082550000	-1.2768790000
C	-0.5000230000	-1.3124770000	-0.0281280000
H	2.5005100000	2.7964200000	-1.0876720000
H	3.1743590000	1.7686440000	-2.3600480000
H	4.1123090000	2.1089130000	-0.9103010000
H	5.1359590000	-1.1240490000	0.2706510000
H	4.7528650000	-0.1475810000	1.6914560000
H	5.1896080000	0.6348600000	0.1710280000
C	0.3500730000	1.0955100000	-1.7418340000
H	-0.0286390000	2.0181410000	-1.3031730000
H	-0.4868890000	0.4646580000	-2.0260640000
H	0.9403080000	1.3203110000	-2.6278560000
C	-1.7967560000	-0.6745680000	-0.1305830000
C	-2.0638150000	0.6147550000	0.4094960000
C	-3.3582940000	1.1322640000	0.3544510000
C	-4.3878780000	0.3888050000	-0.2178210000
C	-4.1493750000	-0.8872420000	-0.7309340000
C	-2.8710500000	-1.4130840000	-0.6735990000
H	-5.3856100000	0.8102440000	-0.2523400000
H	-4.9560010000	-1.4634830000	-1.1657260000
H	-2.6730340000	-2.4064430000	-1.0546220000
H	-3.5757010000	2.1068750000	0.7686350000
O	-1.0198910000	1.2637830000	0.9859090000
C	-1.2777990000	2.4357300000	1.7730940000
H	-0.3227470000	2.7044430000	2.2191500000
H	-1.6366130000	3.2602560000	1.1510780000
H	-2.0024360000	2.2198020000	2.5615500000
O	-0.5704040000	-2.6407100000	0.2475170000
H	0.2356850000	-3.1107920000	-0.0073770000

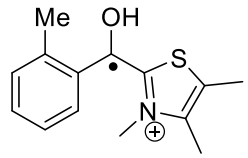
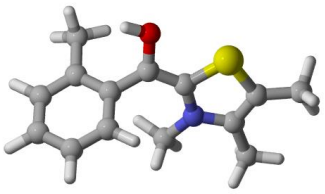
thermodynamic data

Zero-point correction= 0.284776 (Hartree/Particle)
Thermal correction to Energy= 0.303373

Thermal correction to Enthalpy= 0.304317
Thermal correction to Gibbs Free Energy= 0.237527
Sum of electronic and zero-point Energies= -1146.803388
Sum of electronic and thermal Energies= -1146.784792
Sum of electronic and thermal Enthalpies= -1146.783847
Sum of electronic and thermal Free Energies= -1146.850638

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.369	69.717	140.572

(u)B3LYP/6-311+G**	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7622520000	-0.4634220000	-0.0685490000
N	1.1948020000	0.7665610000	0.3585390000
C	2.5745310000	0.9394400000	0.2923010000
C	3.2383270000	-0.1784030000	-0.1351710000
S	2.1241030000	-1.4722270000	-0.4855810000
C	4.7065240000	-0.3912980000	-0.3312950000
C	3.1909270000	2.2469020000	0.6801310000
C	-0.5399620000	-0.9541560000	-0.1935410000
H	3.1227340000	2.4243760000	1.7578470000
H	2.7089630000	3.0833180000	0.1681650000
H	4.2449100000	2.2595710000	0.4111670000
H	4.9672760000	-0.3884530000	-1.3940090000
H	5.0214690000	-1.3516000000	0.0838160000
H	5.2868630000	0.3874150000	0.1621770000
C	0.3157630000	1.7892650000	0.9499190000
H	0.8603440000	2.3088130000	1.7343990000
H	-0.5562080000	1.3093540000	1.3833500000
H	-0.0107440000	2.5053780000	0.1945640000
C	-1.7936570000	-0.1900980000	-0.2613760000
C	-2.8912740000	-0.5027770000	0.5770390000
C	-4.0718460000	0.2253120000	0.3988920000
C	-4.1839050000	1.2148840000	-0.5736350000
C	-3.1000390000	1.5125950000	-1.3997970000

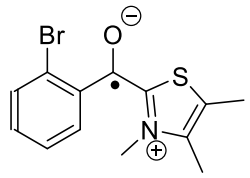
C	-1.9114550000	0.8152530000	-1.2403300000
C	-2.8217860000	-1.5551470000	1.6605150000
H	-5.1169680000	1.7542920000	-0.6863350000
H	-3.1862380000	2.2720430000	-2.1673710000
H	-1.0726080000	1.0197580000	-1.8965090000
H	-4.9179980000	0.0142810000	1.0435670000
H	-3.4695260000	-1.2824230000	2.4950540000
H	-1.8107090000	-1.6922420000	2.0478280000
H	-3.1687460000	-2.5292240000	1.2990010000
O	-0.5811600000	-2.2977780000	-0.3537210000
H	-1.4491930000	-2.5728320000	-0.6780350000

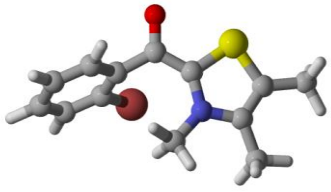
thermodynamic data

Zero-point correction= 0.279623 (Hartree/Particle)
Thermal correction to Energy= 0.297506
Thermal correction to Enthalpy= 0.298450
Thermal correction to Gibbs Free Energy= 0.232500
Sum of electronic and zero-point Energies= -1071.579786
Sum of electronic and thermal Energies= -1071.561904
Sum of electronic and thermal Enthalpies= -1071.560960
Sum of electronic and thermal Free Energies= -1071.626910

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.688	66.567	138.804

(u)B3LYP/6-311+G**	





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9813480000	0.7988510000	-0.1579360000
N	1.3247960000	0.0440270000	0.9473730000
C	2.6751320000	-0.3297900000	0.9830530000
C	3.4013110000	0.1667990000	-0.0491190000
S	2.3991130000	1.1357270000	-1.1300340000
C	4.8570560000	0.0049350000	-0.3557460000
C	3.1782870000	-1.1965850000	2.0977740000
C	-0.2609790000	1.3129030000	-0.6266810000

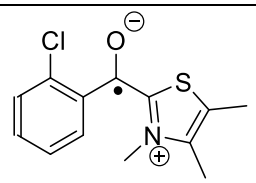
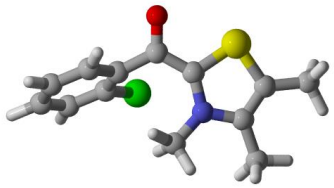
H	2.5792660000	-2.1059390000	2.2006650000
H	3.1668880000	-0.6767690000	3.0614720000
H	4.2060480000	-1.4984450000	1.9037620000
H	5.3648230000	0.9745970000	-0.3829540000
H	5.0086710000	-0.4696310000	-1.3305230000
H	5.3577950000	-0.6082260000	0.3942830000
C	0.4002160000	-0.2351280000	2.0449270000
H	-0.2211340000	-1.1080090000	1.8325290000
H	-0.2462470000	0.6259710000	2.2052900000
H	0.9666310000	-0.4148210000	2.9555980000
O	-0.2605430000	2.1211320000	-1.5834870000
C	-1.5909720000	0.9416060000	-0.0213260000
C	-2.1721990000	-0.3276700000	-0.0974130000
C	-3.4463730000	-0.5848690000	0.4067540000
C	-4.1695840000	0.4457650000	0.9991360000
C	-3.6256140000	1.7286260000	1.0659850000
C	-2.3581390000	1.9685630000	0.5504060000
Br	-1.2519390000	-1.7858950000	-0.9588790000
H	-5.1604040000	0.2467020000	1.3911770000
H	-4.1915680000	2.5392620000	1.5103010000
H	-1.9355610000	2.9664500000	0.5740680000
H	-3.8693170000	-1.5777460000	0.3230350000

thermodynamic data

Zero-point correction= 0.228956 (Hartree/Particle)
Thermal correction to Energy= 0.246400
Thermal correction to Enthalpy= 0.247344
Thermal correction to Gibbs Free Energy= 0.181329
Sum of electronic and zero-point Energies= -3605.447675
Sum of electronic and thermal Energies= -3605.430231
Sum of electronic and thermal Enthalpies= -3605.429287
Sum of electronic and thermal Free Energies= -3605.495302

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	154.618	63.489	138.941

(u)B3LYP/6-311+G**	

xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

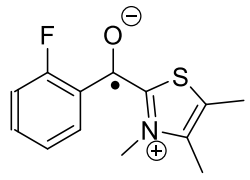
C	0.7845090000	-0.6681070000	-0.1503600000
N	1.1386400000	0.5797920000	-0.6248130000
C	2.5038500000	0.8704950000	-0.4963630000
C	3.2286960000	-0.1547840000	0.0160750000
S	2.2069000000	-1.5491060000	0.3677450000
C	4.6966640000	-0.2390460000	0.2942370000
C	3.0207660000	2.2139770000	-0.9141920000
C	-0.4738490000	-1.3197820000	-0.0064350000
H	2.4522910000	3.0241140000	-0.4486600000
H	2.9765390000	2.3544740000	-1.9992920000
H	4.0612170000	2.3258140000	-0.6140720000
H	5.1562440000	-1.0623000000	-0.2622900000
H	4.8919840000	-0.4150920000	1.3569240000
H	5.2109340000	0.6791770000	0.0085270000
C	0.2122820000	1.4541790000	-1.3430270000
H	-0.3531470000	2.0893420000	-0.6578420000
H	-0.4860790000	0.8484340000	-1.9178100000
H	0.7707230000	2.0831960000	-2.0328040000
O	-0.4944830000	-2.5427870000	0.2655950000
C	-1.7929340000	-0.6102900000	-0.1643340000
C	-2.2283630000	0.4461400000	0.6426060000
C	-3.4989440000	1.0020920000	0.5046030000
C	-4.3681500000	0.4967410000	-0.4564300000
C	-3.9711630000	-0.5742010000	-1.2581450000
C	-2.7049540000	-1.1227810000	-1.0999410000
Cl	-1.1913950000	1.0934960000	1.9191570000
H	-5.3560610000	0.9292790000	-0.5651040000
H	-4.6501330000	-0.9842360000	-1.9968360000
H	-2.3946570000	-1.9720440000	-1.6973680000
H	-3.8016110000	1.8120470000	1.1562010000

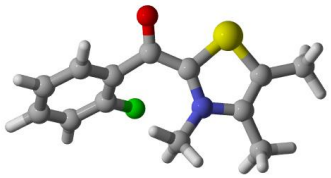
thermodynamic data

Zero-point correction= 0.229586 (Hartree/Particle)
Thermal correction to Energy= 0.246748
Thermal correction to Enthalpy= 0.247692
Thermal correction to Gibbs Free Energy= 0.183233
Sum of electronic and zero-point Energies= -1491.528092
Sum of electronic and thermal Energies= -1491.510931
Sum of electronic and thermal Enthalpies= -1491.509986
Sum of electronic and thermal Free Energies= -1491.574445

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	154.836	63.063	135.664

(u)B3LYP/6-311+G**	





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

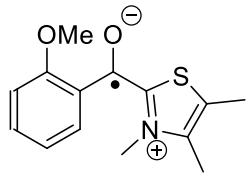
C	0.6945090000	-0.6053810000	-0.1320580000
N	1.0845140000	0.6819410000	-0.4372340000
C	2.4545130000	0.9197480000	-0.2592220000
C	3.1502970000	-0.1827380000	0.1128290000
S	2.0922800000	-1.5866150000	0.2585310000
C	4.6127460000	-0.3370450000	0.3898010000
C	2.9980730000	2.2976500000	-0.4883500000
C	-0.5795620000	-1.2466060000	-0.0884950000
H	2.4321820000	3.0470520000	0.0723270000
H	2.9708990000	2.5817900000	-1.5453260000
H	4.0352760000	2.3537010000	-0.1622220000
H	5.0580500000	-1.0969860000	-0.2604060000
H	4.7936170000	-0.6466470000	1.4241340000
H	5.1510630000	0.5964570000	0.2220080000
C	0.2147740000	1.6544560000	-1.0983320000
H	-0.1848190000	2.3817150000	-0.3887980000
H	-0.6137350000	1.1311250000	-1.5685030000
H	0.7742650000	2.1769520000	-1.8739850000
O	-0.6116410000	-2.5001740000	-0.0389410000
C	-1.8844510000	-0.5060860000	-0.0684410000
C	-2.1616070000	0.5873640000	0.7516000000
C	-3.4111490000	1.1817400000	0.8322430000
C	-4.4493910000	0.6671430000	0.0599080000
C	-4.2214920000	-0.4391860000	-0.7606790000
C	-2.9608640000	-1.0218520000	-0.8088540000
F	-1.1702210000	1.0984710000	1.5353790000
H	-5.4323370000	1.1207210000	0.1107570000
H	-5.0296570000	-0.8520190000	-1.3530450000
H	-2.7786280000	-1.9015510000	-1.4140560000
H	-3.5575190000	2.0198520000	1.5026680000

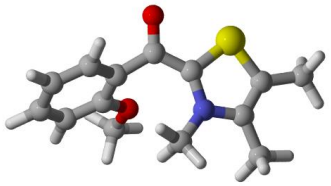
thermodynamic data

Zero-point correction= 0.231070 (Hartree/Particle)
Thermal correction to Energy= 0.247783
Thermal correction to Enthalpy= 0.248727
Thermal correction to Gibbs Free Energy= 0.185623
Sum of electronic and zero-point Energies= -1131.174476
Sum of electronic and thermal Energies= -1131.157764
Sum of electronic and thermal Enthalpies= -1131.156820
Sum of electronic and thermal Free Energies= -1131.219923

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	155.486	62.089	132.813

(u)B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8214240000	-0.7226610000	-0.0469690000
N	1.1743170000	0.4352270000	-0.7113550000
C	2.5301830000	0.7691530000	-0.5938500000
C	3.2542320000	-0.1426230000	0.1008240000
S	2.2419580000	-1.4829430000	0.6443690000
C	4.7145730000	-0.1511890000	0.4273730000
C	3.0376860000	2.0326650000	-1.2211570000
C	-0.4304860000	-1.3725890000	0.1608040000
H	2.4388770000	2.8973510000	-0.9207360000
H	3.0259230000	1.9838500000	-2.3150650000
H	4.0656980000	2.2192150000	-0.9149460000
H	5.2063050000	-1.0371380000	0.0121400000
H	4.8825210000	-0.1637550000	1.5091740000
H	5.2202830000	0.7261360000	0.0221050000
C	0.2696540000	1.1485410000	-1.6101180000
H	-0.2733600000	1.9381850000	-1.0868250000
H	-0.4510760000	0.4474470000	-2.0260910000
H	0.8393630000	1.5838550000	-2.4292950000
O	-0.4207960000	-2.5452850000	0.6069700000
C	-1.7596480000	-0.7253310000	-0.1111250000

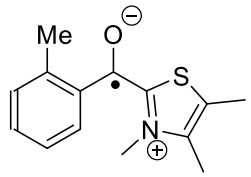
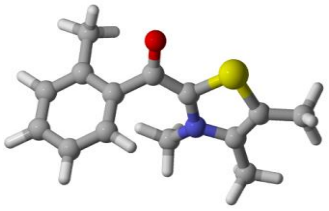
C	-2.1461070000	0.5062430000	0.4546490000
C	-3.4412430000	0.9960140000	0.2631740000
C	-4.3592040000	0.2643200000	-0.4903420000
C	-3.9992050000	-0.9626640000	-1.0395910000
C	-2.7119240000	-1.4511200000	-0.8322010000
H	-5.3599180000	0.6565200000	-0.6335750000
H	-4.7155100000	-1.5397370000	-1.6124560000
H	-2.4225030000	-2.4214070000	-1.2184430000
H	-3.7456590000	1.9356920000	0.7046340000
O	-1.1961730000	1.1617000000	1.1923780000
C	-1.5892930000	2.2803340000	1.9756490000
H	-0.7075480000	2.5669850000	2.5469060000
H	-1.9040480000	3.1239770000	1.3505010000
H	-2.3989980000	2.0174480000	2.6640310000

thermodynamic data

Zero-point correction= 0.271746 (Hartree/Particle)
Thermal correction to Energy= 0.290166
Thermal correction to Enthalpy= 0.291110
Thermal correction to Gibbs Free Energy= 0.224372
Sum of electronic and zero-point Energies= -1146.419621
Sum of electronic and thermal Energies= -1146.401201
Sum of electronic and thermal Enthalpies= -1146.400257
Sum of electronic and thermal Free Energies= -1146.466995

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	182.082	68.285	140.463

(u)B3LYP/6-311+G**		

xyz-matrix

33
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7394870000	-0.5001670000	-0.0532790000
N	1.1580490000	0.7670230000	0.3281680000
C	2.5498900000	0.9415140000	0.2566250000
C	3.2211250000	-0.1665930000	-0.1387170000
S	2.1195740000	-1.5152450000	-0.4348080000

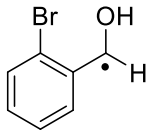
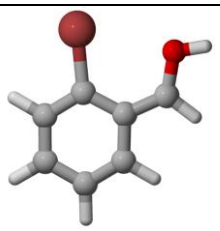
C	4.6883050000	-0.3654320000	-0.3563320000
C	3.1332220000	2.2798310000	0.5960210000
C	-0.5582490000	-1.0718520000	-0.2289430000
H	2.9365320000	2.5617130000	1.6347910000
H	2.7212090000	3.0667240000	-0.0437690000
H	4.2127120000	2.2704000000	0.4560560000
H	4.9130560000	-0.5696390000	-1.4083050000
H	5.0584390000	-1.2151650000	0.2260210000
H	5.2598820000	0.5140880000	-0.0577580000
C	0.3546970000	1.6507080000	1.1795820000
H	0.6884810000	1.5810980000	2.2205770000
H	-0.6888280000	1.3633210000	1.1240020000
H	0.4431670000	2.6838250000	0.8419760000
O	-0.6464940000	-2.3064330000	-0.4155760000
C	-1.7983530000	-0.2226370000	-0.2818310000
C	-2.9227140000	-0.5336540000	0.5118260000
C	-4.0741530000	0.2450670000	0.3592840000
C	-4.1378620000	1.2881310000	-0.5635330000
C	-3.0316020000	1.5771160000	-1.3580260000
C	-1.8699250000	0.8239550000	-1.2094300000
C	-2.9024980000	-1.6687410000	1.5061470000
H	-5.0494540000	1.8670440000	-0.6629410000
H	-3.0732990000	2.3758580000	-2.0901290000
H	-1.0056680000	1.0377410000	-1.8297470000
H	-4.9408480000	0.0242150000	0.9742150000
H	-3.7982860000	-1.6512900000	2.1304280000
H	-2.0268220000	-1.6163490000	2.1596420000
H	-2.8460630000	-2.6308450000	0.9929410000

thermodynamic data

Zero-point correction= 0.266527 (Hartree/Particle)
Thermal correction to Energy= 0.284218
Thermal correction to Enthalpy= 0.285162
Thermal correction to Gibbs Free Energy= 0.219735
Sum of electronic and zero-point Energies= -1071.196651
Sum of electronic and thermal Energies= -1071.178959
Sum of electronic and thermal Enthalpies= -1071.178015
Sum of electronic and thermal Free Energies= -1071.243442

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.349	65.213	137.703

(u)B3LYP/6-311+G**	

xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

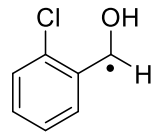
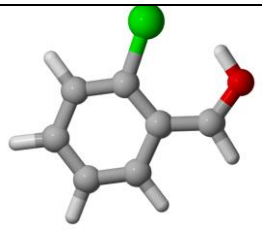
C	0.2255620000	-0.3944460000	0.0000040000
C	0.7760200000	0.9235920000	-0.0000500000
C	2.2067720000	0.9978040000	-0.0001090000
C	3.0088380000	-0.1219600000	-0.0001160000
C	2.4311280000	-1.3985280000	-0.0000620000
C	1.0420720000	-1.5177580000	0.0000010000
H	2.6611320000	1.9830760000	-0.0001370000
H	4.0870200000	-0.0103410000	-0.0001540000
Br	-1.6651880000	-0.7303910000	0.0000710000
C	0.0987470000	2.1556600000	-0.0000860000
H	0.6749220000	3.0736080000	-0.0002580000
H	3.0487310000	-2.2883120000	-0.0000730000
H	0.5829340000	-2.4981190000	0.0000430000
O	-1.2521890000	2.2783980000	0.0000330000
H	-1.4904720000	3.2104150000	0.0003350000

thermodynamic data

Zero-point correction= 0.109072 (Hartree/Particle)
Thermal correction to Energy= 0.117545
Thermal correction to Enthalpy= 0.118490
Thermal correction to Gibbs Free Energy= 0.074027
Sum of electronic and zero-point Energies= -2919.660733
Sum of electronic and thermal Energies= -2919.652259
Sum of electronic and thermal Enthalpies= -2919.651315
Sum of electronic and thermal Free Energies= -2919.695777

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.761	31.398	93.580

(u)B3LYP/6-311+G**	

xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

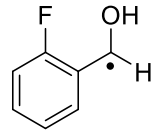
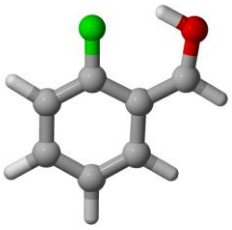
C	-0.0329800000	-0.6056130000	-0.0000510000
C	-0.0265890000	0.8210440000	-0.0000240000
C	-1.3237840000	1.4301800000	0.0000540000
C	-2.4879650000	0.6940300000	0.0000580000
C	-2.4418270000	-0.7078600000	-0.0000060000
C	-1.2018220000	-1.3468120000	-0.0000470000
H	-1.3703270000	2.5137470000	0.0001040000
H	-3.4436700000	1.2054090000	0.0001080000
Cl	1.4892540000	-1.5277240000	-0.0000010000
C	1.0832870000	1.6865710000	-0.0000500000
H	0.9233720000	2.7563460000	-0.0000140000
H	-3.3516380000	-1.2948420000	-0.0000070000
H	-1.1403330000	-2.4280060000	-0.0000570000
O	2.3933370000	1.3724480000	0.0000320000
H	2.5086690000	0.4098240000	0.0000270000

thermodynamic data

Zero-point correction= 0.110304 (Hartree/Particle)
Thermal correction to Energy= 0.118184
Thermal correction to Enthalpy= 0.119129
Thermal correction to Gibbs Free Energy= 0.076801
Sum of electronic and zero-point Energies= -805.747752
Sum of electronic and thermal Energies= -805.739871
Sum of electronic and thermal Enthalpies= -805.738927
Sum of electronic and thermal Free Energies= -805.781254

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.162	30.326	89.085

(u)B3LYP/6-311+G**	

xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

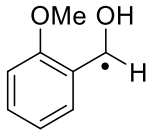
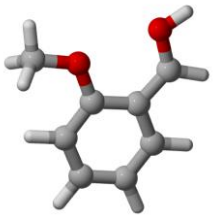
C	-0.0250540000	0.8054780000	-0.0000200000
C	0.3380830000	-0.5654140000	0.0000100000
C	-0.7627010000	-1.4760420000	0.0000420000
C	-2.0721440000	-1.0354750000	0.0000450000
C	-2.3684740000	0.3348440000	0.0000170000
C	-1.3203540000	1.2623750000	-0.0000170000
H	-0.5469280000	-2.5387200000	0.0000620000
H	-2.8777360000	-1.7605540000	0.0000690000
F	0.9907900000	1.7369340000	-0.0000550000
C	1.6569540000	-1.0520480000	0.0000210000
H	1.8563570000	-2.1147110000	0.0000490000
H	-3.3947660000	0.6793060000	0.0000200000
H	-1.5026340000	2.3301110000	-0.0000420000
O	2.7879350000	-0.3123710000	-0.0000270000
H	2.5672580000	0.6288290000	-0.0000330000

thermodynamic data

Zero-point correction= 0.111739 (Hartree/Particle)
Thermal correction to Energy= 0.119248
Thermal correction to Enthalpy= 0.120192
Thermal correction to Gibbs Free Energy= 0.079247
Sum of electronic and zero-point Energies= -445.394660
Sum of electronic and thermal Energies= -445.387151
Sum of electronic and thermal Enthalpies= -445.386207
Sum of electronic and thermal Free Energies= -445.427152

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.829	29.496	86.176

(u)B3LYP/6-311+G**	

xyz-matrix

19
XYZ file generated by gabedit : coordinates in Angstrom

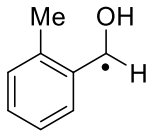
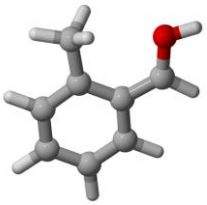
C	0.0912320000	-0.5040080000	0.0001940000
C	-0.0998260000	0.9203010000	-0.0000690000
C	-1.4485160000	1.3842250000	-0.0002090000
C	-2.5281870000	0.5212360000	-0.0001200000
C	-2.3131330000	-0.8592810000	0.0001330000
C	-1.0049580000	-1.3590980000	0.0003050000
H	-1.6175240000	2.4561560000	-0.0004290000
H	-3.5367740000	0.9181870000	-0.0002550000
C	0.9170770000	1.8877670000	-0.0003280000
H	0.6472540000	2.9381010000	0.0001010000
H	-3.1489610000	-1.5486700000	0.0002320000
H	-0.8534980000	-2.4300470000	0.0005990000
O	1.3821780000	-0.9345570000	0.0004280000
C	1.6408410000	-2.3291710000	-0.0005090000
H	2.7253200000	-2.4274100000	-0.0010460000
H	1.2329080000	-2.8140150000	0.8935630000
H	1.2320810000	-2.8129410000	-0.8947770000
O	2.2488990000	1.6000500000	0.0002300000
H	2.7433930000	2.4248760000	0.0003770000

thermodynamic data

Zero-point correction= 0.151402 (Hartree/Particle)
Thermal correction to Energy= 0.161114
Thermal correction to Enthalpy= 0.162058
Thermal correction to Gibbs Free Energy= 0.116003
Sum of electronic and zero-point Energies= -460.633284
Sum of electronic and thermal Energies= -460.623573
Sum of electronic and thermal Enthalpies= -460.622629
Sum of electronic and thermal Free Energies= -460.668684

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.100	36.463	96.931

(u)B3LYP/6-311+G**	

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

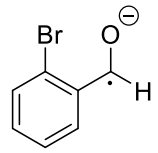
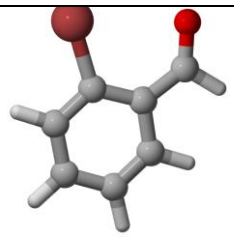
C	-0.0113090000	0.8534770000	0.0000030000
C	0.2915900000	-0.5515270000	0.0000230000
C	-0.8003850000	-1.4722380000	-0.0000380000
C	-2.1138440000	-1.0488300000	-0.0000490000
C	-2.4025330000	0.3203010000	-0.0000310000
C	-1.3491720000	1.2384020000	-0.0000130000
H	-0.5799690000	-2.5350470000	-0.0000660000
H	-2.9161730000	-1.7782820000	-0.0000840000
C	1.0585550000	1.9184710000	0.0000390000
C	1.5790580000	-1.1171730000	0.0001050000
H	1.7045790000	-2.1937430000	0.0000960000
H	-3.4286950000	0.6684830000	-0.0000410000
H	-1.5769210000	2.2998510000	-0.0000230000
H	0.5997910000	2.9094280000	-0.0001470000
H	1.7088220000	1.8417770000	-0.8751110000
H	1.7085150000	1.8419820000	0.8754470000
O	2.7227470000	-0.3684150000	-0.0001660000
H	3.4863170000	-0.9524150000	0.0010260000

thermodynamic data

Zero-point correction= 0.146845 (Hartree/Particle)
Thermal correction to Energy= 0.155443
Thermal correction to Enthalpy= 0.156387
Thermal correction to Gibbs Free Energy= 0.113295
Sum of electronic and zero-point Energies= -385.411813
Sum of electronic and thermal Energies= -385.403216
Sum of electronic and thermal Enthalpies= -385.402272
Sum of electronic and thermal Free Energies= -385.445363

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	97.542	33.060	90.694

(u)B3LYP/6-311+G**	

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

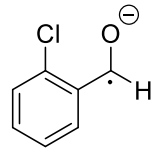
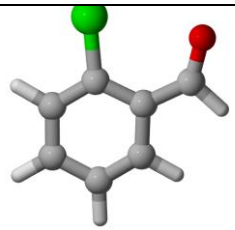
C	-0.2071400000	-0.3808780000	0.0000070000
C	-0.7855850000	0.9386570000	0.0001610000
C	-2.2251550000	0.9363660000	0.0001190000
C	-2.9882160000	-0.2070620000	-0.0000270000
C	-2.3731250000	-1.4825380000	-0.0001580000
C	-0.9693340000	-1.5336510000	-0.0001390000
H	-2.7139320000	1.9079860000	0.0002190000
H	-4.0723250000	-0.1272240000	-0.0000410000
Br	1.7187210000	-0.6419900000	-0.0000350000
C	-0.1169760000	2.2034560000	0.0003190000
H	-0.8402400000	3.0532060000	-0.0000460000
H	-2.9568330000	-2.3957470000	-0.0002690000
H	-0.4648330000	-2.4936450000	-0.0002450000
O	1.1107660000	2.4598710000	-0.0000110000

thermodynamic data

Zero-point correction= 0.095249 (Hartree/Particle)
Thermal correction to Energy= 0.103378
Thermal correction to Enthalpy= 0.104322
Thermal correction to Gibbs Free Energy= 0.060258
Sum of electronic and zero-point Energies= -2919.134325
Sum of electronic and thermal Energies= -2919.126197
Sum of electronic and thermal Enthalpies= -2919.125253
Sum of electronic and thermal Free Energies= -2919.169316

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	64.870	29.844	92.740

(u)B3LYP/6-311+G**	

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

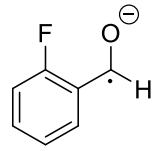
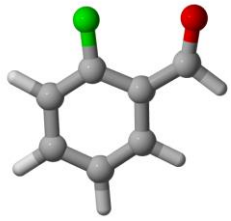
C	-0.0115990000	-0.6085630000	0.0001530000
C	-0.0223970000	0.8323220000	0.0003320000
C	1.2917420000	1.4196960000	0.0000990000
C	2.4563070000	0.6876170000	-0.0001980000
C	2.4168660000	-0.7276610000	-0.0003340000
C	1.1552840000	-1.3475740000	-0.0001490000
H	1.3416870000	2.5061040000	0.0002000000
H	3.4130370000	1.2037350000	-0.0003250000
Cl	-1.5342630000	-1.5331170000	0.0002730000
C	-1.1532310000	1.7095410000	0.0005790000
H	-0.8423040000	2.7811330000	-0.0010580000
H	3.3230640000	-1.3221870000	-0.0005730000
H	1.0825900000	-2.4301830000	-0.0002510000
O	-2.3791790000	1.4415150000	-0.0006910000

thermodynamic data

Zero-point correction= 0.095977 (Hartree/Particle)
Thermal correction to Energy= 0.103791
Thermal correction to Enthalpy= 0.104735
Thermal correction to Gibbs Free Energy= 0.062271
Sum of electronic and zero-point Energies= -805.212885
Sum of electronic and thermal Energies= -805.205070
Sum of electronic and thermal Enthalpies= -805.204126
Sum of electronic and thermal Free Energies= -805.246590

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.130	29.308	89.374

(u)B3LYP/6-311+G**	

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

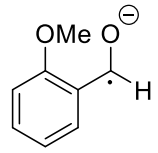
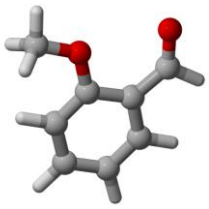
C	0.0265670000	0.8445390000	-0.0000650000
C	-0.4358160000	-0.5119060000	-0.0001850000
C	0.6317860000	-1.4789500000	-0.0001150000
C	1.9676660000	-1.1328890000	0.0000280000
C	2.3676940000	0.2206200000	0.0001270000
C	1.3508860000	1.2043650000	0.0000770000
H	0.3489270000	-2.5289640000	-0.0001940000
H	2.7205320000	-1.9176110000	0.0000570000
F	-0.8926820000	1.8607570000	-0.0000740000
C	-1.7961870000	-0.9494590000	-0.0003000000
H	-1.8739660000	-2.0637100000	0.0004040000
H	3.4134450000	0.5049830000	0.0002390000
H	1.5937060000	2.2627650000	0.0001490000
O	-2.8555100000	-0.2727740000	0.0003260000

thermodynamic data

Zero-point correction=	0.097131 (Hartree/Particle)
Thermal correction to Energy=	0.104583
Thermal correction to Enthalpy=	0.105527
Thermal correction to Gibbs Free Energy=	0.064461
Sum of electronic and zero-point Energies=	-444.855745
Sum of electronic and thermal Energies=	-444.848293
Sum of electronic and thermal Enthalpies=	-444.847348
Sum of electronic and thermal Free Energies=	-444.888415

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.627	28.528	86.431

(u)B3LYP/6-311+G**	

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

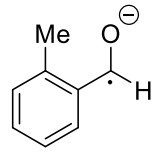
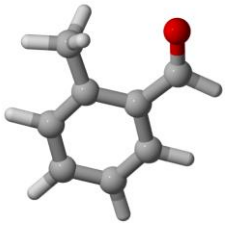
C	-0.1743130000	-0.4738720000	-0.0000440000
C	0.1287310000	0.9418750000	-0.0000420000
C	1.5317040000	1.2567630000	-0.0001110000
C	2.5262610000	0.2984990000	-0.0001600000
C	2.1994610000	-1.0699150000	-0.0001500000
C	0.8262590000	-1.4291390000	-0.0000930000
H	1.8022200000	2.3101620000	-0.0001150000
H	3.5689740000	0.6080930000	-0.0002050000
C	-0.8170780000	2.0149620000	0.0000300000
H	-0.3023960000	3.0079530000	0.0000200000
H	2.9652660000	-1.8375700000	-0.0001820000
H	0.5679170000	-2.4817100000	-0.0001020000
O	-1.5146500000	-0.7984830000	-0.0000070000
C	-1.8743670000	-2.1539950000	0.0003300000
H	-2.9660800000	-2.1765070000	0.0005130000
H	-1.5041150000	-2.6823940000	-0.8911190000
H	-1.5038080000	-2.6820130000	0.8918750000
O	-2.0738410000	2.0013490000	0.0001010000

thermodynamic data

Zero-point correction= 0.137260 (Hartree/Particle)
Thermal correction to Energy= 0.146476
Thermal correction to Enthalpy= 0.147421
Thermal correction to Gibbs Free Energy= 0.102204
Sum of electronic and zero-point Energies= -460.092580
Sum of electronic and thermal Energies= -460.083364
Sum of electronic and thermal Enthalpies= -460.082419
Sum of electronic and thermal Free Energies= -460.127636

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.915	34.773	95.166

(u)B3LYP/6-311+G**	

xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

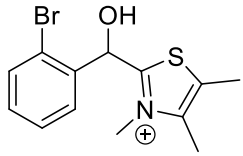
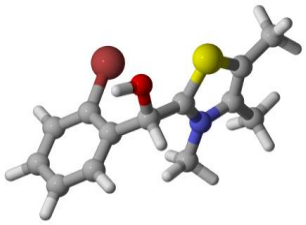
C	0.0324860000	0.8538390000	-0.0000520000
C	0.3553770000	-0.5615760000	-0.0000630000
C	-0.7586890000	-1.4679990000	-0.0000750000
C	-2.0700010000	-1.0425320000	-0.0000920000
C	-2.3741220000	0.3362900000	-0.0000900000
C	-1.2969520000	1.2465880000	-0.0000690000
H	-0.5416650000	-2.5342710000	-0.0000780000
H	-2.8732460000	-1.7764200000	-0.0001100000
C	1.1194790000	1.9013860000	0.0000150000
C	1.6775900000	-1.1026210000	-0.0000350000
H	1.6872400000	-2.2181660000	0.0003430000
H	-3.4002890000	0.6881890000	-0.0001080000
H	-1.5136450000	2.3143140000	-0.0000670000
H	0.6774070000	2.9052210000	-0.0000670000
H	1.7775680000	1.8022530000	-0.8685680000
H	1.7773750000	1.8023360000	0.8687610000
O	2.7872800000	-0.4954630000	0.0003330000

thermodynamic data

Zero-point correction= 0.132815 (Hartree/Particle)
Thermal correction to Energy= 0.140964
Thermal correction to Enthalpy= 0.141908
Thermal correction to Gibbs Free Energy= 0.099582
Sum of electronic and zero-point Energies= -384.876772
Sum of electronic and thermal Energies= -384.868623
Sum of electronic and thermal Enthalpies= -384.867679
Sum of electronic and thermal Free Energies= -384.910005

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	88.456	31.309	89.082

B3LYP/6-311+G**	

xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8840570000	0.5305270000	0.7423970000
N	-1.3199430000	1.1759060000	-0.3373860000
C	-2.6310200000	0.8460580000	-0.7256050000
C	-3.2035670000	-0.0491090000	0.1263060000
S	-2.0896820000	-0.4816610000	1.3969210000
C	-4.5676960000	-0.6668660000	0.0781090000
C	-3.2325050000	1.4619220000	-1.9484510000
C	0.4448330000	0.7039940000	1.4513550000
H	-3.3811610000	2.5394910000	-1.8316480000
H	-4.2041710000	1.0150660000	-2.1493430000
H	-2.6078140000	1.2981550000	-2.8302470000
H	-5.0021360000	-0.7427980000	1.0769110000
H	-4.5286770000	-1.6739580000	-0.3466310000
H	-5.2448160000	-0.0676410000	-0.5302040000
C	-0.5162470000	2.1420480000	-1.1098120000
H	0.3373640000	2.4645800000	-0.5237750000
H	-1.1352940000	3.0042570000	-1.3489050000
H	-0.1636800000	1.6722970000	-2.0286930000
C	1.7170890000	0.6165090000	0.6180070000
C	2.0361560000	-0.4119100000	-0.2819850000
C	3.2661800000	-0.4398650000	-0.9344620000
C	4.2060320000	0.5592460000	-0.6929440000
C	3.9178120000	1.5866830000	0.2004230000
C	2.6853910000	1.6070740000	0.8443010000
H	4.6455870000	2.3637390000	0.3988640000
H	2.4648600000	2.4066920000	1.5448880000
Br	0.8170020000	-1.8391060000	-0.6744230000
H	0.4222980000	1.7155980000	1.8846890000
H	5.1613460000	0.5263720000	-1.2029290000
H	3.4879670000	-1.2434350000	-1.6246580000
O	0.3944560000	-0.2582420000	2.4958180000
H	1.2417080000	-0.2863910000	2.9550840000

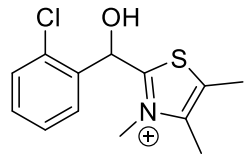
thermodynamic data

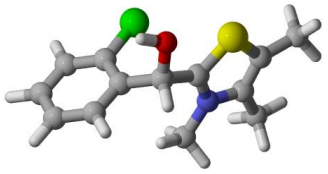
Zero-point correction= 0.253943 (Hartree/Particle)
Thermal correction to Energy= 0.271932

Thermal correction to Enthalpy= 0.272876
Thermal correction to Gibbs Free Energy= 0.206298
Sum of electronic and zero-point Energies= -3606.437577
Sum of electronic and thermal Energies= -3606.419588
Sum of electronic and thermal Enthalpies= -3606.418644
Sum of electronic and thermal Free Energies= -3606.485222

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.640	65.548	140.124

B3LYP/6-311+G**	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7541840000	-0.2372870000	-0.7076960000
N	1.1944590000	0.9881640000	-0.4316170000
C	2.5167580000	1.0409120000	0.0448270000
C	3.0896670000	-0.1938680000	0.0910800000
S	1.9630540000	-1.4108430000	-0.4512160000
C	4.4631750000	-0.5878300000	0.5413510000
C	3.1264520000	2.3515020000	0.4283360000
C	-0.5921010000	-0.6250080000	-1.2862500000
H	3.2250290000	3.0220980000	-0.4302380000
H	4.1217080000	2.1924680000	0.8385050000
H	2.5349240000	2.8625240000	1.1925660000
H	4.8851560000	-1.3587080000	-0.1066000000
H	4.4444280000	-0.9821390000	1.5613110000
H	5.1396630000	0.2662650000	0.5202340000
C	0.3894670000	2.2150410000	-0.5825530000
H	-0.5198520000	1.9947080000	-1.1307550000
H	0.9713420000	2.9556220000	-1.1283500000
H	0.1269740000	2.6031440000	0.4020990000
C	-1.8381030000	-0.1341480000	-0.5617450000
C	-2.0653160000	-0.2450000000	0.8182090000
C	-3.2717890000	0.1560960000	1.3843970000
C	-4.2807950000	0.6713590000	0.5750190000
C	-4.0842170000	0.7870200000	-0.7983640000
C	-2.8733900000	0.3861280000	-1.3527910000
H	-4.8667780000	1.1820240000	-1.4342030000
H	-2.7237600000	0.4718710000	-2.4246470000

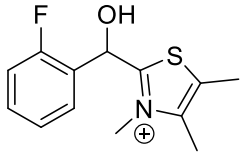
Cl	-0.8403910000	-0.8928650000	1.8986360000
H	-0.6235790000	-0.1926410000	-2.2979530000
H	-5.2185240000	0.9777300000	1.0227450000
H	-3.4162290000	0.0580490000	2.4526820000
O	-0.5218690000	-2.0411740000	-1.3809180000
H	-1.3929250000	-2.3980810000	-1.5890070000

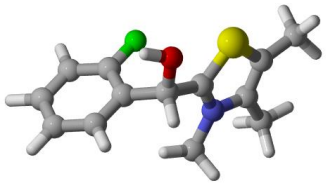
thermodynamic data

Zero-point correction= 0.254261 (Hartree/Particle)
Thermal correction to Energy= 0.271305
Thermal correction to Enthalpy= 0.272249
Thermal correction to Gibbs Free Energy= 0.208068
Sum of electronic and zero-point Energies= -1492.518754
Sum of electronic and thermal Energies= -1492.501710
Sum of electronic and thermal Enthalpies= -1492.500766
Sum of electronic and thermal Free Energies= -1492.564947

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.247	63.190	135.081

B3LYP/6-311+G**	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	0.6690530000	-0.2761940000	-0.6430470000
N	1.1762420000	0.9450120000	-0.4752400000
C	2.4762950000	0.9705630000	0.0634520000
C	2.9519920000	-0.2883070000	0.2952750000
S	1.7678860000	-1.4870060000	-0.1657670000
C	4.2708080000	-0.7182520000	0.8650880000
C	3.1561550000	2.2812420000	0.3131270000
C	-0.6812000000	-0.6380520000	-1.2301260000
H	3.2222430000	2.8870360000	-0.5975930000
H	4.1727170000	2.1133760000	0.6704970000
H	2.6339060000	2.8710660000	1.0757090000
H	4.7586230000	-1.4565500000	0.2201280000
H	4.1443550000	-1.1701020000	1.8553700000
H	4.9478580000	0.1322170000	0.9687670000
C	0.4705230000	2.1859090000	-0.8450410000

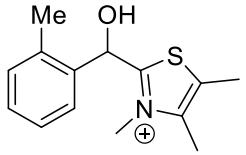
H	-0.5658150000	1.9597900000	-1.0838480000
H	0.9630240000	2.6419700000	-1.7075340000
H	0.4932500000	2.8774400000	-0.0013980000
C	-1.8796800000	-0.1577500000	-0.4292110000
C	-1.9709710000	-0.3327200000	0.9565160000
C	-3.0984120000	0.0236600000	1.6811460000
C	-4.1894700000	0.5669320000	0.9996210000
C	-4.1381160000	0.7512020000	-0.3839820000
C	-2.9913430000	0.3883140000	-1.0897360000
H	-4.9881420000	1.1708150000	-0.9119340000
H	-2.9549330000	0.5230770000	-2.1685370000
F	-0.9090910000	-0.8497540000	1.6151880000
H	-0.7392560000	-0.1721190000	-2.2277890000
H	-5.0797190000	0.8460940000	1.5545170000
H	-3.1108140000	-0.1312110000	2.7547480000
O	-0.6227050000	-2.0508110000	-1.3607630000
H	-1.5275060000	-2.4008840000	-1.3912190000

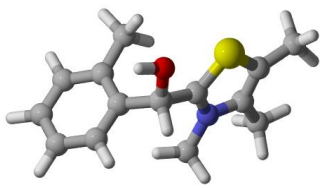
thermodynamic data

Zero-point correction= 0.255782 (Hartree/Particle)
Thermal correction to Energy= 0.273274
Thermal correction to Enthalpy= 0.274218
Thermal correction to Gibbs Free Energy= 0.209245
Sum of electronic and zero-point Energies= -1132.166358
Sum of electronic and thermal Energies= -1132.148866
Sum of electronic and thermal Enthalpies= -1132.147921
Sum of electronic and thermal Free Energies= -1132.212894

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.482	64.284	136.746

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	0.6972030000	-0.2755190000	-0.5804580000
N	1.1449150000	0.9556450000	-0.3381840000
C	2.4759620000	1.0180180000	0.1152140000
C	3.0415880000	-0.2176020000	0.2053240000

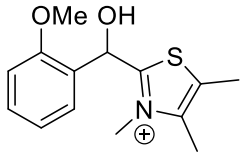
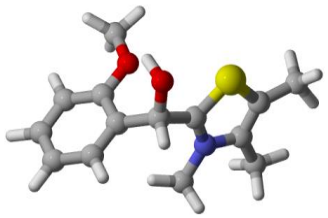
S	1.9022960000	-1.4459520000	-0.2860130000
C	4.4145850000	-0.6066120000	0.6605240000
C	3.0983010000	2.3386980000	0.4390170000
C	-0.6505860000	-0.6714850000	-1.1514260000
H	3.0505120000	3.0290290000	-0.4070700000
H	4.1472050000	2.2032950000	0.6950740000
H	2.6117660000	2.8159430000	1.2947800000
H	4.8481380000	-1.3651420000	0.0054190000
H	4.3921880000	-1.0141350000	1.6751520000
H	5.0835430000	0.2535440000	0.6582430000
C	0.3629900000	2.1845820000	-0.5804440000
H	-0.6843060000	1.9317320000	-0.7065980000
H	0.7397600000	2.6812920000	-1.4757380000
H	0.4643100000	2.8474200000	0.2765450000
C	-1.8900440000	-0.1923430000	-0.4040110000
C	-2.1252620000	-0.4525880000	0.9637090000
C	-3.3333130000	-0.0087700000	1.5115650000
C	-4.2881210000	0.6623620000	0.7507390000
C	-4.0563580000	0.9011960000	-0.5997630000
C	-2.8614260000	0.4701920000	-1.1672950000
H	-4.7962870000	1.4080010000	-1.2071520000
H	-2.6817350000	0.6458060000	-2.2238920000
H	-0.6878010000	-0.2317840000	-2.1595050000
H	-5.2135840000	0.9864250000	1.2120060000
H	-3.5322260000	-0.2039270000	2.5596140000
C	-1.1461870000	-1.1906340000	1.8477120000
H	-1.6157860000	-1.4501670000	2.7970370000
H	-0.2681260000	-0.5797190000	2.0841650000
H	-0.7951590000	-2.1138850000	1.3838820000
O	-0.5652590000	-2.0892380000	-1.2589410000
H	-1.4274780000	-2.4410750000	-1.5093740000

thermodynamic data

Zero-point correction= 0.291774 (Hartree/Particle)
Thermal correction to Energy= 0.309864
Thermal correction to Enthalpy= 0.310808
Thermal correction to Gibbs Free Energy= 0.245178
Sum of electronic and zero-point Energies= -1072.188506
Sum of electronic and thermal Energies= -1072.170415
Sum of electronic and thermal Enthalpies= -1072.169471
Sum of electronic and thermal Free Energies= -1072.235102

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	194.443	67.207	138.131

B3LYP/6-311+G**	

xyz-matrix

36
XYZ file generated by gabedit : coordinates in Angstrom

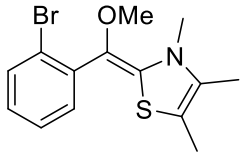
C	-0.8008650000	0.0950610000	0.7189490000
N	-1.2713730000	1.1087150000	-0.0058060000
C	-2.5816430000	0.9274650000	-0.4920860000
C	-3.1083520000	-0.2656690000	-0.1031690000
S	-1.9600870000	-1.1457700000	0.8766260000
C	-4.4497960000	-0.8606160000	-0.4026060000
C	-3.2220620000	1.9863710000	-1.3321970000
C	0.5240870000	-0.0186160000	1.4755090000
H	-3.2488230000	2.9511620000	-0.8190360000
H	-4.2482630000	1.7084230000	-1.5636880000
H	-2.6968610000	2.1220720000	-2.2821230000
H	-4.9322270000	-1.2240960000	0.5075830000
H	-4.3622090000	-1.7033530000	-1.0938650000
H	-5.1111220000	-0.1229320000	-0.8558520000
C	-0.5411540000	2.3675400000	-0.2502630000
H	0.4950960000	2.2510200000	0.0462230000
H	-1.0062560000	3.1720550000	0.3209270000
H	-0.5791100000	2.6035400000	-1.3121510000
C	1.7771950000	0.2414290000	0.6613860000
C	2.1006680000	-0.5707420000	-0.4426550000
C	3.2714800000	-0.3410630000	-1.1642500000
C	4.1316150000	0.6865170000	-0.7755010000
C	3.8415750000	1.4776290000	0.3312420000
C	2.6683680000	1.2447200000	1.0452400000
H	4.5231990000	2.2588010000	0.6429260000
H	2.4437710000	1.8472860000	1.9196720000
H	0.4829410000	0.7274420000	2.2770020000
H	5.0414670000	0.8536080000	-1.3396980000
H	3.5274550000	-0.9586370000	-2.0140890000
O	1.2130590000	-1.5787380000	-0.7063710000
C	1.4794730000	-2.4731450000	-1.7966230000
H	0.6560130000	-3.1839110000	-1.8022990000
H	1.5054100000	-1.9328850000	-2.7463500000
H	2.4211880000	-3.0057240000	-1.6425110000
O	0.5221470000	-1.2770310000	2.1306590000
H	0.9241460000	-1.9277020000	1.5397960000

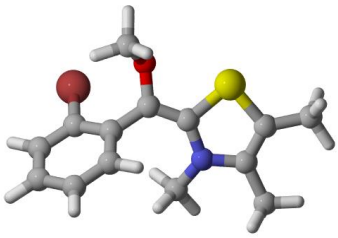
thermodynamic data

Zero-point correction= 0.297091 (Hartree/Particle)
Thermal correction to Energy= 0.315968
Thermal correction to Enthalpy= 0.316912
Thermal correction to Gibbs Free Energy= 0.249213
Sum of electronic and zero-point Energies= -1147.418590
Sum of electronic and thermal Energies= -1147.399714
Sum of electronic and thermal Enthalpies= -1147.398770
Sum of electronic and thermal Free Energies= -1147.466468

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	198.273	70.161	142.484

B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2561550000	-0.2081840000	-0.1988580000
N	1.8502110000	0.9016460000	0.4000140000
C	3.2585020000	0.8171950000	0.4870770000
C	3.7710920000	-0.3475430000	0.0456730000
S	2.4901240000	-1.4502080000	-0.5102630000
C	5.1922820000	-0.8061730000	-0.0336760000
C	4.0276750000	1.9888530000	1.0188750000
C	-0.0492400000	-0.4485010000	-0.4982230000
H	3.7284270000	2.9173560000	0.5228860000
H	5.0942030000	1.8496500000	0.8485310000
H	3.8853390000	2.1276210000	2.0957880000
H	5.4949060000	-1.0082110000	-1.0668640000
H	5.3387050000	-1.7315020000	0.5340760000
H	5.8749510000	-0.0595980000	0.3745160000
C	1.0693490000	1.8320410000	1.2089830000
H	0.2702010000	1.2870290000	1.7169040000
H	0.6120080000	2.6229490000	0.6082920000
H	1.7089850000	2.2887110000	1.9611430000
C	-1.1487240000	0.5299100000	-0.5475200000
C	-2.4059680000	0.3354580000	0.0596190000
C	-3.4406490000	1.2567270000	-0.0763670000

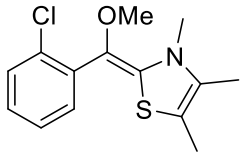
C	-3.2458140000	2.4207570000	-0.8165860000
C	-2.0115810000	2.6525580000	-1.4207580000
C	-0.9930880000	1.7153960000	-1.2947730000
Br	-2.7328440000	-1.1823300000	1.1899110000
H	-4.3890580000	1.0690930000	0.4107400000
H	-1.8497780000	3.5492280000	-2.0083690000
H	-0.0485690000	1.8738120000	-1.8032020000
H	-4.0546020000	3.1352340000	-0.9168070000
O	-0.3270290000	-1.7708380000	-0.8380660000
C	-0.8318820000	-1.9670800000	-2.1609790000
H	-0.9501110000	-3.0435980000	-2.2843680000
H	-1.8034020000	-1.4804720000	-2.2964570000
H	-0.1285490000	-1.5857150000	-2.9099810000

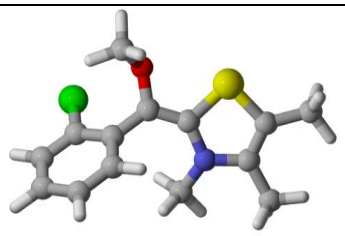
thermodynamic data

Zero-point correction= 0.268243 (Hartree/Particle)
Thermal correction to Energy= 0.287590
Thermal correction to Enthalpy= 0.288534
Thermal correction to Gibbs Free Energy= 0.219284
Sum of electronic and zero-point Energies= -3645.319868
Sum of electronic and thermal Energies= -3645.300521
Sum of electronic and thermal Enthalpies= -3645.299577
Sum of electronic and thermal Free Energies= -3645.368827

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.466	70.273	145.749

B3LYP/6-311+G**





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9464950000	-0.2981130000	-0.0575510000
N	1.4774420000	0.9473930000	0.2754110000
C	2.8899100000	0.9910980000	0.2444080000
C	3.4742210000	-0.1921540000	-0.0251560000
S	2.2638820000	-1.4768470000	-0.2512170000
C	4.9219690000	-0.5445500000	-0.1523970000
C	3.5831960000	2.2982230000	0.4856410000
C	-0.3508240000	-0.6877060000	-0.1876540000

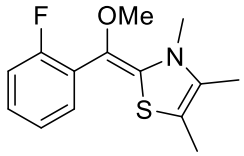
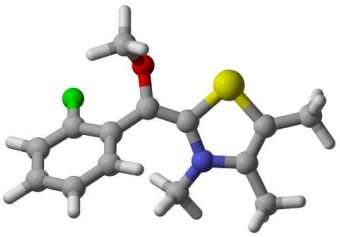
H	3.1569450000	3.0928560000	-0.1343960000
H	4.6412830000	2.2165810000	0.2412860000
H	3.5141910000	2.6200120000	1.5300970000
H	5.1619620000	-0.9132970000	-1.1555320000
H	5.1982910000	-1.3320750000	0.5572010000
H	5.5607450000	0.3166480000	0.0485410000
C	0.6798560000	1.9417670000	0.9863550000
H	-0.0252860000	1.4326030000	1.6474850000
H	0.1077910000	2.5797110000	0.3072340000
H	1.3309880000	2.5695540000	1.5909610000
C	-1.5303860000	0.1831130000	-0.3203060000
C	-2.7206520000	0.0074090000	0.4139090000
C	-3.8390150000	0.8097030000	0.2079270000
C	-3.7993480000	1.8327040000	-0.7360890000
C	-2.6347540000	2.0435740000	-1.4725920000
C	-1.5311060000	1.2231490000	-1.2716150000
Cl	-2.8174230000	-1.2070590000	1.6832510000
H	-4.7290070000	0.6384740000	0.8004150000
H	-2.5937610000	2.8301440000	-2.2175820000
H	-0.6415520000	1.3576790000	-1.8766900000
H	-4.6725420000	2.4556270000	-0.8909600000
O	-0.5326040000	-2.0676140000	-0.2419860000
C	-1.1641650000	-2.5580410000	-1.4260270000
H	-1.1752860000	-3.6442440000	-1.3360980000
H	-2.1931750000	-2.1939520000	-1.5121800000
H	-0.6011540000	-2.2686640000	-2.3206720000

thermodynamic data

Zero-point correction= 0.268902 (Hartree/Particle)
Thermal correction to Energy= 0.287991
Thermal correction to Enthalpy= 0.288936
Thermal correction to Gibbs Free Energy= 0.220870
Sum of electronic and zero-point Energies= -1531.400156
Sum of electronic and thermal Energies= -1531.381066
Sum of electronic and thermal Enthalpies= -1531.380122
Sum of electronic and thermal Free Energies= -1531.448188

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.717	69.818	143.256

B3LYP/6-311+G**	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

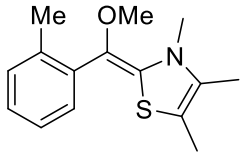
C	-0.8056600000	0.3260780000	0.0488580000
N	-1.3071660000	-0.9639190000	0.2188310000
C	-2.7137780000	-1.0470040000	0.1033130000
C	-3.3256360000	0.1404110000	-0.0692990000
S	-2.1533660000	1.4787770000	-0.0849450000
C	-4.7765930000	0.4602020000	-0.2394240000
C	-3.3702460000	-2.3936970000	0.1585460000
C	0.4811300000	0.7701310000	0.0279000000
H	-2.8793030000	-3.1010550000	-0.5168660000
H	-4.4147900000	-2.3184290000	-0.1402090000
H	-3.3498170000	-2.8273710000	1.1639410000
H	-4.9758290000	0.9329940000	-1.2071680000
H	-5.1192430000	1.1532910000	0.5366680000
H	-5.3928370000	-0.4374540000	-0.1728690000
C	-0.5166090000	-1.9994620000	0.8768070000
H	0.1380570000	-1.5361920000	1.6184380000
H	0.1099850000	-2.5558350000	0.1740920000
H	-1.1778320000	-2.6976870000	1.3858490000
C	1.7007440000	-0.0333400000	-0.1296230000
C	2.8527030000	0.1877430000	0.6417540000
C	4.0300000000	-0.5208170000	0.4715450000
C	4.0935720000	-1.5122130000	-0.5069120000
C	2.9752670000	-1.7677470000	-1.2994850000
C	1.8088160000	-1.0310140000	-1.1183900000
F	2.8179090000	1.1198090000	1.6242050000
H	4.8736990000	-0.2977280000	1.1134800000
H	3.0181130000	-2.5252530000	-2.0737280000
H	0.9565160000	-1.2017770000	-1.7661580000
H	5.0098810000	-2.0731030000	-0.6479370000
O	0.6089750000	2.1520870000	0.1467910000
C	1.2745560000	2.8050950000	-0.9353170000
H	0.7631980000	2.6127370000	-1.8854600000
H	1.2424320000	3.8713810000	-0.7117170000
H	2.3192150000	2.4873010000	-1.0168630000

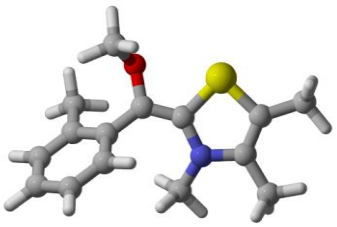
thermodynamic data

Zero-point correction= 0.270206 (Hartree/Particle)
Thermal correction to Energy= 0.289014
Thermal correction to Enthalpy= 0.289958
Thermal correction to Gibbs Free Energy= 0.222702
Sum of electronic and zero-point Energies= -1171.045902
Sum of electronic and thermal Energies= -1171.027094
Sum of electronic and thermal Enthalpies= -1171.026150
Sum of electronic and thermal Free Energies= -1171.093406

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	181.359	68.954	141.552

B3LYP/6-311+G**	





xyz-matrix

37
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7942410000	0.3158560000	0.0332980000
N	-1.2972540000	-0.9743410000	0.2102750000
C	-2.7053240000	-1.0547090000	0.1231960000
C	-3.3196810000	0.1319130000	-0.0453740000
S	-2.1456190000	1.4690010000	-0.0903040000
C	-4.7725990000	0.4534230000	-0.1932990000
C	-3.3646590000	-2.3991470000	0.1968640000
C	0.4915140000	0.7563930000	-0.0068400000
H	-2.8944230000	-3.1090370000	-0.4905950000
H	-4.4164130000	-2.3201840000	-0.0742500000
H	-3.3192670000	-2.8317780000	1.2019580000
H	-4.9865390000	0.9232020000	-1.1595290000
H	-5.1025950000	1.1497660000	0.5855350000
H	-5.3893300000	-0.4429560000	-0.1143260000
C	-0.4892190000	-2.0193410000	0.8299710000
H	0.1501280000	-1.5777130000	1.5984150000
H	0.1559780000	-2.5278630000	0.1089970000
H	-1.1393820000	-2.7541850000	1.2996430000
C	1.7279180000	-0.0364160000	-0.1463820000
C	2.8454530000	0.1789830000	0.6988630000
C	4.0054110000	-0.5689790000	0.4800540000

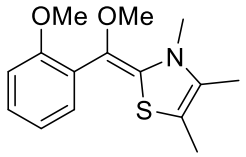
C	4.0906720000	-1.5172220000	-0.5386220000
C	2.9938940000	-1.7299070000	-1.3697850000
C	1.8328820000	-0.9875830000	-1.1762330000
H	4.8572890000	-0.4143450000	1.1351470000
H	3.0464570000	-2.4550180000	-2.1745810000
H	0.9895910000	-1.1227100000	-1.8449260000
H	5.0055390000	-2.0819300000	-0.6796280000
C	2.7924320000	1.1607540000	1.8434690000
H	3.6163160000	0.9857540000	2.5387530000
H	1.8486730000	1.0787570000	2.3894710000
H	2.8528730000	2.1951380000	1.4947400000
O	0.6209210000	2.1478690000	0.0644450000
C	1.1925470000	2.7574590000	-1.0957470000
H	1.1931090000	3.8317360000	-0.9085370000
H	2.2198380000	2.4162030000	-1.2621290000
H	0.5934810000	2.5417150000	-1.9873940000

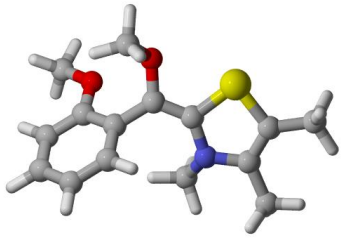
thermodynamic data

Zero-point correction= 0.305920 (Hartree/Particle)
Thermal correction to Energy= 0.325495
Thermal correction to Enthalpy= 0.326439
Thermal correction to Gibbs Free Energy= 0.257938
Sum of electronic and zero-point Energies= -1111.069813
Sum of electronic and thermal Energies= -1111.050238
Sum of electronic and thermal Enthalpies= -1111.049293
Sum of electronic and thermal Free Energies= -1111.117795

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	204.251	71.965	144.173

B3LYP/6-311+G**	





xyz-matrix

38
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9889130000	-0.3114780000	-0.0620250000
N	1.5151010000	0.9578060000	0.2476850000
C	2.9349230000	0.9640570000	0.2690550000

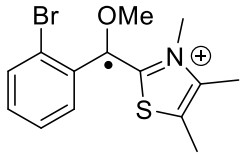
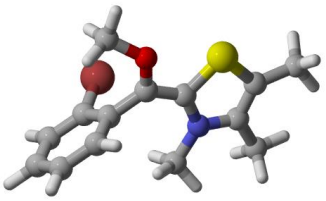
C	3.5117460000	-0.2315630000	0.0542920000
S	2.2987060000	-1.5187670000	-0.1678150000
C	4.9580720000	-0.5979670000	-0.0491070000
C	3.6386090000	2.2717130000	0.4785040000
C	-0.2972730000	-0.6882850000	-0.2583150000
H	3.2572600000	3.0341340000	-0.2086380000
H	4.7073670000	2.1646510000	0.2982060000
H	3.5146930000	2.6524750000	1.4974710000
H	5.2123200000	-0.9606710000	-1.0511640000
H	5.2088430000	-1.3971980000	0.6568710000
H	5.6037320000	0.2526660000	0.1736210000
C	0.8019920000	1.8073410000	1.2079180000
H	0.8534690000	1.3919770000	2.2232160000
H	-0.2409200000	1.9050440000	0.9204830000
H	1.2416520000	2.8036440000	1.2073490000
C	-1.4653510000	0.2006800000	-0.4168830000
C	-2.6535130000	0.0198040000	0.3340670000
C	-3.7547490000	0.8553190000	0.1249920000
C	-3.6889160000	1.8847200000	-0.8149340000
C	-2.5278200000	2.0863910000	-1.5536600000
C	-1.4385340000	1.2405030000	-1.3549870000
H	-4.6620000000	0.7194160000	0.6981810000
H	-2.4735380000	2.8809190000	-2.2886550000
H	-0.5349720000	1.3753400000	-1.9389080000
H	-4.5517310000	2.5246240000	-0.9624100000
O	-2.6317510000	-0.9782080000	1.2585790000
C	-3.7884260000	-1.2149080000	2.0470000000
H	-3.5345760000	-2.0500580000	2.6977770000
H	-4.0440270000	-0.3427330000	2.6592390000
H	-4.6488040000	-1.4881960000	1.4261070000
O	-0.4903550000	-2.0649000000	-0.3289930000
C	-1.1278770000	-2.5359920000	-1.5146260000
H	-0.5550700000	-2.2594540000	-2.4075360000
H	-1.1655340000	-3.6220730000	-1.4280100000
H	-2.1470720000	-2.1460220000	-1.6063910000

thermodynamic data

Zero-point correction= 0.310641 (Hartree/Particle)
Thermal correction to Energy= 0.331298
Thermal correction to Enthalpy= 0.332243
Thermal correction to Gibbs Free Energy= 0.260150
Sum of electronic and zero-point Energies= -1186.291008
Sum of electronic and thermal Energies= -1186.270351
Sum of electronic and thermal Enthalpies= -1186.269407
Sum of electronic and thermal Free Energies= -1186.341499

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	207.893	75.177	151.731

(u)B3LYP/6-311+G**	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.0712860000	0.5622410000	0.3186980000
N	1.4929990000	-0.6439200000	0.8124020000
C	2.8520820000	-0.8925900000	0.6272110000
C	3.5113130000	0.1441950000	0.0258100000
S	2.4177640000	1.4516560000	-0.3407720000
C	4.9593380000	0.2758400000	-0.3269370000
C	3.4529730000	-2.1888900000	1.0727800000
C	-0.2097660000	1.1224310000	0.2671990000
H	2.9215840000	-3.0440070000	0.6476690000
H	3.4436810000	-2.2880890000	2.1624070000
H	4.4891550000	-2.2523310000	0.7483330000
H	5.3927610000	1.1710590000	0.1271210000
H	5.0961910000	0.3539600000	-1.4092410000
H	5.5311390000	-0.5823690000	0.0228660000
C	0.6102550000	-1.6072050000	1.4899160000
H	0.0740950000	-2.2121170000	0.7573580000
H	-0.1006940000	-1.0749910000	2.1150700000
H	1.2132600000	-2.2530750000	2.1204780000
C	-1.4947950000	0.4853740000	0.6376140000
C	-2.1312040000	-0.4662350000	-0.1729500000
C	-3.3559760000	-1.0183180000	0.1925580000
C	-3.9652600000	-0.6145200000	1.3780660000
C	-3.3594090000	0.3420730000	2.1920960000
C	-2.1377360000	0.8901070000	1.8201990000
Br	-1.3433180000	-1.0119690000	-1.8329740000
H	-4.9189360000	-1.0454250000	1.6587770000
H	-3.8363710000	0.6594160000	3.1112440000
H	-1.6599020000	1.6314190000	2.4514490000
H	-3.8317610000	-1.7485410000	-0.4491110000
O	-0.1883990000	2.4072680000	-0.1301800000
C	-1.3812950000	3.0452580000	-0.6493120000
H	-1.0465970000	4.0241340000	-0.9820950000
H	-1.7762310000	2.4735000000	-1.4898490000
H	-2.1341020000	3.1506110000	0.1308860000

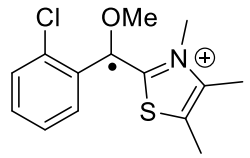
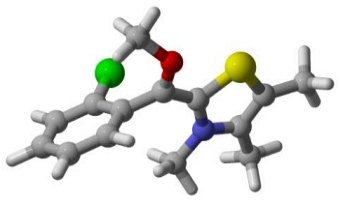
thermodynamic data

Zero-point correction= 0.269527 (Hartree/Particle)

Thermal correction to Energy= 0.288094
Thermal correction to Enthalpy= 0.289038
Thermal correction to Gibbs Free Energy= 0.220294
Sum of electronic and zero-point Energies= -3645.110531
Sum of electronic and thermal Energies= -3645.091964
Sum of electronic and thermal Enthalpies= -3645.091020
Sum of electronic and thermal Free Energies= -3645.159764

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.782	67.905	144.685

(u)B3LYP/6-311+G**	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8707050000	0.4364020000	-0.2675110000
N	-1.3051910000	-0.8432280000	-0.4861810000
C	-2.6785640000	-1.0160990000	-0.3219840000
C	-3.3345500000	0.1464800000	-0.0230540000
S	-2.2202120000	1.4835080000	0.0790450000
C	-4.7946860000	0.3862580000	0.1976980000
C	-3.2926800000	-2.3713980000	-0.4820740000
C	0.4246760000	0.9666960000	-0.2730790000
H	-2.7909530000	-3.1146860000	0.1423110000
H	-3.2528070000	-2.7151670000	-1.5201640000
H	-4.3393850000	-2.3461170000	-0.1873970000
H	-5.1940320000	1.0804220000	-0.5471850000
H	-4.9792030000	0.8176090000	1.1852500000
H	-5.3623490000	-0.5402760000	0.1255840000
C	-0.4293160000	-1.9536550000	-0.8943500000
H	-0.0154700000	-2.4562580000	-0.0187330000
H	0.3782480000	-1.5722940000	-1.5113790000
H	-1.0094310000	-2.6617340000	-1.4790220000
C	1.7051580000	0.2313630000	-0.3431860000
C	2.1758050000	-0.5697620000	0.7087180000
C	3.4036850000	-1.2192380000	0.6254460000
C	4.1835030000	-1.0700310000	-0.5181260000
C	3.7434660000	-0.2691120000	-1.5721660000
C	2.5187660000	0.3797330000	-1.4804470000
Cl	1.2310810000	-0.7472150000	2.1787940000

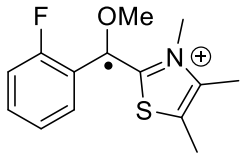
H	5.1392380000	-1.5765480000	-0.5796450000
H	4.3517870000	-0.1515590000	-2.4604500000
H	2.1688270000	0.9979830000	-2.2998060000
H	3.7458100000	-1.8253680000	1.4544540000
O	0.4240910000	2.3122910000	-0.2416140000
C	1.5762020000	3.0428640000	0.2487190000
H	1.2398780000	4.0741680000	0.3155840000
H	1.8646000000	2.6728520000	1.2333610000
H	2.4093030000	2.9647620000	-0.4484350000

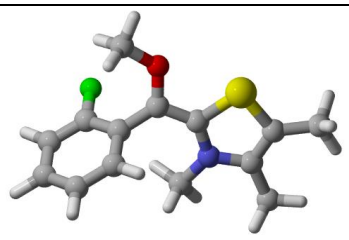
thermodynamic data

Zero-point correction= 0.270259 (Hartree/Particle)
Thermal correction to Energy= 0.289426
Thermal correction to Enthalpy= 0.290370
Thermal correction to Gibbs Free Energy= 0.220115
Sum of electronic and zero-point Energies= -1531.190457
Sum of electronic and thermal Energies= -1531.171289
Sum of electronic and thermal Enthalpies= -1531.170345
Sum of electronic and thermal Free Energies= -1531.240600

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	181.617	69.425	147.864

(u)B3LYP/6-311+G**	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8437400000	0.3572060000	0.0003410000
N	-1.3124880000	-0.9044850000	0.2551340000
C	-2.6991230000	-1.0269230000	0.1647460000
C	-3.3263850000	0.1570650000	-0.1071280000
S	-2.1708870000	1.4538470000	-0.2727420000
C	-4.7859950000	0.4463400000	-0.2640680000
C	-3.3545640000	-2.3565680000	0.3722070000
C	0.4750730000	0.8314040000	-0.0526080000
H	-3.2954530000	-2.6804290000	1.4158300000
H	-2.8979020000	-3.1298930000	-0.2501890000
H	-4.4080630000	-2.3006480000	0.1069980000
H	-5.0241810000	0.7326310000	-1.2925760000

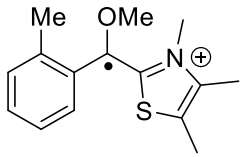
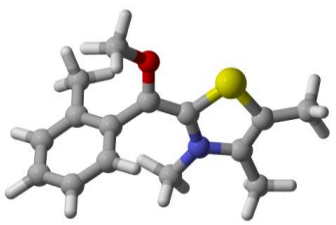
H	-5.0935820000	1.2680970000	0.3878980000
H	-5.3903110000	-0.4225430000	-0.0071920000
C	-0.4633490000	-2.0188290000	0.7081990000
H	-1.0584310000	-2.6815340000	1.3299530000
H	0.3579430000	-1.6283750000	1.3023660000
H	-0.0630290000	-2.5758410000	-0.1398920000
C	1.6852560000	0.0064490000	-0.2153710000
C	2.7232830000	0.0370290000	0.7226880000
C	3.8826960000	-0.7038400000	0.5805360000
C	4.0265550000	-1.5069500000	-0.5493340000
C	3.0166140000	-1.5616280000	-1.5113090000
C	1.8569450000	-0.8132250000	-1.3450970000
F	2.5667560000	0.8021480000	1.8250110000
H	4.9311210000	-2.0890900000	-0.6771020000
H	3.1389520000	-2.1776530000	-2.3934670000
H	1.0813400000	-0.8364160000	-2.1023010000
H	4.6473240000	-0.6483410000	1.3452690000
O	0.5333810000	2.1709570000	-0.0241170000
C	1.7385670000	2.8880180000	-0.3833690000
H	2.1743500000	2.4752630000	-1.2935440000
H	1.4130190000	3.9115290000	-0.5501060000
H	2.4496450000	2.8528080000	0.4412370000

thermodynamic data

Zero-point correction=	0.271785 (Hartree/Particle)
Thermal correction to Energy=	0.290533
Thermal correction to Enthalpy=	0.291477
Thermal correction to Gibbs Free Energy=	0.222504
Sum of electronic and zero-point Energies=	-1170.835408
Sum of electronic and thermal Energies=	-1170.816660
Sum of electronic and thermal Enthalpies=	-1170.815716
Sum of electronic and thermal Free Energies=	-1170.884689

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	182.312	68.497	145.167

(u)B3LYP/6-311+G**	

xyz-matrix

37
XYZ file generated by gabedit : coordinates in Angstrom

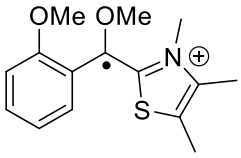
C	-0.8328310000	0.3452900000	-0.0085980000
N	-1.3004170000	-0.9268870000	0.2063080000
C	-2.6874330000	-1.0435000000	0.1398190000
C	-3.3195680000	0.1508780000	-0.0728150000
S	-2.1668510000	1.4521270000	-0.2150320000
C	-4.7818550000	0.4456550000	-0.1886130000
C	-3.3411340000	-2.3801430000	0.3032210000
C	0.4808380000	0.8228880000	-0.0750510000
H	-3.2458430000	-2.7567300000	1.3262240000
H	-2.9097630000	-3.1222160000	-0.3730730000
H	-4.4030420000	-2.3086050000	0.0787510000
H	-5.0395960000	0.7754320000	-1.1992700000
H	-5.0765490000	1.2391030000	0.5032410000
H	-5.3818750000	-0.4333770000	0.0423920000
C	-0.4426500000	-2.0758520000	0.5415460000
H	-1.0093080000	-2.7672950000	1.1588010000
H	0.4226730000	-1.7329260000	1.0998810000
H	-0.1044950000	-2.5843840000	-0.3625700000
C	1.7128350000	0.0165200000	-0.2033500000
C	2.6857820000	-0.0010140000	0.8208160000
C	3.8401620000	-0.7618050000	0.6088800000
C	4.0424160000	-1.4711940000	-0.5721890000
C	3.0782910000	-1.4455640000	-1.5785650000
C	1.9164010000	-0.7072240000	-1.3902210000
C	2.5071380000	0.7477350000	2.1206760000
H	4.9509950000	-2.0467710000	-0.7047260000
H	3.2322200000	-1.9911540000	-2.5016890000
H	1.1659020000	-0.6710420000	-2.1726350000
H	4.5917750000	-0.8012490000	1.3898230000
H	3.0192890000	0.2321480000	2.9346490000
H	1.4566580000	0.8593080000	2.3973670000
H	2.9344570000	1.7545620000	2.0643640000
O	0.5323500000	2.1682900000	-0.0503240000
C	1.6644840000	2.8712560000	-0.6168690000
H	1.4070270000	3.9237340000	-0.5317880000
H	2.5751200000	2.6607870000	-0.0584670000
H	1.7908400000	2.5949780000	-1.6644530000

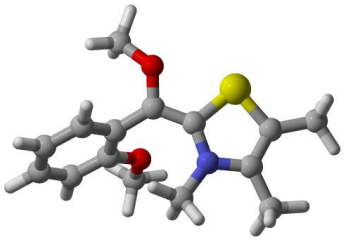
thermodynamic data

Zero-point correction= 0.307048 (Hartree/Particle)
Thermal correction to Energy= 0.326896
Thermal correction to Enthalpy= 0.327840
Thermal correction to Gibbs Free Energy= 0.255426
Sum of electronic and zero-point Energies= -1110.861759
Sum of electronic and thermal Energies= -1110.841912
Sum of electronic and thermal Enthalpies= -1110.840968
Sum of electronic and thermal Free Energies= -1110.913381

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	205.130	71.698	152.408

(u)B3LYP/6-311+G**	





xyz-matrix

38
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8848000000	0.5287990000	-0.2137750000
N	-1.3122910000	-0.6873810000	-0.6673770000
C	-2.6753780000	-0.9203360000	-0.4860220000
C	-3.3332670000	0.1432550000	0.0642830000
S	-2.2326250000	1.4603710000	0.3802880000
C	-4.7860570000	0.3013610000	0.3855210000
C	-3.2739080000	-2.2295490000	-0.8955760000
C	0.4054840000	1.0756530000	-0.1716270000
H	-2.7194590000	-3.0720520000	-0.4750180000
H	-3.2922740000	-2.3454840000	-1.9835670000
H	-4.3004280000	-2.3009700000	-0.5426080000
H	-5.2219880000	1.1340280000	-0.1736540000
H	-4.9370420000	0.5020050000	1.4497520000
H	-5.3462320000	-0.5973740000	0.1311770000
C	-0.4522220000	-1.6526110000	-1.3675550000
H	-0.0527160000	-2.3870930000	-0.6672800000
H	0.3685640000	-1.1250880000	-1.8431910000
H	-1.0363190000	-2.1561650000	-2.1338080000
C	1.6888810000	0.3800280000	-0.3282820000
C	2.0498870000	-0.6977420000	0.5159470000
C	3.3070950000	-1.2917200000	0.3799370000
C	4.1972240000	-0.8288050000	-0.5866230000
C	3.8552850000	0.2308330000	-1.4258240000
C	2.6120890000	0.8320760000	-1.2866100000
H	5.1670540000	-1.3031720000	-0.6799640000
H	4.5489240000	0.5812290000	-2.1795610000
H	2.3312720000	1.6511360000	-1.9394050000
H	3.6010880000	-2.1083180000	1.0247580000
O	1.1203640000	-1.0821210000	1.4294890000
C	1.4812500000	-2.0472240000	2.4268840000
H	0.6139870000	-2.1326690000	3.0777350000
H	1.6989150000	-3.0197810000	1.9768520000

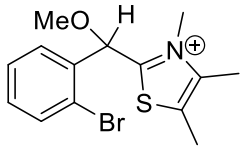
H	2.3417330000	-1.7044430000	3.0069180000
O	0.3738740000	2.4088660000	0.0379830000
C	1.4763280000	3.0813540000	0.6941210000
H	1.7932970000	2.5192480000	1.5733340000
H	2.3124640000	3.2154280000	0.0096160000
H	1.0759470000	4.0490680000	0.9863800000

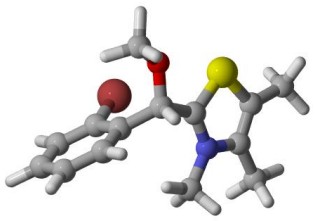
thermodynamic data

Zero-point correction= 0.312405 (Hartree/Particle)
Thermal correction to Energy= 0.332877
Thermal correction to Enthalpy= 0.333822
Thermal correction to Gibbs Free Energy= 0.261632
Sum of electronic and zero-point Energies= -1186.089876
Sum of electronic and thermal Energies= -1186.069403
Sum of electronic and thermal Enthalpies= -1186.068459
Sum of electronic and thermal Free Energies= -1186.140648

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	208.884	74.769	151.936

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9235190000	-0.4794700000	0.6464300000
N	-1.4145270000	0.6954700000	1.0343700000
C	-2.7502460000	0.9248550000	0.6553190000
C	-3.2794190000	-0.1369430000	-0.0128470000
S	-2.0964170000	-1.4095750000	-0.1706480000
C	-4.6473390000	-0.3032120000	-0.6007880000
C	-3.4143700000	2.2216850000	0.9926060000
C	0.4396970000	-1.0819100000	0.9363030000
H	-3.4663270000	2.3854360000	2.0726060000
H	-4.4323770000	2.2283670000	0.6083950000
H	-2.8896910000	3.0707610000	0.5460450000
H	-5.0276130000	-1.3134680000	-0.4365400000
H	-4.6361820000	-0.1218220000	-1.6792860000
H	-5.3536550000	0.3923380000	-0.1479150000
C	-0.6696360000	1.7046110000	1.8111990000

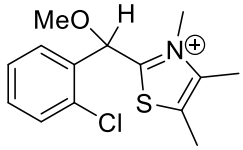
H	0.3133050000	1.3241110000	2.0634430000
H	-1.2216600000	1.9285630000	2.7233130000
H	-0.5584550000	2.6107390000	1.2159540000
C	1.6655070000	-0.2063490000	0.6955170000
C	1.9540710000	0.4636210000	-0.5025160000
C	3.1372800000	1.1811110000	-0.6595080000
C	4.0610020000	1.2369870000	0.3815170000
C	3.8024080000	0.5762680000	1.5786770000
C	2.6165480000	-0.1360430000	1.7241690000
H	4.5183810000	0.6085390000	2.3906310000
H	2.4210630000	-0.6577220000	2.6559060000
Br	0.7493210000	0.4453150000	-1.9952060000
H	0.4400580000	-1.3369140000	2.0091140000
H	4.9802510000	1.7948150000	0.2486940000
H	3.3350980000	1.6900150000	-1.5939600000
O	0.4390840000	-2.2743590000	0.1747170000
C	1.4033430000	-3.2572960000	0.5682330000
H	1.2327330000	-4.1161490000	-0.0773770000
H	2.4234060000	-2.8916890000	0.4252890000
H	1.2551790000	-3.5496520000	1.6140550000

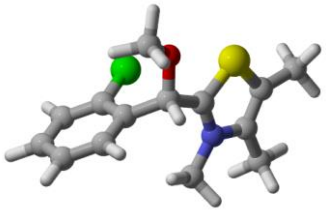
thermodynamic data

Zero-point correction= 0.281926 (Hartree/Particle)
Thermal correction to Energy= 0.301374
Thermal correction to Enthalpy= 0.302319
Thermal correction to Gibbs Free Energy= 0.231954
Sum of electronic and zero-point Energies= -3645.721433
Sum of electronic and thermal Energies= -3645.701984
Sum of electronic and thermal Enthalpies= -3645.701040
Sum of electronic and thermal Free Energies= -3645.771405

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.115	70.078	148.095

B3LYP/6-311+G**	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8087680000	0.3816070000	-0.5148280000

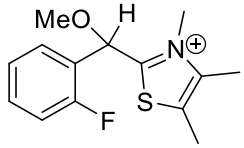
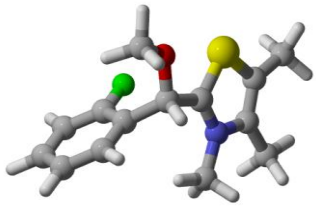
N	-1.2940230000	-0.8347470000	-0.7529660000
C	-2.6364900000	-1.0133380000	-0.3704740000
C	-3.1753740000	0.1278800000	0.1409240000
S	-1.9927550000	1.4110910000	0.1507360000
C	-4.5544120000	0.3706250000	0.6737290000
C	-3.2995300000	-2.3422940000	-0.5468190000
C	0.5736890000	0.9218880000	-0.8299310000
H	-3.4095560000	-2.6070740000	-1.6026040000
H	-4.2946840000	-2.3212310000	-0.1071460000
H	-2.7398550000	-3.1405690000	-0.0526160000
H	-4.9338820000	1.3446810000	0.3582270000
H	-4.5626420000	0.3473930000	1.7671350000
H	-5.2507180000	-0.3861560000	0.3131560000
C	-0.5210420000	-1.9387090000	-1.3539720000
H	0.3829560000	-1.5505720000	-1.8096760000
H	-1.1305570000	-2.4223020000	-2.1146780000
H	-0.2515680000	-2.6598900000	-0.5816020000
C	1.7625890000	0.0754460000	-0.3880010000
C	1.9477820000	-0.4111340000	0.9138290000
C	3.0950510000	-1.1161240000	1.2655940000
C	4.0870710000	-1.3431850000	0.3152640000
C	3.9317030000	-0.8664690000	-0.9835060000
C	2.7795160000	-0.1643480000	-1.3222150000
H	4.7026220000	-1.0332110000	-1.7256390000
H	2.6647150000	0.2149300000	-2.3328570000
Cl	0.7362230000	-0.1594570000	2.1624180000
H	0.6340030000	1.0081830000	-1.9277350000
H	4.9796080000	-1.8891280000	0.5964120000
H	3.2074500000	-1.4779330000	2.2796010000
O	0.5572650000	2.2165540000	-0.2587230000
C	1.5713790000	3.1112270000	-0.7295600000
H	1.3855130000	4.0598970000	-0.2305130000
H	2.5697800000	2.7517990000	-0.4675340000
H	1.4961720000	3.2468770000	-1.8144700000

thermodynamic data

Zero-point correction= 0.282589 (Hartree/Particle)
Thermal correction to Energy= 0.301744
Thermal correction to Enthalpy= 0.302688
Thermal correction to Gibbs Free Energy= 0.233728
Sum of electronic and zero-point Energies= -1531.802209
Sum of electronic and thermal Energies= -1531.783054
Sum of electronic and thermal Enthalpies= -1531.782109
Sum of electronic and thermal Free Energies= -1531.851070

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.347	69.629	145.140

B3LYP/6-311+G**	

xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

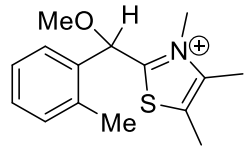
C	-0.7384510000	0.3917160000	-0.4380270000
N	-1.2731800000	-0.7910750000	-0.7328980000
C	-2.6017440000	-0.9562230000	-0.3004320000
C	-3.0722190000	0.1558010000	0.3292750000
S	-1.8465070000	1.3977410000	0.3735780000
C	-4.4109950000	0.3966890000	0.9567700000
C	-3.3168450000	-2.2458290000	-0.5479450000
C	0.6540890000	0.8886330000	-0.7717600000
H	-3.3654520000	-2.4875890000	-1.6130620000
H	-4.3378280000	-2.1821310000	-0.1768930000
H	-2.8327050000	-3.0802150000	-0.0323530000
H	-4.7613290000	1.4126180000	0.7638400000
H	-4.3662340000	0.2586970000	2.0408080000
H	-5.1572590000	-0.2905900000	0.5584780000
C	-0.5800300000	-1.8517500000	-1.4881770000
H	0.4485610000	-1.5604220000	-1.6705470000
H	-1.0931410000	-2.0121310000	-2.4366480000
H	-0.5869930000	-2.7724910000	-0.9063120000
C	1.7918020000	0.0291030000	-0.2382720000
C	1.8243930000	-0.4374960000	1.0765290000
C	2.8903810000	-1.1522340000	1.5935640000
C	3.9813630000	-1.4163440000	0.7672810000
C	3.9880120000	-0.9687980000	-0.5527730000
C	2.9011260000	-0.2518580000	-1.0458760000
H	4.8371040000	-1.1716840000	-1.1933910000
H	2.9122150000	0.1019130000	-2.0719900000
F	0.7586140000	-0.1945230000	1.8797650000
H	0.7438310000	0.9137290000	-1.8701890000
H	4.8249050000	-1.9716950000	1.1589690000
H	2.8579440000	-1.4866440000	2.6229830000
O	0.6620470000	2.2101690000	-0.2644660000
C	1.7295800000	3.0444510000	-0.7267930000
H	1.5526510000	4.0239800000	-0.2876960000
H	2.7004830000	2.6670890000	-0.3956910000
H	1.7129380000	3.1254330000	-1.8195990000

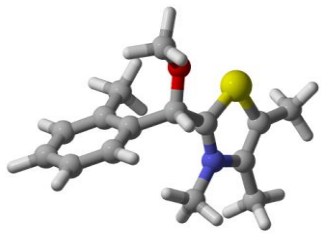
thermodynamic data

Zero-point correction= 0.283903 (Hartree/Particle)
Thermal correction to Energy= 0.302745
Thermal correction to Enthalpy= 0.303689
Thermal correction to Gibbs Free Energy= 0.235470
Sum of electronic and zero-point Energies= -1171.449687
Sum of electronic and thermal Energies= -1171.430844
Sum of electronic and thermal Enthalpies= -1171.429900
Sum of electronic and thermal Free Energies= -1171.498120

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.975	68.764	143.580

B3LYP/6-311+G**		





xyz-matrix

38
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7623990000	0.3143080000	-0.4174480000
N	-1.2617640000	-0.9121700000	-0.5628730000
C	-2.6126840000	-1.0444100000	-0.1873790000
C	-3.1385750000	0.1341730000	0.2463140000
S	-1.9378260000	1.4000090000	0.1744490000
C	-4.5152320000	0.4325460000	0.7558500000
C	-3.2918790000	-2.3732360000	-0.2852770000
C	0.6231250000	0.8186160000	-0.7792260000
H	-3.2484860000	-2.7789830000	-1.2993530000
H	-4.3409980000	-2.2757260000	-0.0134780000
H	-2.8448410000	-3.1063380000	0.3924290000
H	-4.8950210000	1.3695760000	0.3431760000
H	-4.5203930000	0.5211080000	1.8458970000
H	-5.2132390000	-0.3571510000	0.4790200000
C	-0.5203500000	-2.0541270000	-1.1343200000
H	0.5322430000	-1.8051300000	-1.2095000000
H	-0.9225290000	-2.2852800000	-2.1215260000
H	-0.6337780000	-2.9174160000	-0.4811140000
C	1.8060550000	0.0249320000	-0.2308230000
C	2.0056670000	-0.2033040000	1.1472950000
C	3.1563130000	-0.8999050000	1.5322070000

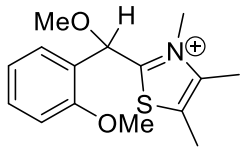
C	4.0887500000	-1.3571200000	0.6035110000
C	3.8928310000	-1.1150660000	-0.7522170000
C	2.7558920000	-0.4227400000	-1.1578970000
H	4.6176540000	-1.4494210000	-1.4845070000
H	2.6070470000	-0.2201460000	-2.2145520000
H	0.6857890000	0.7818040000	-1.8794180000
H	4.9696400000	-1.8898460000	0.9420000000
H	3.3281610000	-1.0788740000	2.5880040000
C	1.0465340000	0.2778790000	2.2120330000
H	1.4967700000	0.1779870000	3.2002410000
H	0.1213930000	-0.3093590000	2.2243190000
H	0.7747150000	1.3246180000	2.0685660000
O	0.5965340000	2.1737830000	-0.3596910000
C	1.6223120000	3.0025520000	-0.9188790000
H	1.4456910000	4.0023570000	-0.5276350000
H	2.6152140000	2.6603350000	-0.6163260000
H	1.5521140000	3.0200810000	-2.0122650000

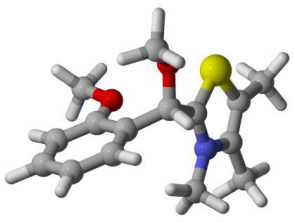
thermodynamic data

Zero-point correction= 0.319863 (Hartree/Particle)
Thermal correction to Energy= 0.339360
Thermal correction to Enthalpy= 0.340304
Thermal correction to Gibbs Free Energy= 0.271494
Sum of electronic and zero-point Energies= -1111.472003
Sum of electronic and thermal Energies= -1111.452506
Sum of electronic and thermal Enthalpies= -1111.451562
Sum of electronic and thermal Free Energies= -1111.520373

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	212.952	71.740	144.824

B3LYP/6-311+G**	





xyz-matrix

39
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8169530000	-0.4410890000	-0.5094100000
N	1.3451240000	0.7152340000	-0.9011090000
C	2.6745650000	0.9233910000	-0.4851520000

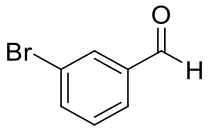
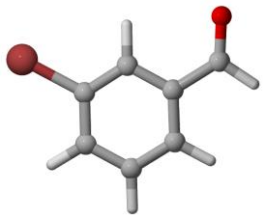
C	3.1519990000	-0.1285050000	0.2338600000
S	1.9325420000	-1.3716140000	0.3811260000
C	4.4942510000	-0.3134970000	0.8727310000
C	3.3825350000	2.1900390000	-0.8475760000
C	-0.5554990000	-0.9933940000	-0.8356030000
H	3.4000030000	2.3511390000	-1.9286750000
H	4.4140700000	2.1520170000	-0.5031890000
H	2.9138410000	3.0625220000	-0.3830170000
H	4.8842300000	-1.3169790000	0.6891490000
H	4.4388860000	-0.1697950000	1.9554900000
H	5.2168850000	0.3991490000	0.4758210000
C	0.6495410000	1.6995830000	-1.7516260000
H	-0.4009900000	1.4395210000	-1.8251920000
H	1.1039170000	1.7066990000	-2.7432480000
H	0.7366250000	2.6872850000	-1.3022730000
C	-1.7373050000	-0.1094670000	-0.4684510000
C	-1.8675270000	0.4673400000	0.8121780000
C	-3.0166840000	1.1941470000	1.1318540000
C	-4.0301330000	1.3503660000	0.1866810000
C	-3.9135350000	0.7904910000	-1.0811360000
C	-2.7681390000	0.0631050000	-1.3952670000
H	-4.7031900000	0.9094760000	-1.8120870000
H	-2.6741630000	-0.3879610000	-2.3785180000
H	-0.5857390000	-1.1433870000	-1.9278740000
H	-4.9156980000	1.9158650000	0.4519470000
H	-3.1306390000	1.6391210000	2.1107690000
O	-0.8227930000	0.2826120000	1.6636130000
C	-0.9570400000	0.6920860000	3.0290050000
H	-0.0450810000	0.3667160000	3.5251970000
H	-1.0488390000	1.7788500000	3.1101050000
H	-1.8181100000	0.2084940000	3.4972640000
O	-0.5627780000	-2.2565990000	-0.1906630000
C	-1.5818330000	-3.1602190000	-0.6265930000
H	-1.4193160000	-4.0832580000	-0.0737290000
H	-2.5792360000	-2.7724070000	-0.4036260000
H	-1.4923240000	-3.3582690000	-1.7011420000

thermodynamic data

Zero-point correction= 0.324568 (Hartree/Particle)
Thermal correction to Energy= 0.345161
Thermal correction to Enthalpy= 0.346105
Thermal correction to Gibbs Free Energy= 0.274090
Sum of electronic and zero-point Energies= -1186.702077
Sum of electronic and thermal Energies= -1186.681484
Sum of electronic and thermal Enthalpies= -1186.680540
Sum of electronic and thermal Free Energies= -1186.752555

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	216.592	75.030	151.569

B3LYP/6-31G*	***m*-Br-PhCHO**

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

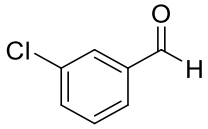
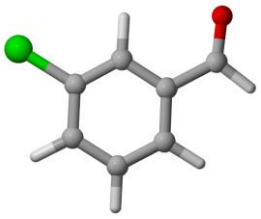
C	-0.6231570000	-0.5212100000	-0.0000020000
C	-1.9008310000	0.0580100000	-0.0000020000
C	-2.0449460000	1.4505790000	-0.0000010000
C	-0.9148730000	2.2673220000	0.0000010000
C	0.3598460000	1.6989580000	0.0000020000
C	0.4904890000	0.3068600000	0.0000000000
H	-3.0408310000	1.8875680000	-0.0000010000
H	-1.0184340000	3.3485650000	0.0000020000
Br	2.2403590000	-0.4620680000	0.0000010000
H	-0.5314550000	-1.6017500000	-0.0000030000
C	-3.1013810000	-0.8123160000	-0.0000050000
H	-4.0692140000	-0.2634440000	0.0000040000
O	-3.0736170000	-2.0266250000	0.0000020000
H	1.2454430000	2.3252070000	0.0000030000

thermodynamic data

Zero-point correction= 0.100070 (Hartree/Particle)
Thermal correction to Energy= 0.107762
Thermal correction to Enthalpy= 0.108706
Thermal correction to Gibbs Free Energy= 0.066207
Sum of electronic and zero-point Energies= -2916.576670
Sum of electronic and thermal Energies= -2916.568978
Sum of electronic and thermal Enthalpies= -2916.568034
Sum of electronic and thermal Free Energies= -2916.610533

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.622	28.053	89.447

B3LYP/6-31G*	***m*-Cl-PhCHO**

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

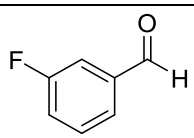
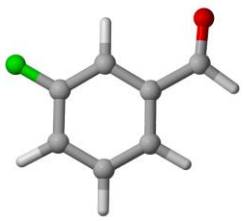
C	-0.1479020000	-0.6350560000	-0.0000030000
C	-1.2983970000	0.1668130000	-0.0000040000
C	-1.1881630000	1.5623730000	-0.0000020000
C	0.0714860000	2.1602190000	0.0000010000
C	1.2219500000	1.3706900000	0.0000020000
C	1.0986790000	-0.0230640000	0.0000000000
H	-2.0881070000	2.1728960000	-0.0000020000
H	0.1655900000	3.2422870000	0.0000030000
Cl	2.5512540000	-1.0108980000	0.0000010000
H	-0.2530600000	-1.7146800000	-0.0000040000
C	-2.6370310000	-0.4715330000	-0.0000080000
H	-3.4893510000	0.2436590000	0.0000070000
O	-2.8296920000	-1.6707760000	0.0000060000
H	2.2074250000	1.8246500000	0.0000040000

thermodynamic data

Zero-point correction= 0.100508 (Hartree/Particle)
Thermal correction to Energy= 0.107981
Thermal correction to Enthalpy= 0.108925
Thermal correction to Gibbs Free Energy= 0.067724
Sum of electronic and zero-point Energies= -805.067469
Sum of electronic and thermal Energies= -805.059996
Sum of electronic and thermal Enthalpies= -805.059052
Sum of electronic and thermal Free Energies= -805.100252

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.759	27.717	86.715

B3LYP/6-31G*	***m*-F-PhCHO**

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

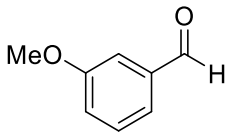
C	-0.0310800000	-0.8274340000	-0.0000080000
C	-0.8851220000	0.2848750000	-0.0000140000
C	-0.3583620000	1.5827170000	-0.0000070000
C	1.0236610000	1.7747160000	0.0000020000
C	1.8823040000	0.6751430000	0.0000070000
C	1.3359520000	-0.6084100000	0.0000020000
H	-1.0321020000	2.4360950000	-0.0000110000
H	1.4371070000	2.7789290000	0.0000060000
F	2.1729260000	-1.6648060000	0.0000060000
H	-0.4408920000	-1.8316810000	-0.0000140000
C	-2.3538170000	0.0836810000	-0.0000310000
H	-2.9491730000	1.0233620000	0.0000310000
O	-2.9017030000	-1.0009860000	0.0000280000
H	2.9611400000	0.7927100000	0.0000150000

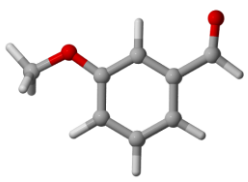
thermodynamic data

Zero-point correction= 0.101937 (Hartree/Particle)
Thermal correction to Energy= 0.109028
Thermal correction to Enthalpy= 0.109972
Thermal correction to Gibbs Free Energy= 0.070103
Sum of electronic and zero-point Energies= -444.703883
Sum of electronic and thermal Energies= -444.696793
Sum of electronic and thermal Enthalpies= -444.695849
Sum of electronic and thermal Free Energies= -444.735717

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.416	26.819	83.911

B3LYP/6-31G*	***m*-OMe-PhCHO**





xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

C	0.2986310000	-0.7097540000	-0.0000270000
C	1.3768770000	0.1778230000	-0.0000300000
C	1.1574780000	1.5640740000	-0.0000040000
C	-0.1467370000	2.0473880000	0.0000150000

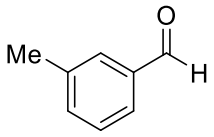
C	-1.2332350000	1.1673090000	0.0000140000
C	-1.0106300000	-0.2193050000	-0.0000070000
H	2.0034140000	2.2470550000	-0.0000040000
H	-0.3325500000	3.1180160000	0.0000310000
H	0.4787790000	-1.7796690000	-0.0000470000
C	2.7628070000	-0.3452220000	-0.0000650000
H	3.5510220000	0.4409440000	0.0000920000
O	3.0622310000	-1.5232920000	0.0000610000
H	-2.2411730000	1.5663720000	0.0000310000
O	-1.9978290000	-1.1592580000	-0.0000100000
C	-3.3480440000	-0.7224670000	0.0000110000
H	-3.9541280000	-1.6298740000	0.0000050000
H	-3.5817180000	-0.1307700000	0.8951800000
H	-3.5817370000	-0.1307460000	-0.8951380000

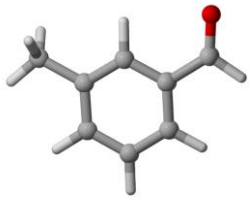
thermodynamic data

Zero-point correction= 0.142929 (Hartree/Particle)
Thermal correction to Energy= 0.151769
Thermal correction to Enthalpy= 0.152714
Thermal correction to Gibbs Free Energy= 0.108876
Sum of electronic and zero-point Energies= -459.952655
Sum of electronic and thermal Energies= -459.943815
Sum of electronic and thermal Enthalpies= -459.942870
Sum of electronic and thermal Free Energies= -459.986708

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.237	33.014	92.264

B3LYP/6-31G*	***m*-Me-PhCHO**





xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

C	0.0119330000	-0.7765740000	0.0000030000
C	-0.9370060000	0.2540930000	0.0000030000
C	-0.5193730000	1.5921130000	0.0000010000
C	0.8410570000	1.8875700000	-0.0000020000
C	1.7777900000	0.8510680000	-0.0000020000
C	1.3803380000	-0.4950970000	0.0000000000
H	-1.2603790000	2.3887440000	0.0000010000
H	1.1776260000	2.9206940000	-0.0000030000

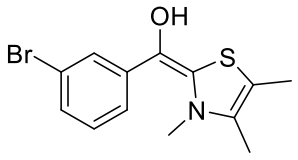
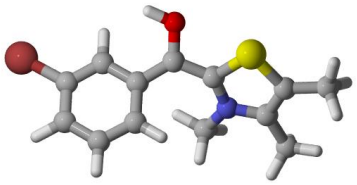
C	2.3988470000	-1.6121020000	0.0000000000
H	-0.3473260000	-1.8027140000	0.0000040000
C	-2.3820040000	-0.0648010000	0.0000070000
H	-3.0511930000	0.8250610000	-0.0000080000
O	-2.8475910000	-1.1885620000	-0.0000060000
H	2.8389830000	1.0899880000	-0.0000040000
H	3.4216750000	-1.2224280000	-0.0000100000
H	2.2859170000	-2.2542410000	-0.8819790000
H	2.2859300000	-2.2542290000	0.8819900000

thermodynamic data

Zero-point correction= 0.137662 (Hartree/Particle)
Thermal correction to Energy= 0.144951
Thermal correction to Enthalpy= 0.145895
Thermal correction to Gibbs Free Energy= 0.105723
Sum of electronic and zero-point Energies= -384.754017
Sum of electronic and thermal Energies= -384.746728
Sum of electronic and thermal Enthalpies= -384.745784
Sum of electronic and thermal Free Energies= -384.785956

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.958	27.890	84.549

B3LYP/6-31G*		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.8282820000	-0.4706860000	0.0268510000
N	-2.3765180000	0.7640450000	-0.3239500000
C	-3.7910510000	0.7859910000	-0.2667550000
C	-4.3518010000	-0.4061200000	0.0279120000
S	-3.1218340000	-1.6715250000	0.2483430000
C	-5.7942870000	-0.7740920000	0.1861460000
C	-4.5068990000	2.0825410000	-0.5093110000
C	-0.5188310000	-0.8309170000	0.1577770000
H	-4.0604010000	2.8957500000	0.0754110000
H	-5.5560320000	1.9998970000	-0.2188690000
H	-4.4860200000	2.3856980000	-1.5642580000
H	-6.0137270000	-1.1336220000	1.1998320000

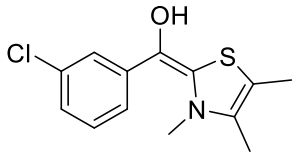
H	-6.0735380000	-1.5768720000	-0.5087760000
H	-6.4491030000	0.0780650000	-0.0155710000
C	-1.6272540000	1.6924240000	-1.1673850000
H	-0.9591680000	1.1231850000	-1.8222710000
H	-1.0127910000	2.3864870000	-0.5841560000
H	-2.3177600000	2.2684710000	-1.7839540000
C	0.6595110000	0.0096190000	0.3460860000
C	1.9234680000	-0.4734300000	-0.0617970000
C	3.0651670000	0.2796190000	0.1772560000
C	3.0166630000	1.5153700000	0.8207140000
C	1.7705850000	1.9870820000	1.2420880000
C	0.6113820000	1.2488920000	1.0226800000
Br	4.7622600000	-0.3985350000	-0.4050660000
H	1.7123690000	2.9346230000	1.7715860000
H	-0.3367910000	1.6040340000	1.4140550000
O	-0.3097920000	-2.2145070000	0.1459590000
H	0.2504930000	-2.4414440000	0.9080190000
H	3.9234810000	2.0821710000	0.9980070000
H	1.9929860000	-1.4233440000	-0.5788200000

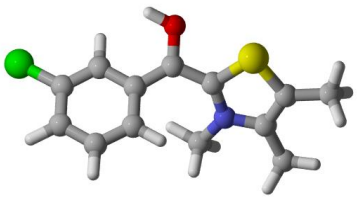
thermodynamic data

Zero-point correction= 0.243094 (Hartree/Particle)
Thermal correction to Energy= 0.260630
Thermal correction to Enthalpy= 0.261574
Thermal correction to Gibbs Free Energy= 0.196713
Sum of electronic and zero-point Energies= -3603.405083
Sum of electronic and thermal Energies= -3603.387547
Sum of electronic and thermal Enthalpies= -3603.386603
Sum of electronic and thermal Free Energies= -3603.451464

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.548	64.930	136.511

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2182470000	-0.4859180000	-0.0125890000
N	-1.7317030000	0.7772280000	-0.3100880000

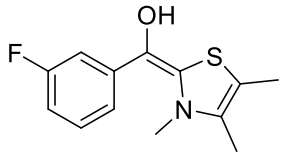
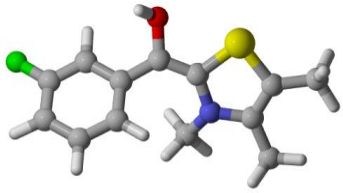
C	-3.1409660000	0.8508460000	-0.1968840000
C	-3.7358100000	-0.3277370000	0.0851600000
S	-2.5478400000	-1.6443910000	0.2217530000
C	-5.1843810000	-0.6460330000	0.2888320000
C	-3.8135650000	2.1809270000	-0.3723760000
C	0.0807680000	-0.8959600000	0.0642260000
H	-3.3151300000	2.9566430000	0.2213050000
H	-4.8543330000	2.1288570000	-0.0468980000
H	-3.8173920000	2.5180550000	-1.4171370000
H	-5.3781870000	-1.0316140000	1.2981320000
H	-5.5218550000	-1.4131960000	-0.4203550000
H	-5.8124480000	0.2368930000	0.1418500000
C	-0.9800780000	1.7021930000	-1.1552680000
H	-0.3330560000	1.1276650000	-1.8258950000
H	-0.3440100000	2.3794840000	-0.5751320000
H	-1.6699540000	2.2961170000	-1.7558230000
C	1.2937390000	-0.1026110000	0.2372910000
C	2.5271370000	-0.6209800000	-0.2166360000
C	3.7025960000	0.0850080000	0.0072590000
C	3.7152660000	1.3070970000	0.6793990000
C	2.4988680000	1.8123120000	1.1457260000
C	1.3081890000	1.1216380000	0.9423190000
Cl	5.2246510000	-0.5825900000	-0.5846920000
H	2.4890460000	2.7486130000	1.6977530000
H	0.3845920000	1.5013750000	1.3676450000
O	0.2389890000	-2.2852490000	0.0081070000
H	0.8117240000	-2.5536790000	0.7471280000
H	4.6473920000	1.8358910000	0.8436890000
H	2.5488890000	-1.5601180000	-0.7575300000

thermodynamic data

Zero-point correction= 0.243605 (Hartree/Particle)
Thermal correction to Energy= 0.260845
Thermal correction to Enthalpy= 0.261789
Thermal correction to Gibbs Free Energy= 0.198418
Sum of electronic and zero-point Energies= -1491.895796
Sum of electronic and thermal Energies= -1491.878556
Sum of electronic and thermal Enthalpies= -1491.877611
Sum of electronic and thermal Free Energies= -1491.940982

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.682	64.577	133.375

B3LYP/6-31G*	

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8978170000	-0.4974360000	-0.0424570000
N	-1.3718880000	0.7921160000	-0.2905180000
C	-2.7730190000	0.9146790000	-0.1321990000
C	-3.4040290000	-0.2482900000	0.1358340000
S	-2.2637630000	-1.6120820000	0.2002000000
C	-4.8570650000	-0.5172850000	0.3754760000
C	-3.3989510000	2.2736710000	-0.2495240000
C	0.3859930000	-0.9572500000	-0.0175230000
H	-2.8557870000	3.0114870000	0.3532490000
H	-4.4321040000	2.2505950000	0.1024460000
H	-3.4168940000	2.6430950000	-1.2831820000
H	-5.0355310000	-0.9240960000	1.3792990000
H	-5.2451770000	-1.2504730000	-0.3437460000
H	-5.4545530000	0.3926730000	0.2724120000
C	-0.6112810000	1.7111640000	-1.1340460000
H	0.0012060000	1.1305320000	-1.8312140000
H	0.0600950000	2.3549370000	-0.5554590000
H	-1.2955990000	2.3389670000	-1.7061020000
C	1.6342200000	-0.2159770000	0.1363990000
C	2.8316870000	-0.7673220000	-0.3697130000
C	4.0320440000	-0.1065190000	-0.1616390000
C	4.1212140000	1.0909220000	0.5402180000
C	2.9399490000	1.6271340000	1.0597900000
C	1.7174430000	0.9870670000	0.8743660000
F	5.1629770000	-0.6475030000	-0.6694720000
H	2.9811200000	2.5466320000	1.6378670000
H	0.8228410000	1.3879170000	1.3398140000
O	0.4889400000	-2.3496520000	-0.1154640000
H	1.0891920000	-2.6558410000	0.5860160000
H	5.0852070000	1.5680140000	0.6798120000
H	2.8187690000	-1.6885420000	-0.9417150000

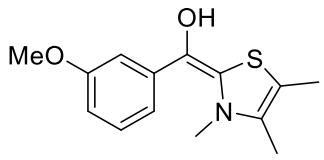
thermodynamic data

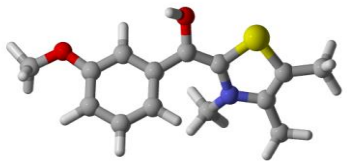
Zero-point correction= 0.244994 (Hartree/Particle)
Thermal correction to Energy= 0.261859
Thermal correction to Enthalpy= 0.262803

Thermal correction to Gibbs Free Energy= 0.200653
Sum of electronic and zero-point Energies= -1131.531667
Sum of electronic and thermal Energies= -1131.514802
Sum of electronic and thermal Enthalpies= -1131.513858
Sum of electronic and thermal Free Energies= -1131.576008

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.319	63.691	130.805

B3LYP/6-31G*	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2749940000	-0.4998340000	-0.0387310000
N	-1.7507900000	0.7892320000	-0.2987360000
C	-3.1545300000	0.9042130000	-0.1594970000
C	-3.7847940000	-0.2608900000	0.1001450000
S	-2.6413340000	-1.6225910000	0.1787470000
C	-5.2392830000	-0.5340730000	0.3253070000
C	-3.7845560000	2.2611060000	-0.2815810000
C	0.0096130000	-0.9497170000	0.0139510000
H	-3.2504090000	2.9993450000	0.3287810000
H	-4.8217440000	2.2340290000	0.0582950000
H	-3.7918090000	2.6330950000	-1.3144870000
H	-5.4273660000	-0.9381390000	1.3286220000
H	-5.6169420000	-1.2716190000	-0.3951950000
H	-5.8393200000	0.3731340000	0.2123240000
C	-0.9902260000	1.6954890000	-1.1570660000
H	-0.3818190000	1.1045260000	-1.8494700000
H	-0.3143080000	2.3428840000	-0.5882260000
H	-1.6742470000	2.3192400000	-1.7342430000
C	1.2501820000	-0.1959910000	0.1888920000
C	2.4593160000	-0.7393070000	-0.2786290000
C	3.6782810000	-0.0890050000	-0.0571370000
C	3.7153870000	1.1224380000	0.6437380000
C	2.5141970000	1.6554050000	1.1267290000
C	1.2998070000	1.0155850000	0.9189370000
H	2.5411100000	2.5808130000	1.6970550000
H	0.3908600000	1.4159300000	1.3561320000
O	0.1238880000	-2.3410860000	-0.0687980000
H	0.7567050000	-2.6273730000	0.6118760000

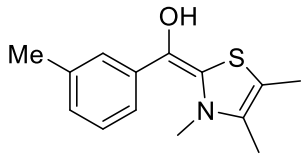
H	4.6489980000	1.6408510000	0.8276990000
H	2.4627540000	-1.6648220000	-0.8447000000
O	4.7784490000	-0.7177860000	-0.5728360000
C	6.0448750000	-0.1083550000	-0.3901250000
H	6.7676430000	-0.7671160000	-0.8755710000
H	6.0887980000	0.8842440000	-0.8583330000
H	6.2996140000	-0.0136090000	0.6741270000

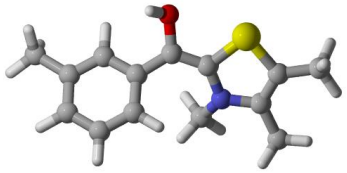
thermodynamic data

Zero-point correction= 0.285929 (Hartree/Particle)
Thermal correction to Energy= 0.304602
Thermal correction to Enthalpy= 0.305547
Thermal correction to Gibbs Free Energy= 0.239280
Sum of electronic and zero-point Energies= -1146.779152
Sum of electronic and thermal Energies= -1146.760479
Sum of electronic and thermal Enthalpies= -1146.759535
Sum of electronic and thermal Free Energies= -1146.825802

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	191.141	69.901	139.470

B3LYP/6-31G*





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9121190000	-0.4985210000	-0.0342460000
N	-1.3927860000	0.7888330000	-0.2948200000
C	-2.7960300000	0.9012060000	-0.1507150000
C	-3.4225370000	-0.2640640000	0.1170920000
S	-2.2753320000	-1.6226850000	0.1969630000
C	-4.8754810000	-0.5399530000	0.3486410000
C	-3.4301460000	2.2557060000	-0.2776030000
C	0.3733610000	-0.9459310000	0.0108950000
H	-2.8964540000	2.9987700000	0.3272840000
H	-4.4661840000	2.2273000000	0.0655840000
H	-3.4417230000	2.6221850000	-1.3124630000
H	-5.0584750000	-0.9434160000	1.3531440000
H	-5.2549770000	-1.2788760000	-0.3695260000

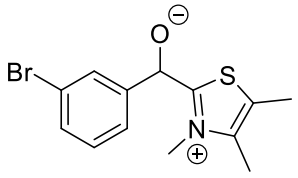
H	-5.4777840000	0.3659850000	0.2375440000
C	-0.6336120000	1.6996080000	-1.1483270000
H	-0.0287300000	1.1133880000	-1.8478790000
H	0.0456350000	2.3416750000	-0.5770190000
H	-1.3181610000	2.3297020000	-1.7177690000
C	1.6164380000	-0.1907380000	0.1670760000
C	2.8230820000	-0.7207170000	-0.3334340000
C	4.0503830000	-0.0759180000	-0.1472180000
C	4.0751650000	1.1291100000	0.5652240000
C	2.8940230000	1.6627710000	1.0886740000
C	1.6788320000	1.0126820000	0.9044840000
H	2.9281110000	2.5842690000	1.6650210000
H	0.7766130000	1.4046050000	1.3644150000
O	0.4891840000	-2.3391230000	-0.0632470000
H	1.1068020000	-2.6221070000	0.6325850000
H	5.0200900000	1.6442820000	0.7205510000
H	2.7869600000	-1.6493870000	-0.8977870000
C	5.3189030000	-0.6724830000	-0.7148360000
H	6.1890800000	-0.0467200000	-0.4923950000
H	5.2571480000	-0.7831850000	-1.8045660000
H	5.5118370000	-1.6709190000	-0.3026560000

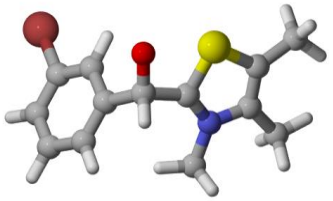
thermodynamic data

Zero-point correction= 0.280664 (Hartree/Particle)
Thermal correction to Energy= 0.297755
Thermal correction to Enthalpy= 0.298700
Thermal correction to Gibbs Free Energy= 0.236138
Sum of electronic and zero-point Energies= -1071.579676
Sum of electronic and thermal Energies= -1071.562584
Sum of electronic and thermal Enthalpies= -1071.561640
Sum of electronic and thermal Free Energies= -1071.624202

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.844	64.781	131.673

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

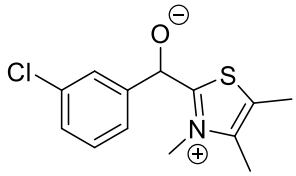
C	-1.7164630000	0.4379840000	0.6407200000
N	-2.3157550000	0.8683300000	-0.4731450000
C	-3.3405360000	0.0211260000	-0.9464070000
C	-3.4897900000	-1.0695660000	-0.1428630000
S	-2.3567230000	-1.0328190000	1.2197000000
C	-4.4504810000	-2.2107020000	-0.2968520000
C	-4.0880310000	0.3903650000	-2.1930900000
C	-0.6054710000	0.9016730000	1.6350290000
H	-4.5511530000	1.3816850000	-2.1161330000
H	-4.8853660000	-0.3316610000	-2.3782360000
H	-3.4382180000	0.3953880000	-3.0774360000
H	-5.0287510000	-2.3655690000	0.6213240000
H	-3.9215620000	-3.1476530000	-0.5094710000
H	-5.1596600000	-2.0376990000	-1.1112470000
C	-1.9592830000	2.1274360000	-1.1325380000
H	-1.0237160000	2.4919820000	-0.7129480000
H	-2.7494980000	2.8691630000	-0.9813440000
H	-1.8223450000	1.9572080000	-2.2024820000
C	0.7237070000	1.1216520000	0.8712150000
C	1.4919170000	-0.0063000000	0.5605370000
C	2.6975690000	0.1536210000	-0.1091080000
C	3.1848920000	1.4150020000	-0.4591750000
C	2.4320790000	2.5369190000	-0.1163780000
C	1.2084780000	2.3912580000	0.5450190000
H	2.8097390000	3.5281490000	-0.3547100000
H	0.6428000000	3.2747410000	0.8375940000
O	-0.5717140000	-0.0536500000	2.5543320000
H	1.1417060000	-0.9799030000	0.8858210000
Br	3.7357560000	-1.3958880000	-0.5623100000
H	-0.9420000000	1.9206080000	1.9755990000
H	4.1366160000	1.5128060000	-0.9699810000

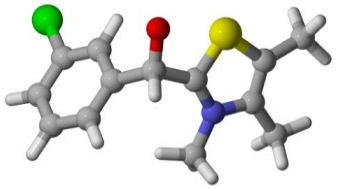
thermodynamic data

Zero-point correction= 0.242027 (Hartree/Particle)
Thermal correction to Energy= 0.259450
Thermal correction to Enthalpy= 0.260394
Thermal correction to Gibbs Free Energy= 0.194515
Sum of electronic and zero-point Energies= -3603.374789
Sum of electronic and thermal Energies= -3603.357367
Sum of electronic and thermal Enthalpies= -3603.356423
Sum of electronic and thermal Free Energies= -3603.422301

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.807	63.657	138.654

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.1509160000	0.2174950000	0.7128360000
N	-1.7407450000	1.0251930000	-0.1731150000
C	-2.8990070000	0.4843860000	-0.7715130000
C	-3.1594000000	-0.7677760000	-0.3005980000
S	-1.9628830000	-1.2695890000	0.9070200000
C	-4.2782370000	-1.6892590000	-0.6850200000
C	-3.6508220000	1.2905000000	-1.7885130000
C	0.0649790000	0.2294730000	1.6926850000
H	-3.9670390000	2.2625090000	-1.3905010000
H	-4.5490380000	0.7545770000	-2.1007640000
H	-3.0525660000	1.4795760000	-2.6888920000
H	-4.7997890000	-2.0663920000	0.2020720000
H	-3.9029570000	-2.5602030000	-1.2360990000
H	-5.0174790000	-1.1892590000	-1.3172310000
C	-1.2442850000	2.3696990000	-0.4783210000
H	-0.2428130000	2.4772710000	-0.0663060000
H	-1.9084760000	3.1242070000	-0.0457690000
H	-1.1961990000	2.5075930000	-1.5605220000
C	1.3714290000	0.4999380000	0.9064920000
C	1.9604740000	-0.5759470000	0.2332990000
C	3.1432930000	-0.3765410000	-0.4674190000
C	3.7811160000	0.8666170000	-0.4967950000
C	3.2069770000	1.9254810000	0.2042550000
C	2.0088430000	1.7437330000	0.9022070000
H	3.7049720000	2.8917430000	0.2168960000
H	1.5858320000	2.5676770000	1.4751270000
O	0.0084560000	-0.9509800000	2.2951940000
H	1.4968950000	-1.5538420000	0.3085020000
Cl	3.8728470000	-1.7284460000	-1.3375510000
H	-0.1045170000	1.1357700000	2.3383820000
H	4.7117990000	0.9904730000	-1.0401640000

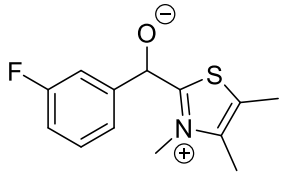
thermodynamic data

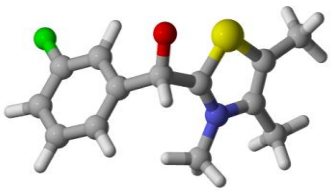
Zero-point correction= 0.242508 (Hartree/Particle)
Thermal correction to Energy= 0.259696
Thermal correction to Enthalpy= 0.260641
Thermal correction to Gibbs Free Energy= 0.196019

Sum of electronic and zero-point Energies= -1491.865576
Sum of electronic and thermal Energies= -1491.848388
Sum of electronic and thermal Enthalpies= -1491.847443
Sum of electronic and thermal Free Energies= -1491.912065

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.962	63.309	136.008

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8501700000	-0.0705010000	-0.6859350000
N	1.4136630000	1.0345360000	-0.1892530000
C	2.6579870000	0.8190000000	0.4411990000
C	3.0102890000	-0.4969120000	0.4013640000
S	1.7918360000	-1.4713010000	-0.4414590000
C	4.2390590000	-1.1451060000	0.9660130000
C	3.3921450000	1.9791640000	1.0452350000
C	-0.4194890000	-0.4869700000	-1.4923700000
H	3.5780690000	2.7748540000	0.3133890000
H	4.3606160000	1.6504680000	1.4268360000
H	2.8427190000	2.4229790000	1.8852660000
H	4.7293250000	-1.7776350000	0.2172080000
H	3.9922730000	-1.7862800000	1.8211260000
H	4.9696340000	-0.4052660000	1.3053380000
C	0.8066980000	2.3623860000	-0.3160020000
H	-0.2346820000	2.2466300000	-0.6106820000
H	1.3432040000	2.9529490000	-1.0651120000
H	0.8457160000	2.8771720000	0.6460110000
C	-1.6942330000	-0.0502200000	-0.7311010000
C	-2.1407480000	-0.8598890000	0.3179390000
C	-3.2920490000	-0.5009440000	1.0009220000
C	-4.0385140000	0.6283310000	0.6702110000
C	-3.6043380000	1.4144910000	-0.3959250000
C	-2.4395560000	1.0773400000	-1.0936500000
H	-4.1848380000	2.2842540000	-0.6930890000
H	-2.1294940000	1.6750660000	-1.9494290000
O	-0.2820730000	-1.7969700000	-1.6568830000
H	-1.6076630000	-1.7751820000	0.5528840000

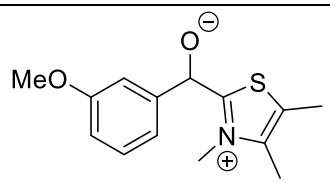
F	-3.7175460000	-1.2767390000	2.0246060000
H	-0.3789710000	0.1456130000	-2.4224530000
H	-4.9409410000	0.8588180000	1.2270220000

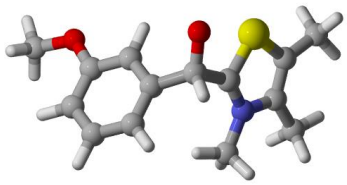
thermodynamic data

Zero-point correction= 0.243970 (Hartree/Particle)
Thermal correction to Energy= 0.260713
Thermal correction to Enthalpy= 0.261657
Thermal correction to Gibbs Free Energy= 0.198672
Sum of electronic and zero-point Energies= -1131.501160
Sum of electronic and thermal Energies= -1131.484417
Sum of electronic and thermal Enthalpies= -1131.483473
Sum of electronic and thermal Free Energies= -1131.546457

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.600	62.392	132.562

B3LYP/6-31G*	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2269340000	0.1467110000	-0.7052590000
N	1.7741360000	1.0126500000	0.1526770000
C	2.9264140000	0.5292680000	0.8093710000
C	3.2248910000	-0.7398610000	0.4131290000
S	2.0717050000	-1.3323170000	-0.7985900000
C	4.3519530000	-1.6142460000	0.8755470000
C	3.6340830000	1.4047300000	1.8008400000
C	0.0423350000	0.0757280000	-1.7174990000
H	3.9335900000	2.3643640000	1.3618790000
H	4.5392300000	0.9095420000	2.1574100000
H	3.0119470000	1.6218610000	2.6785400000
H	4.9252320000	-2.0007230000	0.0248880000
H	3.9776420000	-2.4805470000	1.4346070000
H	5.0458220000	-1.0742710000	1.5261350000
C	1.2376370000	2.3580260000	0.3738670000
H	0.2402270000	2.4138230000	-0.0589210000
H	1.8890480000	3.1055750000	-0.0895130000

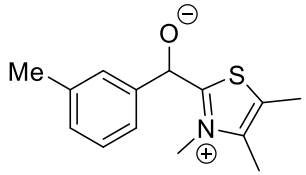
H	1.1675440000	2.5541890000	1.4458510000
C	-1.2902880000	0.3804320000	-0.9915110000
C	-1.8949820000	-0.6437190000	-0.2682240000
C	-3.1107820000	-0.4272900000	0.3899900000
C	-3.7406300000	0.8235150000	0.3108080000
C	-3.1421300000	1.8390480000	-0.4389420000
C	-1.9265010000	1.6262860000	-1.0882780000
H	-3.6443930000	2.7998540000	-0.5252320000
H	-1.4907980000	2.4119460000	-1.7035900000
O	0.1433790000	-1.1400110000	-2.2433740000
H	-1.4359060000	-1.6270010000	-0.2545710000
H	0.2225770000	0.9406850000	-2.4154930000
H	-4.6887640000	1.0068740000	0.8033950000
O	-3.6091700000	-1.4975180000	1.0825440000
C	-4.8646150000	-1.3574050000	1.7224690000
H	-5.0738970000	-2.3225180000	2.1884740000
H	-4.8425830000	-0.5798980000	2.4988380000
H	-5.6623340000	-1.1223550000	1.0047960000

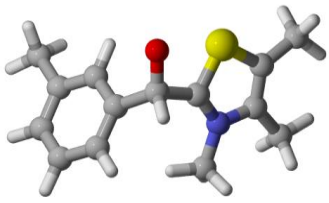
thermodynamic data

Zero-point correction= 0.284738 (Hartree/Particle)
Thermal correction to Energy= 0.303317
Thermal correction to Enthalpy= 0.304261
Thermal correction to Gibbs Free Energy= 0.236812
Sum of electronic and zero-point Energies= -1146.748081
Sum of electronic and thermal Energies= -1146.729502
Sum of electronic and thermal Enthalpies= -1146.728558
Sum of electronic and thermal Free Energies= -1146.796007

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.334	68.628	141.958

B3LYP/6-31G*	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8651690000	-0.0254160000	-0.6955600000
N	1.4303000000	1.0412050000	-0.1226040000
C	2.6644580000	0.7753790000	0.5090430000

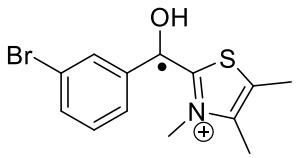
C	3.0074230000	-0.5379990000	0.3899700000
S	1.7907780000	-1.4484040000	-0.5278100000
C	4.2261030000	-1.2300060000	0.9234110000
C	3.3973960000	1.8900110000	1.1950990000
C	-0.3970130000	-0.3833030000	-1.5379020000
H	3.6003470000	2.7277370000	0.5166570000
H	4.3572550000	1.5308210000	1.5708850000
H	2.8371800000	2.2859990000	2.0517730000
H	4.7451010000	-1.7800890000	0.1298670000
H	3.9612900000	-1.9565400000	1.7013600000
H	4.9387170000	-0.5232860000	1.3582130000
C	0.8341490000	2.3789080000	-0.1704390000
H	-0.1975690000	2.2922350000	-0.5060810000
H	1.3978550000	3.0190400000	-0.8562280000
H	0.8436200000	2.8219230000	0.8276600000
C	-1.6774250000	0.0258030000	-0.7726250000
C	-2.1580100000	-0.8258750000	0.2244290000
C	-3.3197050000	-0.5263610000	0.9448110000
C	-4.0143890000	0.6515660000	0.6336180000
C	-3.5633760000	1.4966060000	-0.3806230000
C	-2.3984630000	1.1837000000	-1.0847260000
H	-4.1292270000	2.3904960000	-0.6329890000
H	-2.0673060000	1.8230610000	-1.9026810000
O	-0.2639050000	-1.6850460000	-1.7741640000
H	-1.6183990000	-1.7543610000	0.3955080000
H	-0.3347260000	0.2972900000	-2.4326590000
H	-4.9250350000	0.8962140000	1.1764460000
C	-3.8193770000	-1.4650500000	2.0198940000
H	-4.7357710000	-1.0896310000	2.4871120000
H	-3.0726720000	-1.6032690000	2.8119720000
H	-4.0356170000	-2.4590400000	1.6092820000

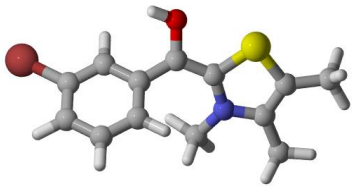
thermodynamic data

Zero-point correction= 0.279654 (Hartree/Particle)
Thermal correction to Energy= 0.296598
Thermal correction to Enthalpy= 0.297542
Thermal correction to Gibbs Free Energy= 0.234204
Sum of electronic and zero-point Energies= -1071.548864
Sum of electronic and thermal Energies= -1071.531920
Sum of electronic and thermal Enthalpies= -1071.530976
Sum of electronic and thermal Free Energies= -1071.594314

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.118	63.447	133.307

(u)B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.8484460000	-0.4792380000	0.0376910000
N	-2.3311690000	0.7342330000	-0.3786350000
C	-3.7238380000	0.8190980000	-0.3954140000
C	-4.3370630000	-0.3560170000	-0.0452460000
S	-3.1611320000	-1.5905540000	0.3262020000
C	-5.7976020000	-0.6798020000	0.0349380000
C	-4.3926610000	2.1010070000	-0.7897750000
C	-0.5214870000	-0.8967810000	0.2245690000
H	-4.2823980000	2.3059130000	-1.8617340000
H	-3.9835800000	2.9540240000	-0.2382140000
H	-5.4607850000	2.0510350000	-0.5762890000
H	-6.0822840000	-0.9788500000	1.0500780000
H	-6.0529030000	-1.5060380000	-0.6383240000
H	-6.4092120000	0.1793650000	-0.2468350000
C	-1.4853080000	1.8044210000	-0.9325470000
H	-2.0204260000	2.2872970000	-1.7495110000
H	-0.5663470000	1.3698440000	-1.3209210000
H	-1.2387630000	2.5461410000	-0.1688170000
C	0.6682560000	-0.0849790000	0.4723050000
C	1.8972780000	-0.4913190000	-0.0891570000
C	3.0562700000	0.2225030000	0.2004270000
C	3.0211570000	1.3312040000	1.0507000000
C	1.8057700000	1.7240610000	1.6168540000
C	0.6339650000	1.0272160000	1.3373270000
H	1.9410210000	-1.3314240000	-0.7750670000
Br	4.7006410000	-0.3171300000	-0.5770000000
H	3.9339260000	1.8739250000	1.2703670000
H	1.7828390000	2.5704090000	2.2964130000
H	-0.2956760000	1.3095040000	1.8218740000
O	-0.3985220000	-2.2455480000	0.2225710000
H	0.4388900000	-2.5062410000	0.6465970000

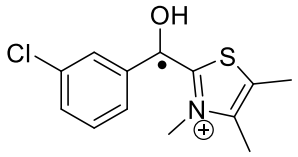
thermodynamic data

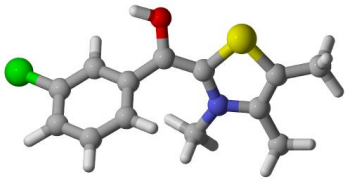
Zero-point correction= 0.244227 (Hartree/Particle)
Thermal correction to Energy= 0.261643
Thermal correction to Enthalpy= 0.262587
Thermal correction to Gibbs Free Energy= 0.196621

Sum of electronic and zero-point Energies= -3603.198047
Sum of electronic and thermal Energies= -3603.180631
Sum of electronic and thermal Enthalpies= -3603.179687
Sum of electronic and thermal Free Energies= -3603.245653

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.183	64.225	138.838

(u)B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2432740000	-0.4893980000	-0.0064510000
N	-1.7083400000	0.7523680000	-0.3537440000
C	-3.0970470000	0.8770360000	-0.3005670000
C	-3.7281330000	-0.2929020000	0.0351750000
S	-2.5737130000	-1.5734740000	0.3032690000
C	-5.1925950000	-0.5788230000	0.1695950000
C	-3.7449010000	2.1910340000	-0.6165360000
C	0.0778040000	-0.9512190000	0.1015150000
H	-3.6836960000	2.4291450000	-1.6855560000
H	-3.2817020000	3.0120980000	-0.0594210000
H	-4.8017860000	2.1649680000	-0.3494740000
H	-5.4321890000	-0.9602770000	1.1684120000
H	-5.5131160000	-1.3321380000	-0.5592990000
H	-5.7879820000	0.3206720000	0.0019750000
C	-0.8573990000	1.8193400000	-0.9063430000
H	-1.4171190000	2.3518490000	-1.6744820000
H	0.0267400000	1.3743330000	-1.3586640000
H	-0.5495420000	2.5206240000	-0.1268110000
C	1.3013480000	-0.1831660000	0.3236510000
C	2.4903820000	-0.6013220000	-0.3098140000
C	3.6817300000	0.0698660000	-0.0473130000
C	3.7182680000	1.1450670000	0.8459730000
C	2.5417360000	1.5471790000	1.4824760000
C	1.3385430000	0.8944910000	1.2309450000
H	2.4795010000	-1.4139940000	-1.0295570000

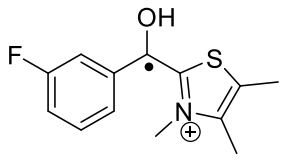
Cl	5.1424800000	-0.4367500000	-0.8522710000
H	4.6566670000	1.6522310000	1.0422500000
H	2.5738410000	2.3662110000	2.1942740000
H	0.4404390000	1.1827880000	1.7684430000
O	0.1600830000	-2.3018580000	0.0432250000
H	1.0061330000	-2.6029930000	0.4207890000

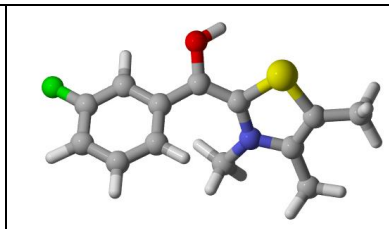
thermodynamic data

Zero-point correction= 0.244677 (Hartree/Particle)
Thermal correction to Energy= 0.261853
Thermal correction to Enthalpy= 0.262797
Thermal correction to Gibbs Free Energy= 0.197910
Sum of electronic and zero-point Energies= -1491.688385
Sum of electronic and thermal Energies= -1491.671208
Sum of electronic and thermal Enthalpies= -1491.670264
Sum of electronic and thermal Free Energies= -1491.735152

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.315	63.884	136.567

(u)B3LYP/6-31G*





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9067800000	-0.5167320000	-0.0992890000
N	-1.3714750000	0.7349830000	-0.4046610000
C	-2.7454140000	0.9044130000	-0.2136930000
C	-3.3791960000	-0.2376960000	0.1946860000
S	-2.2337580000	-1.5452060000	0.3885550000
C	-4.8295950000	-0.4798820000	0.4800480000
C	-3.3782070000	2.2368930000	-0.4803050000
C	0.4148630000	-1.0098630000	-0.1471710000
H	-3.4135860000	2.4642160000	-1.5526750000
H	-2.8345220000	3.0452640000	0.0195700000
H	-4.4038860000	2.2495490000	-0.1104300000

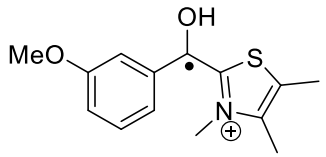
H	-4.9787210000	-0.8455690000	1.5020400000
H	-5.2454810000	-1.2271090000	-0.2056220000
H	-5.4098620000	0.4375480000	0.3643460000
C	-0.5556440000	1.7646060000	-1.0718440000
H	-1.1676230000	2.2646070000	-1.8222430000
H	0.2906620000	1.2870710000	-1.5616220000
H	-0.1847660000	2.4978900000	-0.3520190000
C	1.6385190000	-0.2720920000	0.1140620000
C	2.8462560000	-0.7288980000	-0.4549020000
C	4.0206340000	-0.0560760000	-0.1583290000
C	4.0507910000	1.0465340000	0.6954580000
C	2.8562030000	1.4799730000	1.2758840000
C	1.6573360000	0.8328370000	0.9944210000
H	2.8685080000	-1.5850520000	-1.1183230000
H	4.9966280000	1.5359760000	0.9017210000
H	2.8698070000	2.3169830000	1.9667380000
H	0.7464120000	1.1431300000	1.4963130000
F	5.1628810000	-0.4775500000	-0.7129570000
O	0.5943450000	-2.3417980000	-0.3114240000
H	-0.1524180000	-2.7578580000	-0.7782030000

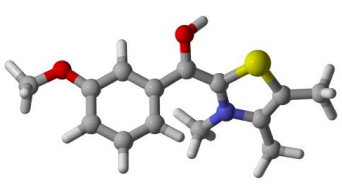
thermodynamic data

Zero-point correction= 0.246017 (Hartree/Particle)
Thermal correction to Energy= 0.262765
Thermal correction to Enthalpy= 0.263709
Thermal correction to Gibbs Free Energy= 0.200676
Sum of electronic and zero-point Energies= -1131.319921
Sum of electronic and thermal Energies= -1131.303173
Sum of electronic and thermal Enthalpies= -1131.302229
Sum of electronic and thermal Free Energies= -1131.365263

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.887	63.128	132.665

(u)B3LYP/6-31G*	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2861020000	-0.5204560000	-0.0897740000

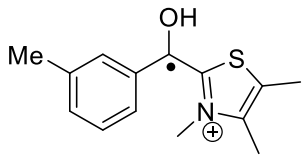
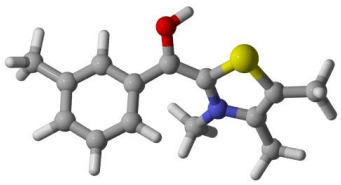
N	-1.7378760000	0.7345880000	-0.4047660000
C	-3.1149980000	0.9101560000	-0.2450540000
C	-3.7642310000	-0.2285700000	0.1459680000
S	-2.6306450000	-1.5438290000	0.3641090000
C	-5.2219580000	-0.4632110000	0.3984230000
C	-3.7342890000	2.2469670000	-0.5221070000
C	0.0336690000	-1.0173290000	-0.1044900000
H	-3.7443670000	2.4778150000	-1.5942270000
H	-3.1969070000	3.0506300000	-0.0079800000
H	-4.7678520000	2.2647510000	-0.1749870000
H	-5.3969010000	-0.8221140000	1.4188120000
H	-5.6248360000	-1.2130220000	-0.2921970000
H	-5.7957980000	0.4556900000	0.2634740000
C	-0.9018230000	1.7588920000	-1.0543610000
H	-1.4943790000	2.2622650000	-1.8181650000
H	-0.0477470000	1.2755610000	-1.5245810000
H	-0.5403820000	2.4889140000	-0.3266940000
C	1.2516820000	-0.2781510000	0.1780290000
C	2.4636770000	-0.7281490000	-0.3711310000
C	3.6644840000	-0.0727030000	-0.0712440000
C	3.6513950000	1.0323130000	0.7965960000
C	2.4444010000	1.4618740000	1.3598640000
C	1.2476650000	0.8257810000	1.0638670000
H	2.4901600000	-1.5821910000	-1.0376100000
H	4.5693330000	1.5507130000	1.0467370000
H	2.4540440000	2.2966540000	2.0541940000
H	0.3297400000	1.1323780000	1.5548400000
O	4.7667940000	-0.5766460000	-0.6660830000
C	6.0368400000	0.0156470000	-0.3890990000
H	6.7602770000	-0.5639010000	-0.9624640000
H	6.0665260000	1.0621830000	-0.7151180000
H	6.2795550000	-0.0490720000	0.6780250000
O	0.2109020000	-2.3510430000	-0.2577190000
H	-0.5290500000	-2.7649700000	-0.7369620000

thermodynamic data

Zero-point correction= 0.287042 (Hartree/Particle)
Thermal correction to Energy= 0.305596
Thermal correction to Enthalpy= 0.306540
Thermal correction to Gibbs Free Energy= 0.239476
Sum of electronic and zero-point Energies= -1146.574554
Sum of electronic and thermal Energies= -1146.556001
Sum of electronic and thermal Enthalpies= -1146.555056
Sum of electronic and thermal Free Energies= -1146.622120

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	191.764	69.399	141.148

(u)B3LYP/6-31G*	

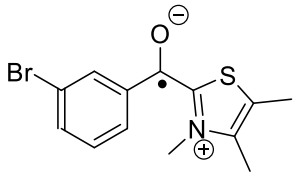
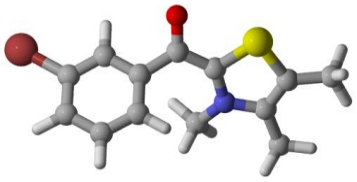
		

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9219930000	-0.5157600000	0.0925320000
N	1.3943800000	0.7315920000	0.4076170000
C	2.7715900000	0.8906080000	0.2290470000
C	3.4002580000	-0.2539880000	-0.1775160000
S	2.2465960000	-1.5533220000	-0.3865960000
C	4.8510680000	-0.5059790000	-0.4522020000
C	3.4116470000	2.2179080000	0.5047390000
C	-0.4038010000	-0.9977070000	0.1244210000
H	3.4386330000	2.4431820000	1.5777660000
H	2.8783250000	3.0311780000	0.0015620000
H	4.4407700000	2.2240190000	0.1443280000
H	5.0071350000	-0.8575530000	-1.4781900000
H	5.2530150000	-1.2676620000	0.2258350000
H	5.4392230000	0.4037210000	-0.3165710000
C	0.5817670000	1.7624160000	1.0756620000
H	1.1920800000	2.2538000000	1.8331760000
H	-0.2713710000	1.2874460000	1.5560290000
H	0.2195220000	2.5025990000	0.3584590000
C	-1.6168220000	-0.2490770000	-0.1410810000
C	-2.8401920000	-0.6962890000	0.4084510000
C	-4.0385250000	-0.0388770000	0.1370380000
C	-4.0038860000	1.0799030000	-0.7149020000
C	-2.8080000000	1.5210460000	-1.2864550000
C	-1.6152500000	0.8648380000	-1.0083070000
H	-2.8379110000	-1.5641170000	1.0596950000
C	-5.3428240000	-0.5090270000	0.7336290000
H	-4.9290160000	1.6031530000	-0.9428860000
H	-2.8140200000	2.3668750000	-1.9672590000
H	-0.6976180000	1.1733200000	-1.5001810000
H	-5.2020750000	-1.3911130000	1.3641450000
H	-6.0621570000	-0.7681190000	-0.0518220000
H	-5.8026600000	0.2749490000	1.3465490000
O	-0.5902370000	-2.3316580000	0.2773750000
H	0.1496870000	-2.7504970000	0.7522380000

(u)B3LYP/6-31G*	

xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	1.8418860000	-0.5107080000	-0.0333770000
N	2.3292400000	0.7266840000	0.3542270000
C	3.7324580000	0.8086020000	0.3458630000
C	4.3407560000	-0.3620670000	0.0238420000
S	3.1607540000	-1.6410870000	-0.2769420000
C	5.8013170000	-0.6747780000	-0.0890420000
C	4.3960220000	2.1126390000	0.6797580000
C	0.5133780000	-1.0094210000	-0.2205080000
H	4.3005890000	2.3694640000	1.7426500000
H	3.9693290000	2.9399070000	0.1005810000
H	5.4625190000	2.0645930000	0.4529250000
H	6.0648820000	-1.0033910000	-1.1021260000
H	6.0854540000	-1.4819000000	0.5979360000
H	6.4180950000	0.1952890000	0.1511800000
C	1.5005790000	1.7267210000	1.0288180000
H	2.0803710000	2.2084730000	1.8180630000
H	0.6411300000	1.2309160000	1.4808950000
H	1.1318350000	2.4911390000	0.3376610000
O	0.3515100000	-2.2541770000	-0.2641980000
C	-0.6659110000	-0.1105980000	-0.4407240000
C	-1.9108210000	-0.5359420000	0.0507920000
C	-3.0435660000	0.2281540000	-0.1976670000
C	-2.9864480000	1.4007520000	-0.9523910000
C	-1.7541250000	1.8024800000	-1.4692300000
C	-0.6024100000	1.0565790000	-1.2175200000
H	-1.9698790000	-1.4625590000	0.6096570000
Br	-4.7317390000	-0.3421620000	0.5057820000
H	-3.8866540000	1.9755740000	-1.1401220000
H	-1.6989650000	2.6971490000	-2.0838120000
H	0.3446530000	1.3605610000	-1.6544820000

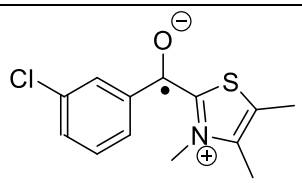
thermodynamic data

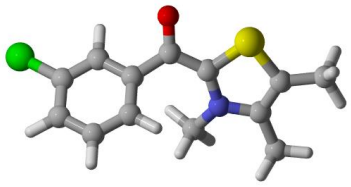
Zero-point correction= 0.231285 (Hartree/Particle)
Thermal correction to Energy= 0.248573
Thermal correction to Enthalpy= 0.249517
Thermal correction to Gibbs Free Energy= 0.183673
Sum of electronic and zero-point Energies= -3602.817059
Sum of electronic and thermal Energies= -3602.799771

Sum of electronic and thermal Enthalpies= -3602.798827
Sum of electronic and thermal Free Energies= -3602.864670

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	155.982	63.028	138.579

(u)B3LYP/6-31G*	





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2303810000	-0.5222970000	0.0060560000
N	1.6920200000	0.7421660000	0.3330990000
C	3.0901670000	0.8678380000	0.2654230000
C	3.7234930000	-0.2933350000	-0.0424530000
S	2.5750630000	-1.6184020000	-0.2530110000
C	5.1880940000	-0.5632810000	-0.2031570000
C	3.7227850000	2.2027030000	0.5304820000
C	-0.0874420000	-1.0681470000	-0.1107940000
H	3.6638520000	2.4898440000	1.5882450000
H	3.2440340000	2.9967920000	-0.0544020000
H	4.7797010000	2.1823400000	0.2590210000
H	5.4219310000	-0.9241090000	-1.2125570000
H	5.5270100000	-1.3320990000	0.5026940000
H	5.7840010000	0.3354180000	-0.0232990000
C	0.8578300000	1.7403000000	1.0034780000
H	1.4495140000	2.2632360000	1.7570340000
H	0.0284290000	1.2359650000	1.4998630000
H	0.4447930000	2.4714900000	0.3013600000
O	-0.2108770000	-2.3180880000	-0.1073490000
C	-1.3030470000	-0.2140920000	-0.3116420000
C	-2.5112070000	-0.6583350000	0.2488970000
C	-3.6780940000	0.0614460000	0.0227810000
C	-3.6894450000	1.2061840000	-0.7768290000
C	-2.4935700000	1.6244510000	-1.3611120000
C	-1.3088870000	0.9242580000	-1.1325520000
H	-2.5180390000	-1.5650560000	0.8428270000
Cl	-5.1841220000	-0.4845490000	0.7564570000

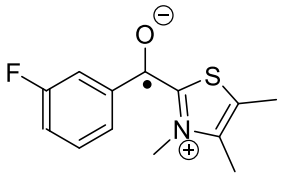
H	-4.6155430000	1.7450340000	-0.9456790000
H	-2.4926530000	2.4964030000	-2.0097970000
H	-0.3914460000	1.2398890000	-1.6212750000

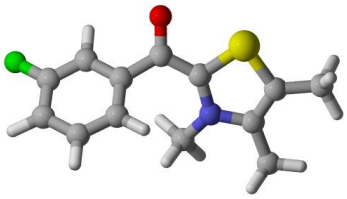
thermodynamic data

Zero-point correction= 0.231783 (Hartree/Particle)
Thermal correction to Energy= 0.248792
Thermal correction to Enthalpy= 0.249736
Thermal correction to Gibbs Free Energy= 0.185367
Sum of electronic and zero-point Energies= -1491.307824
Sum of electronic and thermal Energies= -1491.290814
Sum of electronic and thermal Enthalpies= -1491.289870
Sum of electronic and thermal Free Energies= -1491.354240

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.120	62.677	135.477

(u)B3LYP/6-31G*





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9079460000	-0.5309060000	0.0444110000
N	1.3420860000	0.7571340000	0.3128580000
C	2.7319540000	0.9222560000	0.1852220000
C	3.3887420000	-0.2286570000	-0.1117790000
S	2.2753870000	-1.5941940000	-0.2335790000
C	4.8536180000	-0.4591130000	-0.3237500000
C	3.3341180000	2.2828410000	0.3821250000
C	-0.3956160000	-1.1208080000	0.0022370000
H	3.3137510000	2.6005930000	1.4326400000
H	2.8061030000	3.0442110000	-0.2037730000
H	4.3781210000	2.2850350000	0.0639070000
H	5.0582120000	-0.8463550000	-1.3297420000
H	5.2449220000	-1.1931710000	0.3919810000

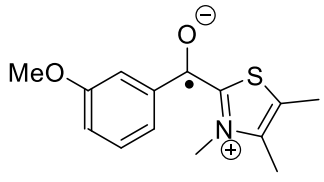
H	5.4275490000	0.4627790000	-0.1977660000
C	0.5012090000	1.7487580000	0.9847190000
H	1.1154840000	2.3521780000	1.6547710000
H	-0.2563500000	1.2320470000	1.5757890000
H	-0.0087840000	2.4065600000	0.2743600000
O	-0.4767630000	-2.3732140000	0.0531910000
C	-1.6452600000	-0.3126160000	-0.1751500000
C	-2.8150820000	-0.7707730000	0.4499750000
C	-4.0040450000	-0.0904420000	0.2395470000
C	-4.0913950000	1.0214430000	-0.5939530000
C	-2.9326460000	1.4532670000	-1.2403610000
C	-1.7187290000	0.7956250000	-1.0351420000
H	-2.7875240000	-1.6537460000	1.0785330000
H	-5.0474850000	1.5147760000	-0.7342940000
H	-2.9820800000	2.3007940000	-1.9187570000
H	-0.8318930000	1.1181540000	-1.5731590000
F	-5.1228440000	-0.5218050000	0.8620690000

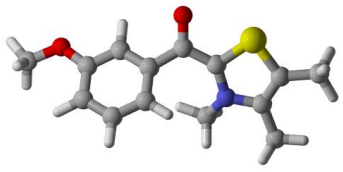
thermodynamic data

Zero-point correction= 0.233289 (Hartree/Particle)
Thermal correction to Energy= 0.249888
Thermal correction to Enthalpy= 0.250832
Thermal correction to Gibbs Free Energy= 0.187878
Sum of electronic and zero-point Energies= -1130.943671
Sum of electronic and thermal Energies= -1130.927072
Sum of electronic and thermal Enthalpies= -1130.926128
Sum of electronic and thermal Free Energies= -1130.989083

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.807	61.741	132.499

(u)B3LYP/6-31G*





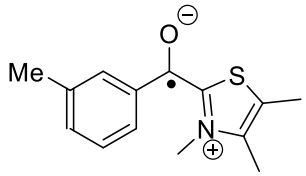
thermodynamic data

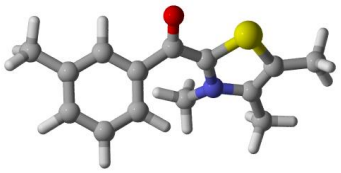
Zero-point correction= 0.274136 (Hartree/Particle)
Thermal correction to Energy= 0.292566
Thermal correction to Enthalpy= 0.293511

Thermal correction to Gibbs Free Energy= 0.226260
Sum of electronic and zero-point Energies= -1146.191215
Sum of electronic and thermal Energies= -1146.172785
Sum of electronic and thermal Enthalpies= -1146.171841
Sum of electronic and thermal Free Energies= -1146.239091

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	183.588	67.983	141.541

(u)B3LYP/6-31G*	





xyz-matrix

33
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9155620000	-0.5165930000	-0.0654460000
N	-1.3820730000	0.7738740000	-0.2885630000
C	-2.7788940000	0.8903890000	-0.1510570000
C	-3.4020260000	-0.2822570000	0.1246250000
S	-2.2523210000	-1.6232250000	0.2076140000
C	-4.8560890000	-0.5543330000	0.3598970000
C	-3.4098390000	2.2426220000	-0.3092760000
C	0.4013970000	-1.0773100000	0.0004280000
H	-3.2775250000	2.6456970000	-1.3210450000
H	-2.9796540000	2.9682170000	0.3924060000
H	-4.4825120000	2.1897390000	-0.1154060000
H	-5.0384280000	-0.9143570000	1.3803390000
H	-5.2265910000	-1.3259870000	-0.3265880000
H	-5.4628970000	0.3425360000	0.2090930000
C	-0.6648430000	1.7262090000	-1.1442110000
H	-1.0771770000	1.7133350000	-2.1613210000
H	0.3866050000	1.4574950000	-1.1863660000
H	-0.7466480000	2.7376460000	-0.7376520000
O	0.4999930000	-2.3283670000	-0.0358870000
C	1.6388280000	-0.2499910000	0.1795890000
C	2.8418340000	-0.7554400000	-0.3372690000
C	4.0567890000	-0.0923640000	-0.1509430000
C	4.0606000000	1.0938760000	0.5987180000
C	2.8789180000	1.5966240000	1.1424730000
C	1.6700080000	0.9322210000	0.9352140000
H	2.8060100000	-1.6955330000	-0.8800940000

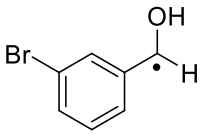
C	5.3348430000	-0.6310770000	-0.7522400000
H	4.9984520000	1.6192280000	0.7666100000
H	2.9020430000	2.5025440000	1.7431620000
H	0.7567950000	1.3147630000	1.3830440000
H	5.2550810000	-1.7020930000	-0.9634920000
H	6.1883800000	-0.4798900000	-0.0818970000
H	5.5739830000	-0.1273690000	-1.6985900000

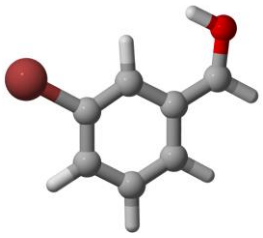
thermodynamic data

Zero-point correction= 0.269023 (Hartree/Particle)
Thermal correction to Energy= 0.286719
Thermal correction to Enthalpy= 0.287663
Thermal correction to Gibbs Free Energy= 0.221732
Sum of electronic and zero-point Energies= -1070.992360
Sum of electronic and thermal Energies= -1070.974664
Sum of electronic and thermal Enthalpies= -1070.973720
Sum of electronic and thermal Free Energies= -1071.039651

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.919	64.829	138.764

(u)B3LYP/6-31G*





xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

C	0.5972830000	-0.4707410000	-0.0000030000
C	1.8950390000	0.1217600000	0.0000020000
C	1.9686120000	1.5470800000	0.0000090000
C	0.8212820000	2.3192900000	0.0000030000
C	-0.4526140000	1.7283170000	-0.0000050000
C	-0.5293370000	0.3333170000	-0.0000050000
H	2.9459680000	2.0222040000	0.0000310000
H	0.9021490000	3.4029530000	0.0000150000
Br	-2.2561150000	-0.4986360000	0.0000010000
H	0.4639790000	-1.5484990000	-0.0000090000
C	3.0829850000	-0.6330410000	-0.0000240000
H	4.0607880000	-0.1664830000	-0.0000110000

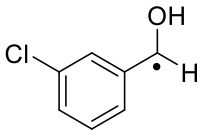
H	-1.3534060000	2.3301570000	-0.0000250000
O	3.1702960000	-1.9856970000	0.0000090000
H	2.2826740000	-2.3783990000	0.0000290000

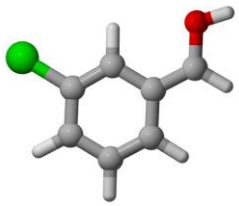
thermodynamic data

Zero-point correction= 0.109858 (Hartree/Particle)
Thermal correction to Energy= 0.118269
Thermal correction to Enthalpy= 0.119213
Thermal correction to Gibbs Free Energy= 0.074648
Sum of electronic and zero-point Energies= -2917.126533
Sum of electronic and thermal Energies= -2917.118123
Sum of electronic and thermal Enthalpies= -2917.117179
Sum of electronic and thermal Free Energies= -2917.161743

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.215	31.140	93.794

(u)B3LYP/6-31G*





xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.1357430000	-0.5943400000	-0.0000110000
C	-1.2759480000	0.2596260000	-0.0000080000
C	-1.0632120000	1.6676440000	0.0000150000
C	0.2201000000	2.1880000000	0.0000110000
C	1.3419150000	1.3464890000	-0.0000030000
C	1.1310600000	-0.0371310000	0.0000140000
H	-1.9219190000	2.3343050000	0.0000310000
H	0.3645890000	3.2650650000	0.0000260000
Cl	2.5338190000	-1.1076050000	0.0000060000
H	-0.2666960000	-1.6695230000	-0.0000030000
C	-2.5831630000	-0.2587940000	-0.0002340000
H	-3.4591500000	0.3829050000	0.0006200000
H	2.3486500000	1.7483010000	-0.0000160000
O	-2.7779010000	-1.6080720000	0.0000330000

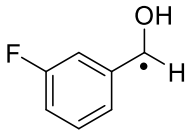
H -3.7272360000 -1.7961510000 0.0002670000

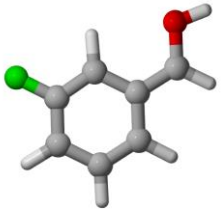
thermodynamic data

Zero-point correction= 0.110329 (Hartree/Particle)
Thermal correction to Energy= 0.118474
Thermal correction to Enthalpy= 0.119418
Thermal correction to Gibbs Free Energy= 0.076516
Sum of electronic and zero-point Energies= -805.617479
Sum of electronic and thermal Energies= -805.609334
Sum of electronic and thermal Enthalpies= -805.608390
Sum of electronic and thermal Free Energies= -805.651292

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.344	30.901	90.296

(u)B3LYP/6-31G*	





xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

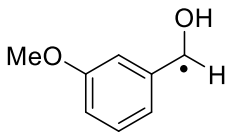
C	0.0212120000	-0.7996660000	0.0002860000
C	0.8470700000	0.3597580000	-0.0000540000
C	0.2159780000	1.6375170000	0.0000350000
C	-1.1655950000	1.7445680000	-0.0001010000
C	-1.9780670000	0.6016410000	0.0001290000
C	-1.3506590000	-0.6451060000	0.0006170000
H	0.8318530000	2.5332180000	-0.0001270000
H	-1.6287950000	2.7275560000	-0.0004120000
F	-2.1269630000	-1.7529290000	-0.0004070000
H	0.4560580000	-1.7919720000	0.0001140000
C	2.2502540000	0.2677340000	-0.0003830000
H	2.8871580000	1.1471960000	0.0005350000
H	-3.0607230000	0.6617540000	-0.0001290000
O	2.8505490000	-0.9571400000	0.0001440000
H	3.8115650000	-0.8429490000	-0.0006400000

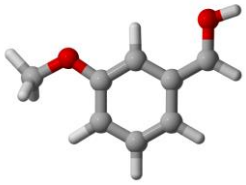
thermodynamic data

Zero-point correction= 0.111759 (Hartree/Particle)
Thermal correction to Energy= 0.119512
Thermal correction to Enthalpy= 0.120456
Thermal correction to Gibbs Free Energy= 0.078904
Sum of electronic and zero-point Energies= -445.253398
Sum of electronic and thermal Energies= -445.245645
Sum of electronic and thermal Enthalpies= -445.244701
Sum of electronic and thermal Free Energies= -445.286253

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.995	29.987	87.454

(u)B3LYP/6-31G*	





xyz-matrix

19
XYZ file generated by gabedit : coordinates in Angstrom

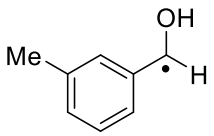
C	-0.2775700000	-0.6668030000	0.0002410000
C	-1.3518770000	0.2572820000	-0.0000430000
C	-1.0472970000	1.6503900000	-0.0001190000
C	0.2685820000	2.0718180000	0.0000470000
C	1.3327150000	1.1541190000	0.0003140000
C	1.0431030000	-0.2194930000	0.0004290000
H	-1.8571520000	2.3755480000	-0.0003470000
H	0.4921700000	3.1357680000	-0.0000130000
H	-0.4701500000	-1.7333720000	0.0004020000
C	-2.6957920000	-0.1633990000	-0.0003600000
H	-3.5219190000	0.5414090000	-0.0003480000
H	2.3540960000	1.5153330000	0.0004550000
O	1.9952240000	-1.2038370000	0.0007860000
C	3.3582710000	-0.8187540000	-0.0008350000
H	3.9323500000	-1.7476290000	-0.0014970000
H	3.6151810000	-0.2351990000	-0.8954000000
H	3.6173400000	-0.2352100000	0.8931260000
O	-2.9936890000	-1.4962370000	-0.0001130000
H	-3.9550070000	-1.6070080000	0.0001910000

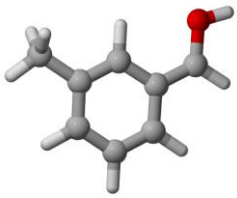
thermodynamic data

Zero-point correction= 0.152663 (Hartree/Particle)
Thermal correction to Energy= 0.162212
Thermal correction to Enthalpy= 0.163156
Thermal correction to Gibbs Free Energy= 0.117509
Sum of electronic and zero-point Energies= -460.500295
Sum of electronic and thermal Energies= -460.490746
Sum of electronic and thermal Enthalpies= -460.489802
Sum of electronic and thermal Free Energies= -460.535449

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.789	36.241	96.071

(u)B3LYP/6-31G*		





xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

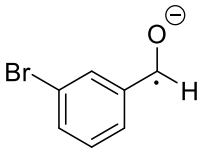
C	-0.0182780000	-0.7493050000	0.0002630000
C	0.8989850000	0.3374590000	-0.0000550000
C	0.3689910000	1.6597440000	-0.0002010000
C	-0.9992790000	1.8644280000	-0.0000760000
C	-1.8858060000	0.7768230000	0.0002100000
C	-1.3957870000	-0.5393820000	0.0002850000
H	1.0509250000	2.5071660000	-0.0003070000
H	-1.3918380000	2.8783610000	-0.0000870000
C	-2.3446610000	-1.7180090000	-0.0002500000
H	0.3747370000	-1.7618760000	0.0004810000
C	2.2923470000	0.1411360000	0.0001860000
H	2.9938830000	0.9703150000	-0.0005330000
H	-2.9587070000	0.9516110000	0.0004190000
H	-3.3892880000	-1.3909360000	0.0079950000
H	-2.1879610000	-2.3576960000	0.8770450000
H	-2.1990800000	-2.3478530000	-0.8866160000
O	2.8046610000	-1.1261640000	-0.0000390000
H	3.7709730000	-1.0771400000	-0.0002550000

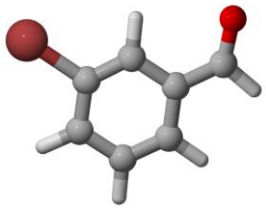
thermodynamic data

Zero-point correction= 0.147361 (Hartree/Particle)
Thermal correction to Energy= 0.155345
Thermal correction to Enthalpy= 0.156290
Thermal correction to Gibbs Free Energy= 0.114349
Sum of electronic and zero-point Energies= -385.301212
Sum of electronic and thermal Energies= -385.293228
Sum of electronic and thermal Enthalpies= -385.292284
Sum of electronic and thermal Free Energies= -385.334225

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	97.481	31.116	88.272

(u)B3LYP/6-31G*	





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.6224380000	-0.5167770000	0.0000540000
C	-1.9497050000	0.0453470000	0.0000770000
C	-2.0404870000	1.4770470000	0.0000380000
C	-0.9166160000	2.2775050000	-0.0000070000
C	0.3895960000	1.7253980000	-0.0000260000
C	0.4648060000	0.3206870000	0.0000060000
H	-3.0315560000	1.9319870000	0.0000500000
H	-1.0262900000	3.3626810000	-0.0000270000
Br	2.2552900000	-0.4724500000	-0.0000110000
H	-0.5226820000	-1.5961190000	0.0000840000
C	-3.1006420000	-0.7973780000	0.0001060000
H	-4.0697340000	-0.2349920000	-0.0001210000
H	1.2800780000	2.3422210000	-0.0000570000
O	-3.1140060000	-2.0576250000	-0.0001310000

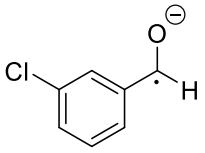
thermodynamic data

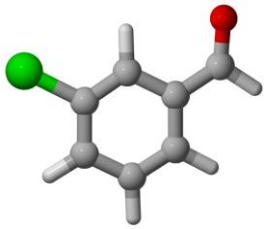
Zero-point correction= 0.096243 (Hartree/Particle)
Thermal correction to Energy= 0.104201
Thermal correction to Enthalpy= 0.105145

Thermal correction to Gibbs Free Energy= 0.061667
Sum of electronic and zero-point Energies= -2916.590288
Sum of electronic and thermal Energies= -2916.582329
Sum of electronic and thermal Enthalpies= -2916.581385
Sum of electronic and thermal Free Energies= -2916.624863

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.387	29.649	91.507

(u)B3LYP/6-31G*	





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.1446280000	-0.6330200000	-0.0000200000
C	-1.3456200000	0.1634780000	0.0000190000
C	-1.1725430000	1.5871200000	0.0000410000
C	0.0796870000	2.1671270000	0.0000220000
C	1.2613500000	1.3842520000	-0.0000160000
C	1.0802360000	-0.0118780000	-0.0000360000
H	-2.0630160000	2.2166400000	0.0000700000
H	0.1705810000	3.2540580000	0.0000370000
Cl	2.5659420000	-1.0334900000	-0.0000910000
H	-0.2446040000	-1.7126880000	-0.0000380000
C	-2.6318150000	-0.4528490000	0.0000470000
H	-3.4816860000	0.2773340000	0.0001490000
H	2.2508770000	1.8263350000	-0.0000330000
O	-2.8766460000	-1.6897160000	0.0001270000

thermodynamic data

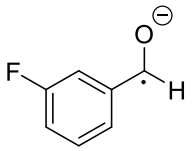
Zero-point correction= 0.096688 (Hartree/Particle)
Thermal correction to Energy= 0.104421
Thermal correction to Enthalpy= 0.105365
Thermal correction to Gibbs Free Energy= 0.063216

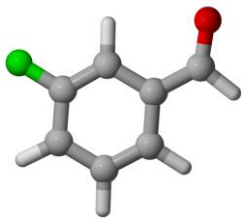
Sum of electronic and zero-point Energies= -805.080347
Sum of electronic and thermal Energies= -805.072614
Sum of electronic and thermal Enthalpies= -805.071670
Sum of electronic and thermal Free Energies= -805.113819

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.525	29.318	88.710

Alpha-HOMO (6311) spin density (6311)

(u)B3LYP/6-31G*	





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	0.0226570000	-0.8287410000	0.0002160000
C	0.9302140000	0.2906720000	0.0002310000
C	0.3361040000	1.5959310000	0.0000750000
C	-1.0332410000	1.7739840000	-0.0001300000
C	-1.9221070000	0.6691160000	-0.0001630000
C	-1.3318540000	-0.6036890000	0.0000500000
H	0.9962860000	2.4641980000	0.0000840000
H	-1.4451150000	2.7840630000	-0.0002800000
F	-2.1805010000	-1.6877150000	-0.0001360000
H	0.4252890000	-1.8361050000	0.0003190000
C	2.3431530000	0.0992320000	0.0003360000
H	2.9291710000	1.0546660000	-0.0002790000
H	-3.0015560000	0.7789800000	-0.0003490000
O	2.9563590000	-1.0044250000	-0.0002460000

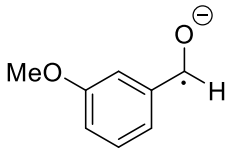
thermodynamic data

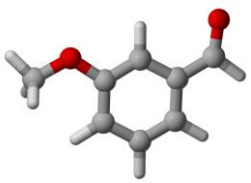
Zero-point correction= 0.098161 (Hartree/Particle)
Thermal correction to Energy= 0.105462
Thermal correction to Enthalpy= 0.106406
Thermal correction to Gibbs Free Energy= 0.065685
Sum of electronic and zero-point Energies= -444.710990
Sum of electronic and thermal Energies= -444.703689

Sum of electronic and thermal Enthalpies= -444.702745
Sum of electronic and thermal Free Energies= -444.743466

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	66.178	28.290	85.706

(u)B3LYP/6-31G*	





xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

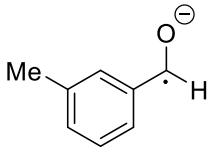
C	0.2904310000	-0.7111510000	0.0000730000
C	1.4211180000	0.1757120000	0.0002260000
C	1.1322050000	1.5798270000	0.0001380000
C	-0.1635260000	2.0476890000	-0.0000530000
C	-1.2773670000	1.1656810000	-0.0002020000
C	-1.0030090000	-0.2181730000	-0.0001510000
H	1.9665520000	2.2827920000	0.0002530000
H	-0.3490720000	3.1230330000	-0.0000850000
H	0.4649200000	-1.7822690000	0.0001800000
C	2.7601910000	-0.3167190000	0.0003590000
H	3.5374290000	0.4914910000	-0.0004650000
H	-2.2879120000	1.5580040000	-0.0004610000
O	-2.0126950000	-1.1850160000	-0.0003450000
C	-3.3415090000	-0.7365260000	0.0005810000
H	-3.9727290000	-1.6324030000	0.0009160000
H	-3.5812800000	-0.1338990000	0.8914810000
H	-3.5825130000	-0.1337660000	-0.8899080000
O	3.1243700000	-1.5263620000	-0.0006210000

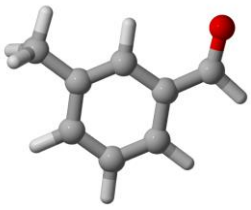
thermodynamic data

Zero-point correction= 0.138806 (Hartree/Particle)
Thermal correction to Energy= 0.147914
Thermal correction to Enthalpy= 0.148859
Thermal correction to Gibbs Free Energy= 0.103795
Sum of electronic and zero-point Energies= -459.950946
Sum of electronic and thermal Energies= -459.941838
Sum of electronic and thermal Enthalpies= -459.940894
Sum of electronic and thermal Free Energies= -459.985957

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	92.818	34.466	94.845

(u)B3LYP/6-31G*	





xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

C	0.0116270000	-0.7766480000	-0.0000030000
C	-0.9781590000	0.2668660000	0.0000030000
C	-0.4802870000	1.6117690000	0.0000190000
C	0.8765120000	1.8765550000	-0.0000050000
C	1.8295270000	0.8333640000	0.0000490000
C	1.3684900000	-0.5101240000	-0.0000070000
H	-1.1979670000	2.4339780000	0.0000460000
H	1.2203300000	2.9129910000	0.0000410000
C	2.3738560000	-1.6422570000	0.0000140000
H	-0.3518640000	-1.8023930000	0.0000150000
C	-2.3729510000	-0.0313490000	-0.0000120000
H	-3.0293140000	0.8783550000	-0.0000170000
H	2.8966160000	1.0514660000	-0.0003960000
H	3.0333400000	-1.6042460000	-0.8810600000
H	1.8758310000	-2.6189080000	0.0001500000
H	3.0335080000	-1.6041390000	0.8809600000
O	-2.9065220000	-1.1770200000	-0.0000100000

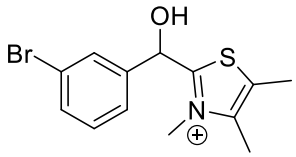
thermodynamic data

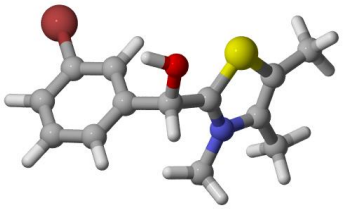
Zero-point correction= 0.133834 (Hartree/Particle)
Thermal correction to Energy= 0.142036
Thermal correction to Enthalpy= 0.142980
Thermal correction to Gibbs Free Energy= 0.100324
Sum of electronic and zero-point Energies= -384.751875
Sum of electronic and thermal Energies= -384.743673
Sum of electronic and thermal Enthalpies= -384.742729
Sum of electronic and thermal Free Energies= -384.785385

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin

Total	89.129	31.176	89.778

B3LYP/6-31G*	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

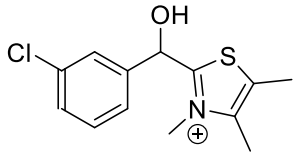
C	-1.6775090000	0.6582760000	0.5140850000
N	-2.2088580000	0.6925290000	-0.7083200000
C	-3.1840070000	-0.2925710000	-0.9526950000
C	-3.3804930000	-1.0926780000	0.1367580000
S	-2.3514170000	-0.5922530000	1.4578300000
C	-4.3047910000	-2.2611610000	0.3072380000
C	-3.8591680000	-0.3624210000	-2.2877740000
C	-0.6243090000	1.5837170000	1.0901370000
H	-4.3330980000	0.5888830000	-2.5538650000
H	-4.6378840000	-1.1258000000	-2.2740110000
H	-3.1552830000	-0.6267430000	-3.0858790000
H	-4.9161160000	-2.1543520000	1.2093320000
H	-3.7443400000	-3.1991060000	0.3912540000
H	-4.9814120000	-2.3509120000	-0.5450830000
C	-1.8464180000	1.6942100000	-1.7286760000
H	-0.9118670000	2.1758180000	-1.4505080000
H	-2.6440990000	2.4370210000	-1.8124210000
H	-1.7092490000	1.1932960000	-2.6873580000
C	0.7468510000	1.4147520000	0.4472370000
C	1.3516330000	0.1507810000	0.3993480000
C	2.6299330000	0.0239780000	-0.1381700000
C	3.3199510000	1.1377620000	-0.6243900000
C	2.7169880000	2.3931240000	-0.5650650000
C	1.4345230000	2.5367940000	-0.0306000000
H	3.2527420000	3.2635920000	-0.9309610000
H	0.9784400000	3.5224170000	0.0267890000
H	0.8416390000	-0.7272160000	0.7826570000
Br	3.4444710000	-1.6920300000	-0.2111280000
H	-0.9610800000	2.6206720000	0.9308420000
H	4.3154110000	1.0203190000	-1.0379580000
O	-0.6290490000	1.2722610000	2.4749940000
H	0.2276870000	1.5260400000	2.8550690000

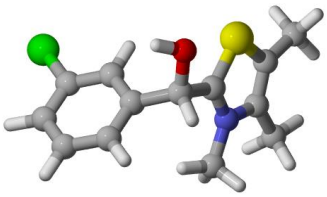
thermodynamic data

Zero-point correction= 0.256180 (Hartree/Particle)
Thermal correction to Energy= 0.274044
Thermal correction to Enthalpy= 0.274989
Thermal correction to Gibbs Free Energy= 0.207658
Sum of electronic and zero-point Energies= -3603.806357
Sum of electronic and thermal Energies= -3603.788493
Sum of electronic and thermal Enthalpies= -3603.787548
Sum of electronic and thermal Free Energies= -3603.854879

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.965	65.043	141.709

B3LYP/6-31G*	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.1280380000	0.5419730000	0.6005740000
N	-1.6636050000	0.8628230000	-0.5774630000
C	-2.8021140000	0.1135140000	-0.9286080000
C	-3.1210390000	-0.8041470000	0.0317210000
S	-1.9985110000	-0.7076140000	1.3680610000
C	-4.2344810000	-1.8082940000	0.0585480000
C	-3.4989200000	0.3749480000	-2.2282050000
C	0.0802510000	1.1689650000	1.2676790000
H	-3.8029030000	1.4232770000	-2.3232320000
H	-4.3988080000	-0.2369610000	-2.2995110000
H	-2.8643070000	0.1255470000	-3.0869120000
H	-4.7882070000	-1.7607430000	1.0018690000
H	-3.8490330000	-2.8281280000	-0.0528990000
H	-4.9429270000	-1.6274400000	-0.7525930000
C	-1.1449740000	1.9372750000	-1.4448920000
H	-0.1359850000	2.1997900000	-1.1354870000
H	-1.8000600000	2.8098680000	-1.3781220000
H	-1.1126070000	1.5802510000	-2.4746100000
C	1.3908140000	0.8766690000	0.5470860000
C	1.7642940000	-0.4465970000	0.2741720000
C	2.9924610000	-0.6984520000	-0.3335190000
C	3.8583680000	0.3466810000	-0.6694820000

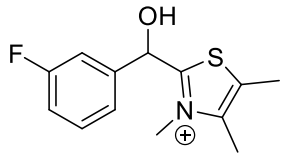
C	3.4836850000	1.6587570000	-0.3860090000
C	2.2551560000	1.9287130000	0.2213730000
H	4.1561590000	2.4740680000	-0.6341280000
H	1.9791100000	2.9547040000	0.4531930000
H	1.1166270000	-1.2770750000	0.5368860000
Cl	3.4517820000	-2.3477170000	-0.6800040000
H	-0.0732030000	2.2598890000	1.2877730000
H	4.8109810000	0.1293860000	-1.1403300000
O	0.0423380000	0.6425890000	2.5854050000
H	0.9347980000	0.6860540000	2.9655710000

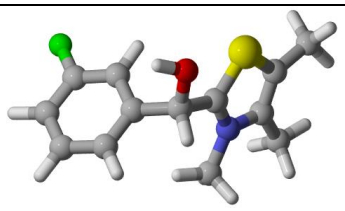
thermodynamic data

Zero-point correction= 0.256604 (Hartree/Particle)
Thermal correction to Energy= 0.274242
Thermal correction to Enthalpy= 0.275187
Thermal correction to Gibbs Free Energy= 0.209357
Sum of electronic and zero-point Energies= -1492.296813
Sum of electronic and thermal Energies= -1492.279175
Sum of electronic and thermal Enthalpies= -1492.278231
Sum of electronic and thermal Free Energies= -1492.344061

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	172.090	64.732	138.550

B3LYP/6-31G*	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8484680000	-0.0946360000	-0.7370300000
N	1.3784110000	1.0119290000	-0.2149060000
C	2.6084810000	0.8205060000	0.4417170000
C	3.0042030000	-0.4863620000	0.4061870000
S	1.8371780000	-1.4564210000	-0.4604690000
C	4.2273530000	-1.1274310000	0.9910430000
C	3.3105940000	1.9829850000	1.0733310000
C	-0.4423640000	-0.2180590000	-1.5218780000
H	3.4840890000	2.7928670000	0.3561500000
H	4.2819910000	1.6692450000	1.4573770000
H	2.7416860000	2.3914780000	1.9170500000
H	4.7166470000	-1.7838510000	0.2643520000

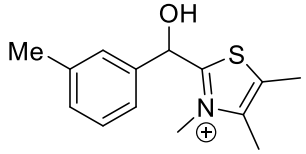
H	3.9749500000	-1.7304620000	1.8707540000
H	4.9541120000	-0.3726410000	1.2989380000
C	0.7631110000	2.3471730000	-0.3374550000
H	-0.2876650000	2.2413210000	-0.5982550000
H	1.2873710000	2.9233940000	-1.1045180000
H	0.8354610000	2.8615410000	0.6209120000
C	-1.6894960000	0.0294650000	-0.6828360000
C	-1.9114620000	-0.7121340000	0.4862680000
C	-3.0876520000	-0.5039040000	1.1950740000
C	-4.0520910000	0.4128760000	0.7805550000
C	-3.8248990000	1.1382750000	-0.3868000000
C	-2.6496110000	0.9500620000	-1.1206270000
H	-4.5695550000	1.8487120000	-0.7318030000
H	-2.4914090000	1.5084640000	-2.0399680000
H	-1.2001330000	-1.4487510000	0.8465490000
F	-3.2965850000	-1.2093290000	2.3149880000
H	-0.4130030000	0.5242200000	-2.3356920000
H	-4.9561120000	0.5389210000	1.3666630000
O	-0.3842310000	-1.5333070000	-2.0525810000
H	-1.2868610000	-1.8276950000	-2.2561980000

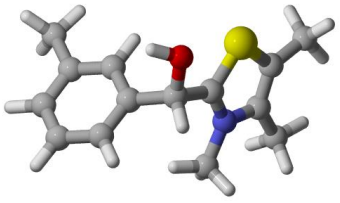
thermodynamic data

Zero-point correction= 0.258174 (Hartree/Particle)
Thermal correction to Energy= 0.275348
Thermal correction to Enthalpy= 0.276292
Thermal correction to Gibbs Free Energy= 0.212093
Sum of electronic and zero-point Energies= -1131.933819
Sum of electronic and thermal Energies= -1131.916645
Sum of electronic and thermal Enthalpies= -1131.915701
Sum of electronic and thermal Free Energies= -1131.979901

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	172.783	63.798	135.119

B3LYP/6-31G*	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8626270000	0.0595650000	-0.7490640000

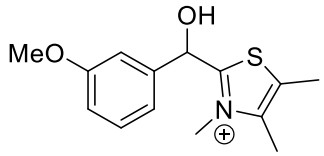
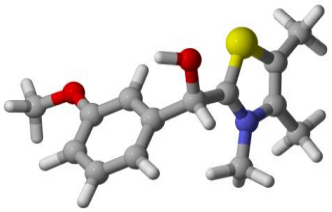
N	1.3989460000	1.0344640000	-0.0147630000
C	2.6154380000	0.6994770000	0.6096020000
C	2.9938820000	-0.5818520000	0.3272880000
S	1.8287950000	-1.3461210000	-0.7293660000
C	4.2007300000	-1.3438670000	0.7872220000
C	3.3221240000	1.7096100000	1.4602170000
C	-0.4186480000	0.1105970000	-1.5568430000
H	3.5179760000	2.6369010000	0.9105670000
H	4.2831580000	1.3144250000	1.7913150000
H	2.7447060000	1.9620960000	2.3575820000
H	4.7486530000	-1.7672580000	-0.0611730000
H	3.9179000000	-2.1701540000	1.4490500000
H	4.8865420000	-0.6957480000	1.3367490000
C	0.8012890000	2.3767410000	0.1156160000
H	-0.2459130000	2.3370840000	-0.1756900000
H	1.3448130000	3.0834280000	-0.5172860000
H	0.8623170000	2.6944890000	1.1566200000
C	-1.6728640000	0.2079670000	-0.6996610000
C	-1.9326960000	-0.7489920000	0.2939120000
C	-3.1106600000	-0.7094580000	1.0448900000
C	-4.0306950000	0.3198990000	0.7809790000
C	-3.7860990000	1.2706370000	-0.2063450000
C	-2.6069230000	1.2175660000	-0.9538980000
H	-4.5155700000	2.0507380000	-0.4024410000
H	-2.4253290000	1.9482820000	-1.7391270000
H	-1.2138410000	-1.5441110000	0.4801240000
H	-0.3684170000	0.9971770000	-2.2093080000
H	-4.9519280000	0.3692730000	1.3559370000
C	-3.3989850000	-1.7443540000	2.1056210000
H	-3.6193820000	-1.2731830000	3.0702740000
H	-2.5539630000	-2.4244630000	2.2465870000
H	-4.2732230000	-2.3493500000	1.8370300000
O	-0.3681740000	-1.0740690000	-2.3400820000
H	-1.2775630000	-1.3416010000	-2.5501770000

thermodynamic data

Zero-point correction= 0.293790 (Hartree/Particle)
Thermal correction to Energy= 0.312135
Thermal correction to Enthalpy= 0.313079
Thermal correction to Gibbs Free Energy= 0.245591
Sum of electronic and zero-point Energies= -1071.987617
Sum of electronic and thermal Energies= -1071.969272
Sum of electronic and thermal Enthalpies= -1071.968328
Sum of electronic and thermal Free Energies= -1072.035816

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	195.868	66.979	142.041

B3LYP/6-31G*	

xyz-matrix

36
XYZ file generated by gabedit : coordinates in Angstrom

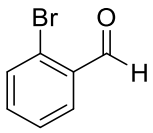
C	-1.2168890000	0.5636260000	0.5298120000
N	-1.7237290000	0.7346530000	-0.6910810000
C	-2.8433470000	-0.0684270000	-0.9804440000
C	-3.1765450000	-0.8714170000	0.0725480000
S	-2.0922640000	-0.5998390000	1.4176250000
C	-4.2797460000	-1.8799320000	0.1919750000
C	-3.5076200000	0.0304250000	-2.3191090000
C	-0.0404630000	1.2885970000	1.1519490000
H	-3.8102660000	1.0584170000	-2.5470470000
H	-4.4053190000	-0.5886260000	-2.3393010000
H	-2.8508740000	-0.3170490000	-3.1255750000
H	-4.9013480000	-1.6843820000	1.0721470000
H	-3.8783090000	-2.8953160000	0.2844980000
H	-4.9283140000	-1.8561800000	-0.6862180000
C	-1.1900970000	1.7062760000	-1.6640540000
H	-0.1819610000	1.9940260000	-1.3735890000
H	-1.8400110000	2.5847380000	-1.6995600000
H	-1.1504130000	1.2394480000	-2.6484200000
C	1.2931300000	0.9496000000	0.4997640000
C	1.7068090000	-0.3800790000	0.3991260000
C	2.9627770000	-0.6906790000	-0.1449930000
C	3.8002990000	0.3461310000	-0.5876420000
C	3.3782040000	1.6711030000	-0.4771340000
C	2.1321690000	1.9859550000	0.0642020000
H	4.0370020000	2.4669290000	-0.8116040000
H	1.8246730000	3.0236410000	0.1653230000
H	1.0833450000	-1.2004340000	0.7425520000
H	-0.2188160000	2.3703750000	1.0449630000
H	4.7743270000	0.1296570000	-1.0100200000
O	3.2642310000	-2.0077500000	-0.1991660000
C	4.5365960000	-2.4040930000	-0.7134990000
H	4.5536160000	-3.4919890000	-0.6464970000
H	4.6537310000	-2.1001570000	-1.7604410000
H	5.3536660000	-1.9877340000	-0.1129020000
O	-0.1023480000	0.9221360000	2.5233020000
H	0.8008780000	0.9118890000	2.8791590000

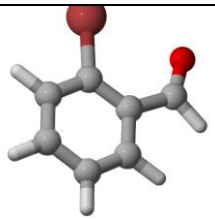
thermodynamic data

Zero-point correction= 0.299213 (Hartree/Particle)
Thermal correction to Energy= 0.318188
Thermal correction to Enthalpy= 0.319132
Thermal correction to Gibbs Free Energy= 0.251049
Sum of electronic and zero-point Energies= -1147.188341
Sum of electronic and thermal Energies= -1147.169367
Sum of electronic and thermal Enthalpies= -1147.168422
Sum of electronic and thermal Free Energies= -1147.236505

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	199.666	70.073	143.292

B3LYP/6-31G*	***o*-Br-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	0.1914030000	-0.3830450000	0.0000030000
C	0.7870320000	0.8926300000	0.0000180000
C	2.1909940000	0.9651030000	0.0000120000
C	2.9850830000	-0.1758010000	-0.0000030000
C	2.3716210000	-1.4296740000	-0.0000140000
C	0.9802760000	-1.5328740000	-0.0000110000
H	2.6538970000	1.9497950000	0.0000220000
H	4.0675060000	-0.0912030000	-0.0000050000
Br	-1.6955180000	-0.6346360000	0.0000040000
C	0.0675650000	2.1936550000	0.0000440000
H	0.7634870000	3.0630390000	-0.0000600000
O	-1.1321800000	2.3688160000	-0.0000450000
H	2.9723490000	-2.3349510000	-0.0000270000
H	0.4994770000	-2.5048980000	-0.0000210000

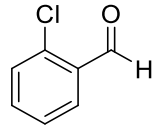
thermodynamic data

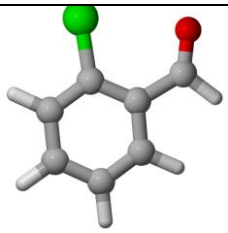
Zero-point correction= 0.100081 (Hartree/Particle)
Thermal correction to Energy= 0.107754

Thermal correction to Enthalpy= 0.108698
Thermal correction to Gibbs Free Energy= 0.066345
Sum of electronic and zero-point Energies= -2916.570669
Sum of electronic and thermal Energies= -2916.562996
Sum of electronic and thermal Enthalpies= -2916.562052
Sum of electronic and thermal Free Energies= -2916.604405

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.617	27.966	89.139

B3LYP/6-31G*	***o*-Cl-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

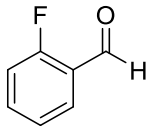
C	0.0348190000	-0.6107430000	0.0000000000
C	-0.0209790000	0.7975230000	0.0000020000
C	-1.2880850000	1.4060900000	0.0000010000
C	-2.4616230000	0.6610520000	0.0000000000
C	-2.3807240000	-0.7324470000	-0.0000010000
C	-1.1380350000	-1.3662980000	-0.0000010000
H	-1.3337380000	2.4931640000	0.0000020000
H	-3.4270460000	1.1576920000	-0.0000010000
Cl	1.5500850000	-1.4827810000	0.0000010000
C	1.1472400000	1.7172560000	0.0000040000
H	0.8413080000	2.7884810000	-0.0000060000
O	2.3208230000	1.4145880000	-0.0000040000
H	-3.2850840000	-1.3344770000	-0.0000030000
H	-1.0691550000	-2.4488760000	-0.0000020000

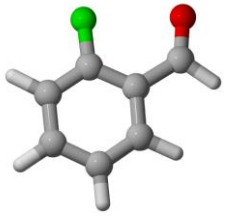
thermodynamic data

Zero-point correction= 0.100458 (Hartree/Particle)
Thermal correction to Energy= 0.107940
Thermal correction to Enthalpy= 0.108884
Thermal correction to Gibbs Free Energy= 0.067699
Sum of electronic and zero-point Energies= -805.060401
Sum of electronic and thermal Energies= -805.052919
Sum of electronic and thermal Enthalpies= -805.051975
Sum of electronic and thermal Free Energies= -805.093160

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.734	27.681	86.682

B3LYP/6-31G*	***o*-F-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

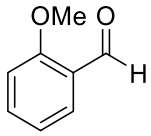
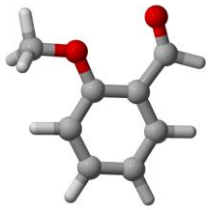
C	-0.0048900000	0.8425140000	0.0000000000
C	-0.3842240000	-0.5095870000	0.0000000000
C	0.6381580000	-1.4728230000	0.0000000000
C	1.9807000000	-1.1079380000	0.0000000000
C	2.3226350000	0.2476340000	0.0000000000
C	1.3303280000	1.2287180000	0.0000000000
H	0.3570720000	-2.5238230000	0.0000000000
H	2.7554340000	-1.8683760000	0.0000000000
F	-0.9396930000	1.8003810000	0.0000000000
C	-1.7925170000	-0.9688280000	0.0000000000
H	-1.8848620000	-2.0793510000	0.0000000000
O	-2.7811960000	-0.2653410000	-0.0000010000
H	3.3672330000	0.5460110000	0.0000000000
H	1.5707940000	2.2866980000	0.0000000000

thermodynamic data

Zero-point correction= 0.101956 (Hartree/Particle)
Thermal correction to Energy= 0.109083
Thermal correction to Enthalpy= 0.110027
Thermal correction to Gibbs Free Energy= 0.070114
Sum of electronic and zero-point Energies= -444.699429
Sum of electronic and thermal Energies= -444.692302
Sum of electronic and thermal Enthalpies= -444.691358
Sum of electronic and thermal Free Energies= -444.731271

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.451	26.780	84.005

B3LYP/6-31G*	***o*-OMe-PhCHO**

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

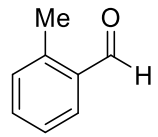
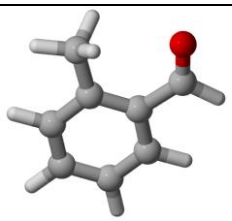
C	-0.2126750000	-0.4574340000	-0.0000220000
C	0.2104360000	0.8987050000	-0.0000460000
C	1.5846940000	1.1761080000	-0.0000190000
C	2.5407360000	0.1656130000	0.0000150000
C	2.1102830000	-1.1613720000	0.0000320000
C	0.7507750000	-1.4767080000	0.0000140000
H	1.8955250000	2.2190530000	-0.0000330000
H	3.5995890000	0.4044800000	0.0000300000
C	-0.7084010000	2.0585490000	-0.0001050000
H	-0.1594960000	3.0301870000	0.0001580000
O	-1.9227520000	2.0441150000	0.0000980000
H	2.8374730000	-1.9692680000	0.0000610000
H	0.4478600000	-2.5169880000	0.0000280000
O	-1.5436020000	-0.6859970000	-0.0000390000
C	-2.0129320000	-2.0268340000	0.0000040000
H	-3.1013270000	-1.9545940000	0.0000000000
H	-1.6831420000	-2.5688160000	-0.8956020000
H	-1.6831440000	-2.5687580000	0.8956450000

thermodynamic data

Zero-point correction= 0.142975 (Hartree/Particle)
Thermal correction to Energy= 0.151814
Thermal correction to Enthalpy= 0.152758
Thermal correction to Gibbs Free Energy= 0.108987
Sum of electronic and zero-point Energies= -459.947808
Sum of electronic and thermal Energies= -459.938969
Sum of electronic and thermal Enthalpies= -459.938025
Sum of electronic and thermal Free Energies= -459.981796

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.265	32.958	92.125

B3LYP/6-31G*	***o*-Me-PhCHO**

xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

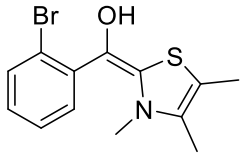
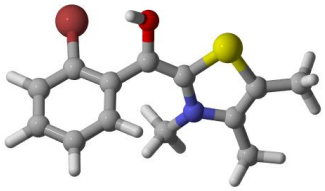
C	0.0567000000	0.8489320000	-0.0000010000
C	0.3103790000	-0.5464840000	-0.0000020000
C	-0.7578200000	-1.4577110000	-0.0000010000
C	-2.0786140000	-1.0224610000	0.0000010000
C	-2.3353130000	0.3490640000	0.0000020000
C	-1.2795730000	1.2632130000	0.0000010000
H	-0.5358220000	-2.5230560000	-0.0000020000
H	-2.8953970000	-1.7383230000	0.0000010000
C	1.1594190000	1.8782870000	-0.0000020000
C	1.6706650000	-1.1257640000	-0.0000050000
H	1.6778970000	-2.2398440000	0.0000060000
O	2.7220020000	-0.5110100000	0.0000050000
H	-3.3598460000	0.7120440000	0.0000030000
H	-1.4965560000	2.3286300000	0.0000020000
H	0.7363730000	2.8879340000	-0.0000020000
H	1.8111400000	1.7691180000	-0.8725770000
H	1.8111410000	1.7691190000	0.8725730000

thermodynamic data

Zero-point correction= 0.138214 (Hartree/Particle)
Thermal correction to Energy= 0.146013
Thermal correction to Enthalpy= 0.146957
Thermal correction to Gibbs Free Energy= 0.105954
Sum of electronic and zero-point Energies= -384.752071
Sum of electronic and thermal Energies= -384.744272
Sum of electronic and thermal Enthalpies= -384.743328
Sum of electronic and thermal Free Energies= -384.784331

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.625	29.645	86.299

B3LYP/6-31G*	

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2377910000	-0.2546300000	-0.2997890000
N	1.8340640000	0.7490090000	0.4663300000
C	3.2428960000	0.6590870000	0.5200510000
C	3.7534210000	-0.4161360000	-0.1177480000
S	2.4718130000	-1.4173280000	-0.8389460000
C	5.1771220000	-0.8465260000	-0.2859380000
C	4.0139300000	1.7277650000	1.2376700000
C	-0.0763320000	-0.4520340000	-0.6005130000
H	3.7004180000	2.7285580000	0.9165380000
H	5.0816290000	1.6312520000	1.0319520000
H	3.8877780000	1.6773260000	2.3271600000
H	5.4674170000	-0.8870270000	-1.3439890000
H	5.3385530000	-1.8493130000	0.1313450000
H	5.8644420000	-0.1645760000	0.2223550000
C	1.0548300000	1.5083690000	1.4357390000
H	0.2695070000	0.8642910000	1.8462560000
H	0.5711400000	2.3847630000	0.9888320000
H	1.6995960000	1.8403850000	2.2500650000
C	-1.1672620000	0.5273070000	-0.5389980000
C	-2.4703570000	0.2373890000	-0.0748460000
C	-3.4979170000	1.1769700000	-0.1206780000
C	-3.2542760000	2.4569900000	-0.6190310000
C	-1.9757730000	2.7846440000	-1.0745630000
C	-0.9629130000	1.8313880000	-1.0467620000
Br	-2.8745200000	-1.4563610000	0.7246920000
H	-4.4799390000	0.9066770000	0.2526180000
H	-1.7737450000	3.7739330000	-1.4761750000
H	0.0169800000	2.0712040000	-1.4497800000
O	-0.3543530000	-1.7218500000	-1.1117640000
H	-0.9805950000	-1.6257140000	-1.8474020000
H	-4.0585830000	3.1863680000	-0.6486070000

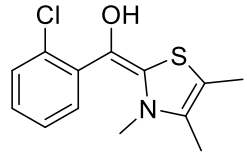
thermodynamic data

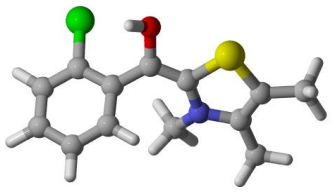
Zero-point correction= 0.242708 (Hartree/Particle)
Thermal correction to Energy= 0.260410
Thermal correction to Enthalpy= 0.261354
Thermal correction to Gibbs Free Energy= 0.195998

Sum of electronic and zero-point Energies= -3603.400118
Sum of electronic and thermal Energies= -3603.382416
Sum of electronic and thermal Enthalpies= -3603.381472
Sum of electronic and thermal Free Energies= -3603.446828

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.410	65.165	137.554

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9028580000	-0.3870150000	-0.1625770000
N	1.4219490000	0.7830980000	0.3945470000
C	2.8329700000	0.8499210000	0.3598050000
C	3.4268250000	-0.2566870000	-0.1365330000
S	2.2300070000	-1.4891120000	-0.5975340000
C	4.8790440000	-0.5599330000	-0.3360100000
C	3.5158280000	2.0957930000	0.8423760000
C	-0.3940630000	-0.7677960000	-0.3421480000
H	3.0761120000	2.9923380000	0.3885720000
H	4.5752240000	2.0755150000	0.5799080000
H	3.4540230000	2.2144000000	1.9321280000
H	5.1150010000	-0.7421570000	-1.3926460000
H	5.1744190000	-1.4594780000	0.2201470000
H	5.5113520000	0.2625740000	0.0096220000
C	0.6157850000	1.6101200000	1.2829140000
H	-0.0709680000	0.9682430000	1.8451630000
H	0.0152590000	2.3473840000	0.7375080000
H	1.2623170000	2.1343890000	1.9871860000
C	-1.5842180000	0.0889430000	-0.3687370000
C	-2.8366260000	-0.2695410000	0.1840400000
C	-3.9601080000	0.5455340000	0.0551660000
C	-3.8719340000	1.7613880000	-0.6221510000
C	-2.6505950000	2.1521740000	-1.1742860000
C	-1.5401020000	1.3227130000	-1.0596360000
Cl	-3.0227700000	-1.7444000000	1.1310250000
H	-4.8958260000	0.2279760000	0.5034730000
H	-2.5688750000	3.0898580000	-1.7172730000
H	-0.6047530000	1.6031840000	-1.5354540000

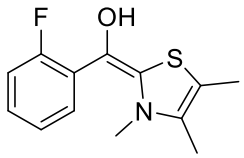
O	-0.5456810000	-2.1257120000	-0.6312380000
H	-1.1872180000	-2.2152880000	-1.3545330000
H	-4.7512690000	2.3919720000	-0.7159460000

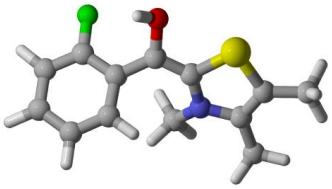
thermodynamic data

Zero-point correction= 0.243151 (Hartree/Particle)
Thermal correction to Energy= 0.260600
Thermal correction to Enthalpy= 0.261545
Thermal correction to Gibbs Free Energy= 0.197650
Sum of electronic and zero-point Energies= -1491.889606
Sum of electronic and thermal Energies= -1491.872156
Sum of electronic and thermal Enthalpies= -1491.871211
Sum of electronic and thermal Free Energies= -1491.935106

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.529	64.841	134.478

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7471330000	-0.4568180000	-0.0373180000
N	1.2186910000	0.8115100000	0.3113620000
C	2.6213730000	0.9433470000	0.1941930000
C	3.2574760000	-0.1944860000	-0.1572550000
S	2.1180960000	-1.5459430000	-0.3592200000
C	4.7149820000	-0.4471050000	-0.3867030000
C	3.2490540000	2.2832140000	0.4446830000
C	-0.5318500000	-0.9233640000	-0.1004670000
H	2.7287420000	3.0753120000	-0.1073810000
H	4.2919910000	2.2822080000	0.1221650000
H	3.2388160000	2.5611440000	1.5068070000
H	4.9141930000	-0.7751850000	-1.4153290000
H	5.0885420000	-1.2348300000	0.2808990000
H	5.3112750000	0.4506900000	-0.2016220000
C	0.4177150000	1.6994370000	1.1450210000
H	-0.1850180000	1.0989210000	1.8350510000
H	-0.2672320000	2.3208610000	0.5567260000
H	1.0718800000	2.3511570000	1.7248290000

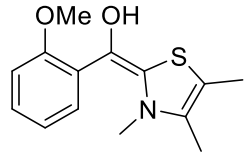
C	-1.7715420000	-0.1512310000	-0.1983630000
C	-2.9721990000	-0.5800140000	0.4028130000
C	-4.1732270000	0.1006240000	0.2663380000
C	-4.2172270000	1.2696700000	-0.4961120000
C	-3.0536150000	1.7288860000	-1.1171180000
C	-1.8608290000	1.0219960000	-0.9809250000
F	-2.9638760000	-1.6946510000	1.1679540000
H	-5.0522360000	-0.2887410000	0.7703560000
H	-3.0795320000	2.6257920000	-1.7298420000
H	-0.9717310000	1.3549360000	-1.5084500000
O	-0.6189080000	-2.3166870000	-0.1544040000
H	-1.2940290000	-2.5565000000	-0.8093250000
H	-5.1533420000	1.8091870000	-0.6059870000

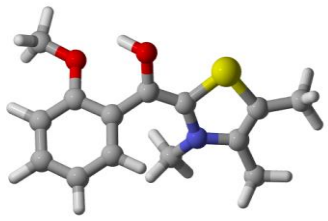
thermodynamic data

Zero-point correction= 0.244662 (Hartree/Particle)
Thermal correction to Energy= 0.261729
Thermal correction to Enthalpy= 0.262673
Thermal correction to Gibbs Free Energy= 0.199880
Sum of electronic and zero-point Energies= -1131.527580
Sum of electronic and thermal Energies= -1131.510513
Sum of electronic and thermal Enthalpies= -1131.509569
Sum of electronic and thermal Free Energies= -1131.572362

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.238	63.937	132.160

B3LYP/6-31G*	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9523510000	-0.3792240000	-0.1477650000
N	1.5255830000	0.8120460000	0.3257920000
C	2.9422970000	0.7811070000	0.3313070000
C	3.4790040000	-0.3861150000	-0.0802000000
S	2.2245520000	-1.5739560000	-0.5049600000
C	4.9152780000	-0.7747380000	-0.2455620000
C	3.6915630000	2.0153020000	0.7420270000

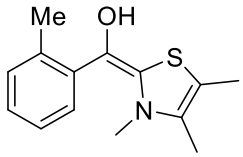
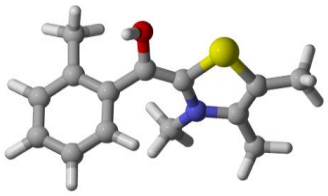
C	-0.3534390000	-0.7056950000	-0.3484250000
H	3.2882700000	2.9050770000	0.2434910000
H	4.7459570000	1.9304810000	0.4714230000
H	3.6496960000	2.1967910000	1.8242450000
H	5.1496520000	-1.0292110000	-1.2876860000
H	5.1580910000	-1.6558580000	0.3631350000
H	5.5874370000	0.0317310000	0.0607720000
C	0.7865050000	1.6290870000	1.2868670000
H	0.1985860000	0.9809890000	1.9485460000
H	0.0954530000	2.3194320000	0.7938060000
H	1.4847840000	2.2086190000	1.8906470000
C	-1.5154060000	0.1953960000	-0.3801260000
C	-2.7809540000	-0.2261540000	0.1055060000
C	-3.8990440000	0.6028150000	0.0279120000
C	-3.7855740000	1.8790300000	-0.5342410000
C	-2.5592740000	2.3151470000	-1.0279460000
C	-1.4480390000	1.4733340000	-0.9600570000
H	-4.8589440000	0.2714650000	0.4072040000
H	-2.4681500000	3.2959410000	-1.4863710000
H	-0.5025370000	1.7903710000	-1.3902390000
O	-0.5602960000	-2.0286270000	-0.7440920000
H	-1.3497600000	-2.3391940000	-0.2663600000
H	-4.6624100000	2.5182530000	-0.5875630000
O	-2.8130540000	-1.4875510000	0.6641760000
C	-4.0475200000	-1.9859660000	1.1592820000
H	-3.8356110000	-2.9870830000	1.5389010000
H	-4.4287060000	-1.3612300000	1.9765760000
H	-4.8033830000	-2.0481270000	0.3661370000

thermodynamic data

Zero-point correction= 0.286354 (Hartree/Particle)
Thermal correction to Energy= 0.304851
Thermal correction to Enthalpy= 0.305796
Thermal correction to Gibbs Free Energy= 0.240048
Sum of electronic and zero-point Energies= -1146.776674
Sum of electronic and thermal Energies= -1146.758176
Sum of electronic and thermal Enthalpies= -1146.757232
Sum of electronic and thermal Free Energies= -1146.822979

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	191.297	69.619	138.377

B3LYP/6-31G*	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7420430000	-0.4416430000	-0.0853600000
N	1.2105390000	0.8115980000	0.3169080000
C	2.6148290000	0.9440140000	0.2495870000
C	3.2598920000	-0.1793120000	-0.1313210000
S	2.1217560000	-1.5149790000	-0.4282770000
C	4.7228020000	-0.4295680000	-0.3249720000
C	3.2394480000	2.2679820000	0.5784590000
C	-0.5333020000	-0.9056810000	-0.1908300000
H	2.7589540000	3.0845250000	0.0256420000
H	4.2984910000	2.2653080000	0.3139940000
H	3.1724310000	2.5099460000	1.6473480000
H	4.9529840000	-0.7156580000	-1.3598340000
H	5.0737480000	-1.2458780000	0.3203820000
H	5.3164980000	0.4569890000	-0.0850890000
C	0.3625400000	1.7197680000	1.0757270000
H	-0.2718790000	1.1402400000	1.7554830000
H	-0.2955120000	2.3125480000	0.4303990000
H	0.9819030000	2.3965140000	1.6647590000
C	-1.7954910000	-0.1495510000	-0.2471400000
C	-2.9433590000	-0.5581970000	0.4854030000
C	-4.1304270000	0.1641760000	0.3284170000
C	-4.2163120000	1.2729530000	-0.5164490000
C	-3.0904940000	1.6786190000	-1.2318380000
C	-1.9005570000	0.9646470000	-1.1037260000
H	-5.0058830000	-0.1418860000	0.8974310000
H	-3.1412580000	2.5330590000	-1.9019640000
H	-1.0322580000	1.2505600000	-1.6918530000
O	-0.6177950000	-2.2984560000	-0.3539540000
H	-1.1561710000	-2.4689890000	-1.1451230000
H	-5.1548950000	1.8124570000	-0.6120930000
C	-2.8922970000	-1.7136610000	1.4577130000
H	-3.7814390000	-1.7211710000	2.0964460000
H	-2.0046480000	-1.6482920000	2.0978550000
H	-2.8264660000	-2.6814250000	0.9498970000

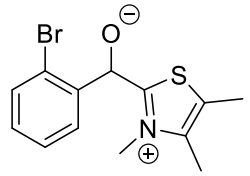
thermodynamic data

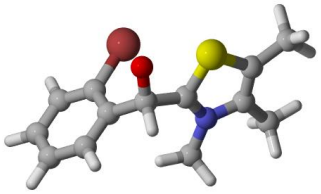
Zero-point correction= 0.280820 (Hartree/Particle)
Thermal correction to Energy= 0.298586
Thermal correction to Enthalpy= 0.299530
Thermal correction to Gibbs Free Energy= 0.235666
Sum of electronic and zero-point Energies= -1071.576486

Sum of electronic and thermal Energies= -1071.558720
Sum of electronic and thermal Enthalpies= -1071.557776
Sum of electronic and thermal Free Energies= -1071.621641

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	187.366	66.772	134.414

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8704870000	0.5216520000	0.6858760000
N	-1.3960200000	1.2269010000	-0.3170740000
C	-2.7212100000	0.8723150000	-0.6459730000
C	-3.1840000000	-0.1167180000	0.1696650000
S	-1.9590620000	-0.6113850000	1.3473160000
C	-4.5304790000	-0.7764390000	0.1578360000
C	-3.4121530000	1.5714690000	-1.7780970000
C	0.4285140000	0.5333110000	1.5390280000
H	-3.4722520000	2.6550790000	-1.6173870000
H	-4.4323800000	1.1981410000	-1.8834960000
H	-2.9009100000	1.4064480000	-2.7348100000
H	-5.0241570000	-0.6837160000	1.1323930000
H	-4.4449530000	-1.8471560000	-0.0626010000
H	-5.1914880000	-0.3342800000	-0.5927530000
C	-0.6463940000	2.2667250000	-1.0274120000
H	0.3571710000	2.3227000000	-0.6085670000
H	-1.1472970000	3.2320790000	-0.9136000000
H	-0.5755930000	2.0161200000	-2.0889420000
C	1.7249680000	0.5815270000	0.6938200000
C	2.0905740000	-0.3719220000	-0.2640170000
C	3.3244830000	-0.3431410000	-0.9100640000
C	4.2453060000	0.6576630000	-0.5953020000
C	3.9176940000	1.6204340000	0.3579900000
C	2.6728170000	1.5733920000	0.9862150000
H	4.6283740000	2.4005220000	0.6175540000
H	2.4223150000	2.3129550000	1.7440910000
O	0.3316380000	-0.4930750000	2.3631120000
Br	0.8817460000	-1.7776500000	-0.7634590000
H	0.3755730000	1.5604680000	2.0133000000

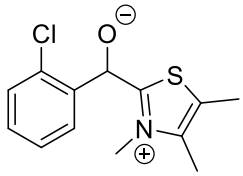
H	5.2109640000	0.6753520000	-1.0931090000
H	3.5597710000	-1.1001090000	-1.6508290000

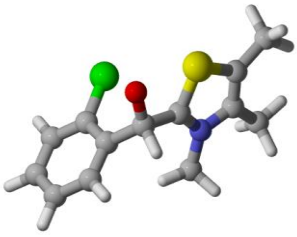
thermodynamic data

Zero-point correction= 0.241900 (Hartree/Particle)
Thermal correction to Energy= 0.259368
Thermal correction to Enthalpy= 0.260312
Thermal correction to Gibbs Free Energy= 0.194815
Sum of electronic and zero-point Energies= -3603.371586
Sum of electronic and thermal Energies= -3603.354119
Sum of electronic and thermal Enthalpies= -3603.353174
Sum of electronic and thermal Free Energies= -3603.418671

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.756	63.667	137.849

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7436260000	-0.0826240000	0.6805360000
N	-1.2611720000	1.0809130000	0.2816240000
C	-2.6018270000	1.0028060000	-0.1504070000
C	-3.0813570000	-0.2685300000	-0.0439100000
S	-1.8542890000	-1.3723220000	0.5978360000
C	-4.4456430000	-0.7799100000	-0.3983290000
C	-3.2892540000	2.2394710000	-0.6467080000
C	0.5690610000	-0.5857120000	1.3364300000
H	-3.3145980000	3.0291890000	0.1144580000
H	-4.3214040000	2.0120990000	-0.9193860000
H	-2.7976100000	2.6528530000	-1.5362890000
H	-4.9087550000	-1.2916130000	0.4534220000
H	-4.3964320000	-1.5009790000	-1.2231070000
H	-5.1150890000	0.0291490000	-0.7035600000
C	-0.4925130000	2.3286830000	0.2890410000
H	0.5267030000	2.1099530000	0.6043260000
H	-0.9467840000	3.0442390000	0.9803400000
H	-0.4698670000	2.7581290000	-0.7156310000
C	1.8493290000	-0.1057370000	0.6069700000

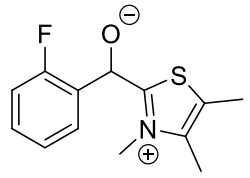
C	2.1443170000	-0.3363300000	-0.7445210000
C	3.3714680000	0.0141480000	-1.3061760000
C	4.3540580000	0.6054980000	-0.5113050000
C	4.0966750000	0.8452080000	0.8374240000
C	2.8599170000	0.4907210000	1.3759480000
H	4.8550360000	1.2988920000	1.4698540000
H	2.6640090000	0.6594830000	2.4328090000
O	0.4415860000	-1.8949650000	1.4497150000
Cl	0.9532340000	-1.0675350000	-1.8258580000
H	0.5772740000	-0.0004630000	2.3059690000
H	5.3123140000	0.8709490000	-0.9491670000
H	3.5507450000	-0.1794520000	-2.3588580000

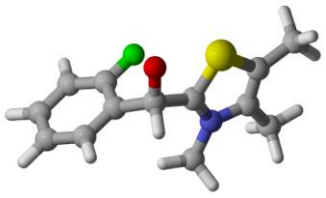
thermodynamic data

Zero-point correction= 0.242287 (Hartree/Particle)
Thermal correction to Energy= 0.259564
Thermal correction to Enthalpy= 0.260509
Thermal correction to Gibbs Free Energy= 0.196031
Sum of electronic and zero-point Energies= -1491.859579
Sum of electronic and thermal Energies= -1491.842301
Sum of electronic and thermal Enthalpies= -1491.841357
Sum of electronic and thermal Free Energies= -1491.905834

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.879	63.363	135.704

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.6552420000	-0.2879190000	-0.6105710000
N	1.1868800000	0.9328340000	-0.5292460000
C	2.5043630000	0.9582750000	-0.0260630000
C	2.9465010000	-0.2988760000	0.2606040000
S	1.7139860000	-1.5195250000	-0.1031690000
C	4.2775030000	-0.7108210000	0.8147030000
C	3.2093580000	2.2727280000	0.1265500000
C	-0.6638070000	-0.9202830000	-1.1078910000
H	3.2800920000	2.8141070000	-0.8250960000

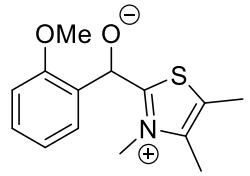
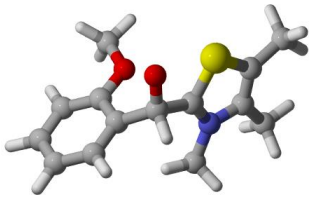
H	4.2261090000	2.1139230000	0.4903900000
H	2.7023770000	2.9298320000	0.8443700000
H	4.7649880000	-1.4467280000	0.1645560000
H	4.1688970000	-1.1722850000	1.8035720000
H	4.9550060000	0.1414010000	0.9183720000
C	0.4525300000	2.1352960000	-0.9320100000
H	-0.5680290000	1.8514840000	-1.1855270000
H	0.9338040000	2.5981210000	-1.7985110000
H	0.4270480000	2.8502170000	-0.1059350000
C	-1.8933060000	-0.2776260000	-0.4269120000
C	-1.9987500000	-0.1440650000	0.9598300000
C	-3.1486080000	0.3045970000	1.5942080000
C	-4.2669690000	0.6224490000	0.8186870000
C	-4.2066180000	0.4967120000	-0.5690390000
C	-3.0295260000	0.0497640000	-1.1755700000
H	-5.0738220000	0.7369680000	-1.1780570000
H	-2.9864200000	-0.0667470000	-2.2564930000
O	-0.5362700000	-2.2232560000	-0.9061800000
F	-0.9155620000	-0.4180600000	1.7312500000
H	-0.7268510000	-0.5836120000	-2.1855070000
H	-5.1766560000	0.9674020000	1.3023650000
H	-3.1557410000	0.3956950000	2.6759530000

thermodynamic data

Zero-point correction= 0.243961 (Hartree/Particle)
Thermal correction to Energy= 0.260776
Thermal correction to Enthalpy= 0.261720
Thermal correction to Gibbs Free Energy= 0.198812
Sum of electronic and zero-point Energies= -1131.499346
Sum of electronic and thermal Energies= -1131.482531
Sum of electronic and thermal Enthalpies= -1131.481587
Sum of electronic and thermal Free Energies= -1131.544495

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.639	62.346	132.402

B3LYP/6-31G*	

xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7552270000	0.2384000000	0.7317000000
N	-1.2901100000	1.1429670000	-0.0895500000
C	-2.6062350000	0.8443320000	-0.5019570000
C	-3.0444760000	-0.3203670000	0.0530250000
S	-1.8084840000	-1.0483410000	1.0990950000
C	-4.3743580000	-0.9897810000	-0.1246930000
C	-3.3139790000	1.7793540000	-1.4365620000
C	0.5473380000	0.0686680000	1.5386840000
H	-3.3968130000	2.7912790000	-1.0205260000
H	-4.3262260000	1.4207880000	-1.6324790000
H	-2.8011180000	1.8612320000	-2.4033280000
H	-4.8697450000	-1.1466520000	0.8408410000
H	-4.2635670000	-1.9744050000	-0.5950540000
H	-5.0477240000	-0.3971060000	-0.7505350000
C	-0.5598240000	2.3383900000	-0.5179430000
H	0.4641730000	2.2691910000	-0.1523050000
H	-1.0373660000	3.2368120000	-0.1156980000
H	-0.5440930000	2.3939870000	-1.6092210000
C	1.8156790000	0.2285950000	0.6687160000
C	2.0229250000	-0.5154760000	-0.5131710000
C	3.2511260000	-0.4673560000	-1.1789140000
C	4.2909940000	0.3210810000	-0.6734650000
C	4.1054720000	1.0660380000	0.4859240000
C	2.8715080000	1.0078280000	1.1427090000
H	4.9105490000	1.6763320000	0.8858600000
H	2.7250150000	1.5642370000	2.0664690000
O	0.4312780000	-1.0963670000	2.1630270000
H	0.5473320000	0.9856970000	2.2017430000
H	5.2425840000	0.3456520000	-1.1983330000
H	3.4076840000	-1.0359270000	-2.0890340000
O	0.9478440000	-1.2298600000	-0.9703230000
C	1.1470030000	-2.1614140000	-2.0177520000
H	0.1997930000	-2.6928660000	-2.1307300000
H	1.3971570000	-1.6654270000	-2.9665180000
H	1.9382200000	-2.8800760000	-1.7692760000

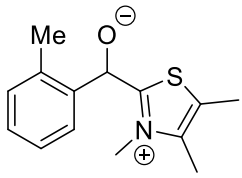
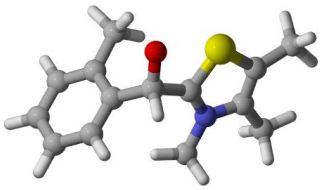
thermodynamic data

Zero-point correction= 0.284845 (Hartree/Particle)
Thermal correction to Energy= 0.303431
Thermal correction to Enthalpy= 0.304375
Thermal correction to Gibbs Free Energy= 0.237478
Sum of electronic and zero-point Energies= -1146.744114
Sum of electronic and thermal Energies= -1146.725529
Sum of electronic and thermal Enthalpies= -1146.724584
Sum of electronic and thermal Free Energies= -1146.791482

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	190.406	68.543	140.798

B3LYP/6-31G*	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

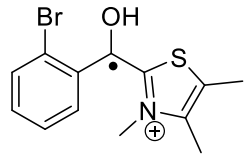
C	0.6791770000	-0.1408480000	-0.5680810000
N	1.1811040000	1.0464440000	-0.2148590000
C	2.5220800000	1.0043140000	0.2230600000
C	3.0169600000	-0.2645540000	0.1820070000
S	1.8053220000	-1.4137850000	-0.4132460000
C	4.3853260000	-0.7412130000	0.5679930000
C	3.1956400000	2.2714250000	0.6590340000
C	-0.6259930000	-0.7096990000	-1.1957030000
H	3.1962570000	3.0299250000	-0.1334070000
H	4.2354210000	2.0713470000	0.9240610000
H	2.7116090000	2.7133300000	1.5391850000
H	4.8520740000	-1.3029360000	-0.2495160000
H	4.3426360000	-1.4086140000	1.4372820000
H	5.0488060000	0.0907640000	0.8201530000
C	0.4107010000	2.2911560000	-0.2995300000
H	-0.6250270000	2.0480760000	-0.5319340000
H	0.8255780000	2.9357020000	-1.0803220000
H	0.4475370000	2.8145960000	0.6586870000
C	-1.8963900000	-0.2065600000	-0.4651150000
C	-2.2569810000	-0.6541240000	0.8263030000
C	-3.4553130000	-0.1908780000	1.3828390000
C	-4.2966870000	0.6901350000	0.7001950000
C	-3.9481010000	1.1182980000	-0.5783610000
C	-2.7579850000	0.6611250000	-1.1484860000
H	-4.5999010000	1.7866110000	-1.1356600000
H	-2.4972380000	0.9672070000	-2.1608310000
O	-0.4346700000	-2.0251750000	-1.2512230000
H	-0.6468190000	-0.1884440000	-2.1957120000
H	-5.2228370000	1.0245080000	1.1609720000
H	-3.7375160000	-0.5391680000	2.3746550000
C	-1.3916810000	-1.6215060000	1.5995940000
H	-1.9609140000	-2.0986730000	2.4043420000
H	-0.5342500000	-1.1139610000	2.0649460000
H	-0.9954430000	-2.3758490000	0.9143520000

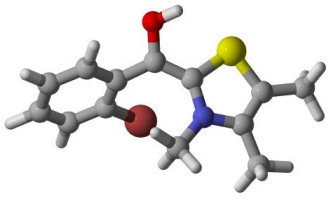
thermodynamic data

Zero-point correction= 0.279957 (Hartree/Particle)
Thermal correction to Energy= 0.297480
Thermal correction to Enthalpy= 0.298424
Thermal correction to Gibbs Free Energy= 0.234310
Sum of electronic and zero-point Energies= -1071.546890
Sum of electronic and thermal Energies= -1071.529367
Sum of electronic and thermal Enthalpies= -1071.528423
Sum of electronic and thermal Free Energies= -1071.592537

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.671	65.333	134.939

(u)B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8804840000	0.8845650000	0.0533040000
N	1.2695570000	-0.0456670000	0.9766960000
C	2.6062620000	-0.4305950000	0.8839440000
C	3.2970860000	0.2462400000	-0.0860850000
S	2.2428490000	1.3508140000	-0.9354310000
C	4.7395520000	0.1545190000	-0.4786430000
C	3.1522350000	-1.4764780000	1.8079540000
C	-0.3905730000	1.4551220000	-0.1532090000
H	2.5344760000	-2.3805290000	1.7952710000
H	3.2091270000	-1.1171060000	2.8425310000
H	4.1606010000	-1.7596960000	1.5050810000
H	5.2573630000	1.1038500000	-0.2989670000
H	4.8479260000	-0.0883200000	-1.5415260000
H	5.2536380000	-0.6188090000	0.0953190000
C	0.3868760000	-0.5511080000	2.0396400000
H	-0.0962130000	-1.4751870000	1.7137030000
H	-0.3701200000	0.1990140000	2.2609000000
H	0.9786530000	-0.7338020000	2.9354010000
C	-1.7050800000	0.8797260000	0.1214830000
C	-2.0746270000	-0.4492770000	-0.1850780000
C	-3.3601880000	-0.9148950000	0.0725030000

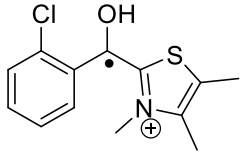
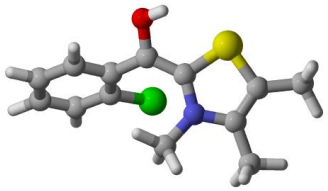
C	-4.3115170000	-0.0573270000	0.6279510000
C	-3.9830950000	1.2715320000	0.9092160000
C	-2.7002420000	1.7341990000	0.6493970000
Br	-0.8672350000	-1.6498430000	-1.0533480000
H	-5.3128040000	-0.4286110000	0.8235760000
H	-4.7255320000	1.9433760000	1.3274600000
H	-2.4389790000	2.7657040000	0.8603800000
H	-3.6200520000	-1.9358280000	-0.1836460000
O	-0.4603040000	2.6653060000	-0.7577050000
H	0.3620640000	3.1773010000	-0.6509100000

thermodynamic data

Zero-point correction= 0.244290 (Hartree/Particle)
Thermal correction to Energy= 0.261602
Thermal correction to Enthalpy= 0.262546
Thermal correction to Gibbs Free Energy= 0.197437
Sum of electronic and zero-point Energies= -3603.193925
Sum of electronic and thermal Energies= -3603.176613
Sum of electronic and thermal Enthalpies= -3603.175669
Sum of electronic and thermal Free Energies= -3603.240779

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.158	64.212	137.035

(u)B3LYP/6-31G*		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7547440000	0.6768030000	-0.1616140000
N	-1.1591470000	-0.5020900000	-0.7239590000
C	-2.5108100000	-0.7962980000	-0.5456650000
C	-3.1957030000	0.1893490000	0.1139650000
S	-2.1196940000	1.4902400000	0.5663660000
C	-4.6479310000	0.2742670000	0.4703420000
C	-3.0743080000	-2.0794650000	-1.0765080000
C	0.5329940000	1.2456100000	-0.1230130000
H	-2.4721710000	-2.9385530000	-0.7631550000

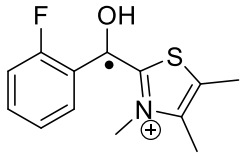
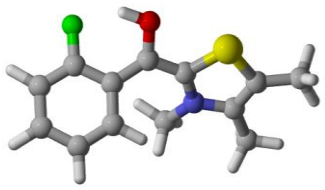
H	-3.1245990000	-2.0802290000	-2.1721100000
H	-4.0874490000	-2.2313620000	-0.7031340000
H	-5.1296970000	1.1155540000	-0.0413030000
H	-4.7858400000	0.4159100000	1.5479540000
H	-5.1755170000	-0.6369600000	0.1820280000
C	-0.2875550000	-1.3446940000	-1.5584830000
H	0.1378360000	-2.1577470000	-0.9658460000
H	0.5145110000	-0.7334770000	-1.9674830000
H	-0.8746360000	-1.7546030000	-2.3796910000
C	1.8286260000	0.5710870000	-0.1421060000
C	2.1365250000	-0.5907360000	0.6043460000
C	3.4103000000	-1.1506460000	0.5649860000
C	4.4079990000	-0.5569650000	-0.2096370000
C	4.1400670000	0.6096550000	-0.9308470000
C	2.8709960000	1.1698090000	-0.8871400000
Cl	0.9619930000	-1.3246820000	1.6860380000
H	5.3985800000	-1.0006050000	-0.2325860000
H	4.9189520000	1.0809220000	-1.5213390000
H	2.6557750000	2.0780930000	-1.4395780000
H	3.6223680000	-2.0326360000	1.1592680000
O	0.6376640000	2.5881370000	0.0256570000
H	-0.1629050000	3.0543440000	-0.2768130000

thermodynamic data

Zero-point correction= 0.244580 (Hartree/Particle)
Thermal correction to Energy= 0.261745
Thermal correction to Enthalpy= 0.262690
Thermal correction to Gibbs Free Energy= 0.198572
Sum of electronic and zero-point Energies= -1491.681135
Sum of electronic and thermal Energies= -1491.663970
Sum of electronic and thermal Enthalpies= -1491.663026
Sum of electronic and thermal Free Energies= -1491.727144

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.248	63.994	134.947

(u)B3LYP/6-31G*	

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7642570000	-0.4534220000	0.0453260000
N	1.2681190000	0.7673460000	0.3994580000
C	2.6485210000	0.8941070000	0.2106650000
C	3.2334160000	-0.2574830000	-0.2408080000
S	2.0474230000	-1.5228760000	-0.4470040000
C	4.6747780000	-0.5407740000	-0.5362690000
C	3.3275750000	2.1925870000	0.5254750000
C	-0.5704990000	-0.9174560000	0.0463000000
H	3.3749470000	2.3785060000	1.6054560000
H	2.8120110000	3.0390270000	0.0595630000
H	4.3520480000	2.1829560000	0.1518830000
H	4.8088890000	-0.8853920000	-1.5675500000
H	5.0650400000	-1.3203170000	0.1281980000
H	5.2880230000	0.3518720000	-0.3982030000
C	0.5091010000	1.7825140000	1.1499590000
H	1.1336010000	2.1558100000	1.9620960000
H	-0.3822420000	1.3244610000	1.5723450000
H	0.2169890000	2.6143680000	0.5045380000
C	-1.7782860000	-0.1242810000	-0.1389650000
C	-3.0320560000	-0.5773870000	0.3203840000
C	-4.2098160000	0.1212900000	0.1306880000
C	-4.1657030000	1.3280320000	-0.5702100000
C	-2.9509330000	1.8013990000	-1.0800870000
C	-1.7789980000	1.0856040000	-0.8735420000
F	-3.0845880000	-1.7683950000	0.9732320000
H	-5.0819520000	1.8862440000	-0.7332560000
H	-2.9254450000	2.7196170000	-1.6577480000
H	-0.8521620000	1.4328370000	-1.3184220000
H	-5.1358570000	-0.2847790000	0.5230760000
O	-0.6279300000	-2.2653860000	0.0902660000
H	-1.5529220000	-2.5703610000	0.1091760000

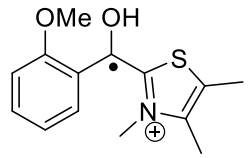
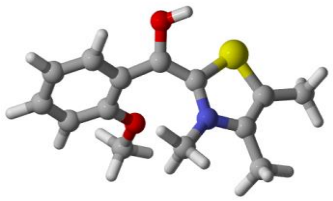
thermodynamic data

Zero-point correction= 0.246149 (Hartree/Particle)
Thermal correction to Energy= 0.262952
Thermal correction to Enthalpy= 0.263896
Thermal correction to Gibbs Free Energy= 0.200571
Sum of electronic and zero-point Energies= -1131.326815

Sum of electronic and thermal Energies= -1131.310012
Sum of electronic and thermal Enthalpies= -1131.309068
Sum of electronic and thermal Free Energies= -1131.372392

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	165.005	63.082	133.278

(u)B3LYP/6-31G*	

xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7808320000	-0.7140500000	-0.0878810000
N	1.2070080000	0.3959770000	-0.7610880000
C	2.5566090000	0.7045130000	-0.5795230000
C	3.2171150000	-0.1986420000	0.2063280000
S	2.1218630000	-1.4426420000	0.7678030000
C	4.6577050000	-0.2434770000	0.6143410000
C	3.1395930000	1.9146570000	-1.2444560000
C	-0.5009470000	-1.3016050000	-0.0469560000
H	2.5416720000	2.8094950000	-1.0420270000
H	3.2033860000	1.7906300000	-2.3322370000
H	4.1493990000	2.0999030000	-0.8770530000
H	5.1501480000	-1.1415170000	0.2235880000
H	4.7630500000	-0.2543950000	1.7049210000
H	5.1997710000	0.6248650000	0.2343980000
C	0.3730450000	1.1371470000	-1.7172510000
H	0.0182350000	2.0666950000	-1.2686550000
H	-0.4816550000	0.5237840000	-1.9945760000
H	0.9609510000	1.3537010000	-2.6098330000
C	-1.8033060000	-0.6719890000	-0.1397520000
C	-2.0791260000	0.6189500000	0.4006060000
C	-3.3819890000	1.1224140000	0.3612710000
C	-4.4119330000	0.3622780000	-0.1934920000
C	-4.1653780000	-0.9151930000	-0.7070040000
C	-2.8781590000	-1.4261190000	-0.6670370000
H	-5.4168980000	0.7730510000	-0.2161740000
H	-4.9725770000	-1.5030110000	-1.1308250000

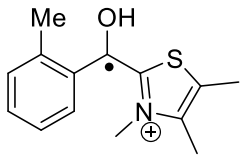
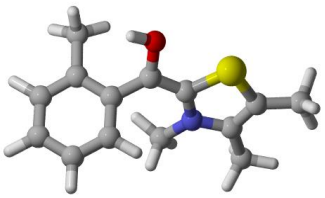
H	-2.6715690000	-2.4189610000	-1.0505410000
H	-3.6038140000	2.0996510000	0.7725090000
O	-1.0316390000	1.2814320000	0.9561560000
C	-1.2901940000	2.4643090000	1.7219930000
H	-0.3304720000	2.7485340000	2.1544740000
H	-1.6619500000	3.2765960000	1.0871920000
H	-2.0085350000	2.2605110000	2.5227110000
O	-0.5639340000	-2.6340490000	0.2195120000
H	0.2433730000	-3.0973130000	-0.0675420000

thermodynamic data

Zero-point correction= 0.287390 (Hartree/Particle)
Thermal correction to Energy= 0.305839
Thermal correction to Enthalpy= 0.306783
Thermal correction to Gibbs Free Energy= 0.240413
Sum of electronic and zero-point Energies= -1146.576552
Sum of electronic and thermal Energies= -1146.558103
Sum of electronic and thermal Enthalpies= -1146.557159
Sum of electronic and thermal Free Energies= -1146.623529

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	191.917	69.239	139.687

(u)B3LYP/6-31G*	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7643750000	-0.4584470000	-0.0616410000
N	1.2099150000	0.7648630000	0.3741800000
C	2.5923060000	0.9296540000	0.2949570000
C	3.2426700000	-0.1906940000	-0.1538560000
S	2.1135620000	-1.4755810000	-0.5014590000
C	4.7089630000	-0.4235530000	-0.3543270000
C	3.2184330000	2.2313370000	0.6953620000
C	-0.5458710000	-0.9414150000	-0.1730780000
H	3.1680140000	2.3926770000	1.7791560000

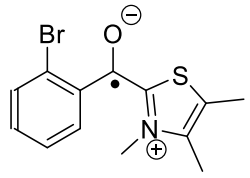
H	2.7312170000	3.0798480000	0.2034590000
H	4.2714730000	2.2463310000	0.4129790000
H	4.9316560000	-0.6737720000	-1.3978040000
H	5.0627230000	-1.2533540000	0.2682580000
H	5.2904410000	0.4615590000	-0.0895420000
C	0.3420260000	1.7745100000	1.0013750000
H	0.9124460000	2.3035230000	1.7635990000
H	-0.5038030000	1.2775780000	1.4724750000
H	-0.0298150000	2.4868760000	0.2606340000
C	-1.7933940000	-0.1717140000	-0.2491460000
C	-2.9272250000	-0.5255020000	0.5296110000
C	-4.0992450000	0.2174680000	0.3448290000
C	-4.1719690000	1.2607140000	-0.5779210000
C	-3.0544960000	1.5985380000	-1.3459350000
C	-1.8729330000	0.8873830000	-1.1786250000
C	-2.9063980000	-1.6375040000	1.5572870000
H	-5.1009460000	1.8102680000	-0.6967210000
H	-3.1091280000	2.3999830000	-2.0760240000
H	-1.0085610000	1.1195160000	-1.7949150000
H	-4.9716080000	-0.0259480000	0.9452940000
H	-3.6095220000	-1.4187670000	2.3657340000
H	-1.9175560000	-1.7840150000	2.0008800000
H	-3.2171420000	-2.5987500000	1.1264700000
O	-0.5885660000	-2.2890390000	-0.3088210000
H	-1.4612050000	-2.5606410000	-0.6426370000

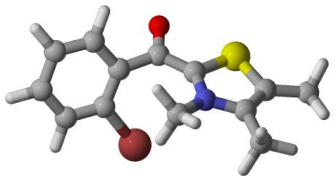
thermodynamic data

Zero-point correction= 0.282183 (Hartree/Particle)
Thermal correction to Energy= 0.299856
Thermal correction to Enthalpy= 0.300800
Thermal correction to Gibbs Free Energy= 0.235582
Sum of electronic and zero-point Energies= -1071.376744
Sum of electronic and thermal Energies= -1071.359071
Sum of electronic and thermal Enthalpies= -1071.358127
Sum of electronic and thermal Free Energies= -1071.423345

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.163	66.102	137.264

(u)B3LYP/6-31G*	





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9463150000	0.8325510000	-0.0263480000
N	1.3013630000	-0.1091390000	0.9214750000
C	2.6571750000	-0.4662050000	0.8878450000
C	3.3758900000	0.2289870000	-0.0322560000
S	2.3605220000	1.3781600000	-0.9065870000
C	4.8344260000	0.1448660000	-0.3624190000
C	3.1694060000	-1.5249890000	1.8193450000
C	-0.2977340000	1.4267810000	-0.3908270000
H	2.5780380000	-2.4453600000	1.7472940000
H	3.1533280000	-1.2006110000	2.8678850000
H	4.2026430000	-1.7757370000	1.5736630000
H	5.3331890000	1.1097470000	-0.2050940000
H	4.9920930000	-0.1339770000	-1.4119420000
H	5.3454420000	-0.5954950000	0.2588850000
C	0.3828450000	-0.5882270000	1.9511800000
H	-0.1989930000	-1.4432140000	1.5940010000
H	-0.3012170000	0.2161320000	2.2248360000
H	0.9479770000	-0.8790070000	2.8369860000
O	-0.2787960000	2.4253560000	-1.1537020000
C	-1.6381620000	0.9329440000	0.0863250000
C	-2.1558430000	-0.3459890000	-0.1542800000
C	-3.4449660000	-0.7094820000	0.2361070000
C	-4.2557320000	0.2260290000	0.8760990000
C	-3.7793320000	1.5200030000	1.1030690000
C	-2.4931660000	1.8653630000	0.7001700000
Br	-1.1115830000	-1.6619350000	-1.0858340000
H	-5.2600620000	-0.0540560000	1.1814200000
H	-4.4124310000	2.2587480000	1.5864230000
H	-2.1210290000	2.8750290000	0.8451940000
H	-3.8078430000	-1.7097190000	0.0252770000

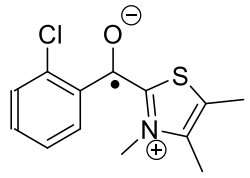
thermodynamic data

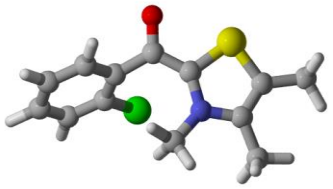
Zero-point correction= 0.231583 (Hartree/Particle)
Thermal correction to Energy= 0.248731
Thermal correction to Enthalpy= 0.249675
Thermal correction to Gibbs Free Energy= 0.184879
Sum of electronic and zero-point Energies= -3602.816498

Sum of electronic and thermal Energies= -3602.799349
Sum of electronic and thermal Enthalpies= -3602.798405
Sum of electronic and thermal Free Energies= -3602.863201

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.081	62.904	136.375

(u)B3LYP/6-31G*	





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7881870000	-0.6568240000	-0.1190170000
N	1.1542470000	0.5791570000	-0.6191470000
C	2.5247980000	0.8556140000	-0.5029310000
C	3.2400350000	-0.1724090000	0.0242150000
S	2.2037100000	-1.5515360000	0.3999660000
C	4.7093370000	-0.2672250000	0.2993750000
C	3.0538400000	2.1876670000	-0.9471130000
C	-0.4720870000	-1.3068420000	0.0265000000
H	2.4952540000	3.0143920000	-0.4927980000
H	3.0061280000	2.3130360000	-2.0366750000
H	4.0996620000	2.2951770000	-0.6544650000
H	5.1636570000	-1.0976740000	-0.2559630000
H	4.9069810000	-0.4427330000	1.3643380000
H	5.2323010000	0.6482030000	0.0100730000
C	0.2343110000	1.4360070000	-1.3634680000
H	-0.3429250000	2.0833970000	-0.6966590000
H	-0.4565330000	0.8131230000	-1.9340680000
H	0.7991640000	2.0548260000	-2.0609450000
O	-0.4830490000	-2.5326320000	0.3033210000
C	-1.7975910000	-0.6109540000	-0.1441060000
C	-2.2428070000	0.4798060000	0.6169490000
C	-3.5230690000	1.0143410000	0.4596380000
C	-4.3945000000	0.4506590000	-0.4697580000
C	-3.9905680000	-0.6568840000	-1.2198660000
C	-2.7148780000	-1.1825980000	-1.0436070000
Cl	-1.2105210000	1.1987740000	1.8597040000
H	-5.3899700000	0.8678030000	-0.5934920000

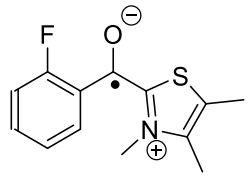
H	-4.6714320000	-1.1130740000	-1.9328990000
H	-2.3972670000	-2.0603280000	-1.5981560000
H	-3.8308990000	1.8540930000	1.0738970000

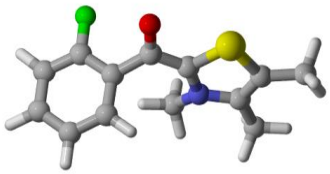
thermodynamic data

Zero-point correction= 0.231793 (Hartree/Particle)
Thermal correction to Energy= 0.248829
Thermal correction to Enthalpy= 0.249773
Thermal correction to Gibbs Free Energy= 0.185706
Sum of electronic and zero-point Energies= -1491.304148
Sum of electronic and thermal Energies= -1491.287112
Sum of electronic and thermal Enthalpies= -1491.286168
Sum of electronic and thermal Free Energies= -1491.350234

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.142	62.693	134.840

(u)B3LYP/6-31G*	





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7520750000	-0.4675410000	-0.0646550000
N	1.1833720000	0.8172160000	0.2454330000
C	2.5818050000	0.9622680000	0.1971480000
C	3.2395130000	-0.1785260000	-0.1310060000
S	2.1203450000	-1.5235590000	-0.3758610000
C	4.7079230000	-0.4133790000	-0.3109120000
C	3.1878000000	2.3037000000	0.4892740000
C	-0.5410900000	-1.0600340000	-0.1923150000
H	2.9836850000	2.6347780000	1.5149820000
H	2.8040270000	3.0757140000	-0.1895420000
H	4.2713730000	2.2660330000	0.3662830000
H	4.9469210000	-0.6902330000	-1.3456460000
H	5.0565710000	-1.2314700000	0.3317500000
H	5.2921230000	0.4761960000	-0.0608000000
C	0.3731500000	1.7560530000	1.0243350000
H	0.5319670000	1.6086130000	2.1008760000

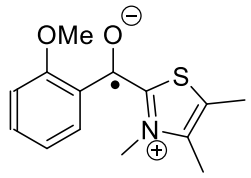
H	-0.6794410000	1.6097940000	0.7991010000
H	0.6410780000	2.7808230000	0.7603880000
O	-0.6167210000	-2.3023920000	-0.3366110000
C	-1.8025400000	-0.2426640000	-0.2567600000
C	-2.8805420000	-0.5221220000	0.5905360000
C	-4.1033890000	0.1293370000	0.4835710000
C	-4.2749600000	1.0902970000	-0.5140840000
C	-3.2236560000	1.3918340000	-1.3820320000
C	-2.0029040000	0.7283650000	-1.2502530000
F	-2.7257980000	-1.4308880000	1.5716800000
H	-5.2294590000	1.6001510000	-0.6099150000
H	-3.3564020000	2.1322700000	-2.1656400000
H	-1.1870160000	0.9500380000	-1.9334890000
H	-4.8977050000	-0.1246690000	1.1780800000

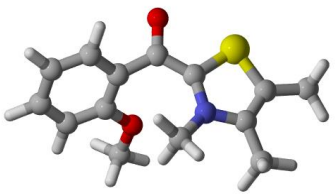
thermodynamic data

Zero-point correction= 0.233181 (Hartree/Particle)
Thermal correction to Energy= 0.249933
Thermal correction to Enthalpy= 0.250877
Thermal correction to Gibbs Free Energy= 0.186909
Sum of electronic and zero-point Energies= -1130.939589
Sum of electronic and thermal Energies= -1130.922837
Sum of electronic and thermal Enthalpies= -1130.921892
Sum of electronic and thermal Free Energies= -1130.985860

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.836	61.770	134.632

(u)B3LYP/6-31G*	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8235980000	-0.7027390000	-0.0365610000
N	1.1910230000	0.4622670000	-0.6847870000
C	2.5538840000	0.7723840000	-0.5696100000
C	3.2672830000	-0.1652520000	0.1065240000
S	2.2378510000	-1.5032030000	0.6275670000
C	4.7299730000	-0.1989520000	0.4267460000

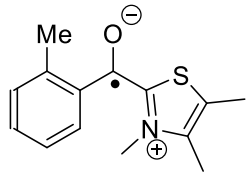
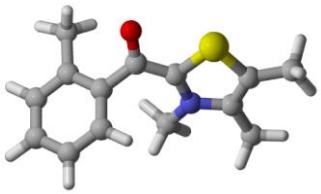
C	3.0759360000	2.0409030000	-1.1783910000
C	-0.4295810000	-1.3584260000	0.1560740000
H	2.4876070000	2.9108760000	-0.8633710000
H	3.0618290000	2.0126500000	-2.2757440000
H	4.1095340000	2.2112390000	-0.8719750000
H	5.2129370000	-1.0796740000	-0.0159080000
H	4.9029590000	-0.2456280000	1.5094270000
H	5.2459510000	0.6864180000	0.0451680000
C	0.2938200000	1.1954470000	-1.5728170000
H	-0.2323790000	1.9929430000	-1.0405880000
H	-0.4436470000	0.5052600000	-1.9837830000
H	0.8651210000	1.6244710000	-2.3975930000
O	-0.4057090000	-2.5438470000	0.5772020000
C	-1.7668690000	-0.7241490000	-0.1079160000
C	-2.1645070000	0.5170560000	0.4359450000
C	-3.4689450000	0.9876670000	0.2470650000
C	-4.3891740000	0.2230780000	-0.4740260000
C	-4.0217960000	-1.0167180000	-0.9941460000
C	-2.7237420000	-1.4836410000	-0.7925150000
H	-5.3982320000	0.6014240000	-0.6154040000
H	-4.7406490000	-1.6198230000	-1.5412190000
H	-2.4248980000	-2.4623510000	-1.1552170000
H	-3.7778540000	1.9387100000	0.6661700000
O	-1.2120560000	1.1997870000	1.1483980000
C	-1.6108490000	2.3416930000	1.8892740000
H	-0.7284640000	2.6561230000	2.4499990000
H	-1.9333530000	3.1631010000	1.2345290000
H	-2.4212980000	2.1020190000	2.5892570000

thermodynamic data

Zero-point correction= 0.274455 (Hartree/Particle)
Thermal correction to Energy= 0.292744
Thermal correction to Enthalpy= 0.293688
Thermal correction to Gibbs Free Energy= 0.227272
Sum of electronic and zero-point Energies= -1146.189196
Sum of electronic and thermal Energies= -1146.170907
Sum of electronic and thermal Enthalpies= -1146.169963
Sum of electronic and thermal Free Energies= -1146.236379

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	183.699	67.847	139.785

(u)B3LYP/6-31G*	

xyz-matrix

33
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7476920000	-0.4732880000	-0.0840660000
N	1.1834280000	0.7735620000	0.3367430000
C	2.5766370000	0.9357920000	0.2785010000
C	3.2354320000	-0.1810590000	-0.1270990000
S	2.1167640000	-1.5084140000	-0.4519440000
C	4.7051180000	-0.4043680000	-0.3113710000
C	3.1867100000	2.2554880000	0.6510980000
C	-0.5537870000	-1.0477310000	-0.2346360000
H	3.1045990000	2.4643100000	1.7257000000
H	2.7114320000	3.0855510000	0.1152380000
H	4.2487200000	2.2650770000	0.4000450000
H	4.9429210000	-0.6762070000	-1.3475930000
H	5.0641770000	-1.2209720000	0.3279340000
H	5.2829190000	0.4891150000	-0.0602560000
C	0.3047860000	1.7396940000	0.9935110000
H	0.8907890000	2.3578860000	1.6741640000
H	-0.4528880000	1.2051790000	1.5690390000
H	-0.2084260000	2.3832270000	0.2722560000
O	-0.6254920000	-2.2891890000	-0.4182160000
C	-1.8030820000	-0.2126040000	-0.2658850000
C	-2.9305660000	-0.5680900000	0.5105690000
C	-4.0932020000	0.1994590000	0.3802620000
C	-4.1691560000	1.2767980000	-0.5053100000
C	-3.0638850000	1.6078400000	-1.2870530000
C	-1.8909640000	0.8628480000	-1.1620730000
C	-2.8993570000	-1.7404500000	1.4631950000
H	-5.0908160000	1.8471970000	-0.5869430000
H	-3.1145190000	2.4313640000	-1.9946190000
H	-1.0314280000	1.1001910000	-1.7848640000
H	-4.9605170000	-0.0580940000	0.9842290000
H	-3.8214160000	-1.7879400000	2.0513100000
H	-2.0536460000	-1.6747170000	2.1584700000
H	-2.7744300000	-2.6799530000	0.9176580000

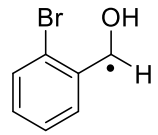
thermodynamic data

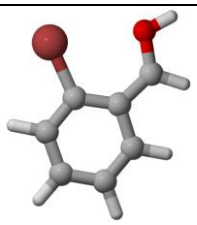
Zero-point correction= 0.269203 (Hartree/Particle)
Thermal correction to Energy= 0.286729

Thermal correction to Enthalpy= 0.287673
Thermal correction to Gibbs Free Energy= 0.222751
Sum of electronic and zero-point Energies= -1070.990933
Sum of electronic and thermal Energies= -1070.973407
Sum of electronic and thermal Enthalpies= -1070.972463
Sum of electronic and thermal Free Energies= -1071.037384

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.925	64.763	136.639

(u)B3LYP/6-31G*	





xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.2287070000	-0.3960900000	-0.0001230000
C	-0.7668020000	0.9280670000	-0.0000510000
C	-2.1976510000	1.0145760000	-0.0000390000
C	-3.0108530000	-0.1007280000	-0.0000060000
C	-2.4442540000	-1.3840850000	-0.0000390000
C	-1.0538320000	-1.5146580000	-0.0001060000
H	-2.6443840000	2.0061360000	-0.0001690000
H	-4.0905220000	0.0210740000	-0.0000600000
Br	1.6554290000	-0.7378130000	0.0000540000
C	-0.0734660000	2.1525540000	0.0005690000
H	-0.6417380000	3.0786630000	0.0008870000
H	-3.0711800000	-2.2703770000	0.0000990000
H	-0.5968320000	-2.4984780000	-0.0001210000
O	1.2801620000	2.2610280000	-0.0003430000
H	1.5167240000	3.2003970000	-0.0010240000

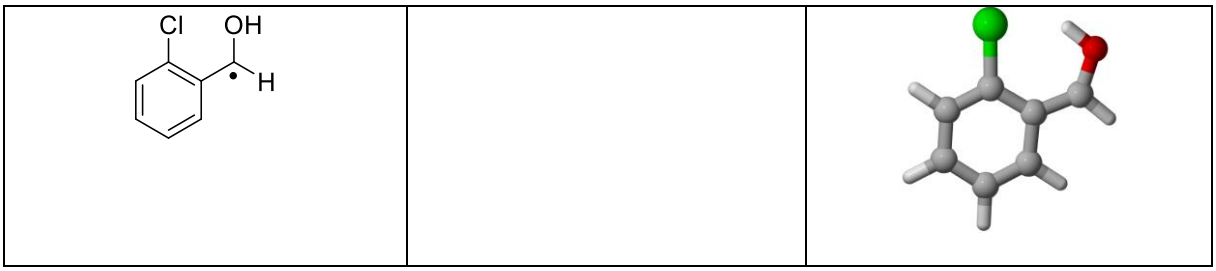
thermodynamic data

Zero-point correction= 0.110066 (Hartree/Particle)
Thermal correction to Energy= 0.118379
Thermal correction to Enthalpy= 0.119323
Thermal correction to Gibbs Free Energy= 0.075283
Sum of electronic and zero-point Energies= -2917.119523
Sum of electronic and thermal Energies= -2917.111211

Sum of electronic and thermal Enthalpies= -2917.110267
Sum of electronic and thermal Free Energies= -2917.154307

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.284	31.001	92.691

(u)B3LYP/6-31G*	



xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

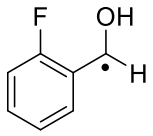
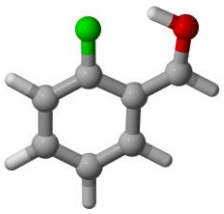
C	0.0366290000	-0.6092560000	0.0001310000
C	0.0200000000	0.8199810000	0.0001090000
C	1.3150760000	1.4371630000	-0.0001030000
C	2.4865270000	0.7078470000	-0.0001400000
C	2.4503630000	-0.6959440000	0.0000180000
C	1.2126080000	-1.3442090000	0.0001200000
H	1.3540280000	2.5235080000	-0.0002050000
H	3.4405100000	1.2276920000	-0.0002700000
Cl	-1.4799490000	-1.5419160000	-0.0000630000
C	-1.0944310000	1.6823680000	0.0002850000
H	-0.9352520000	2.7548540000	0.0002010000
H	3.3663810000	-1.2778560000	0.0000260000
H	1.1567660000	-2.4280440000	0.0001090000
O	-2.4075090000	1.3769270000	-0.0001220000
H	-2.5238610000	0.4092940000	-0.0003380000

thermodynamic data

Zero-point correction= 0.111018 (Hartree/Particle)
Thermal correction to Energy= 0.118855
Thermal correction to Enthalpy= 0.119799
Thermal correction to Gibbs Free Energy= 0.077598
Sum of electronic and zero-point Energies= -805.617048
Sum of electronic and thermal Energies= -805.609211
Sum of electronic and thermal Enthalpies= -805.608267
Sum of electronic and thermal Free Energies= -805.650468

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.583	30.175	88.820

(u)B3LYP/6-31G*	

xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

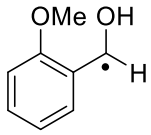
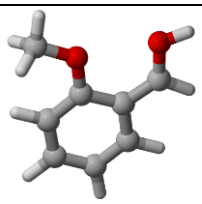
C	-0.0157930000	0.8026970000	-0.0000370000
C	0.3345770000	-0.5748850000	-0.0001140000
C	-0.7730140000	-1.4783960000	-0.0000080000
C	-2.0817630000	-1.0261490000	0.0000350000
C	-2.3680240000	0.3479990000	-0.0000120000
C	-1.3109320000	1.2693780000	-0.0000300000
H	-0.5639150000	-2.5449900000	0.0000520000
H	-2.8947600000	-1.7468250000	0.0000530000
F	1.0053740000	1.7248480000	0.0000870000
C	1.6558110000	-1.0588070000	0.0000790000
H	1.8643630000	-2.1223710000	0.0001740000
H	-3.3941250000	0.7009970000	0.0000170000
H	-1.4837700000	2.3408890000	-0.0000150000
O	2.7815400000	-0.3091090000	-0.0000390000
H	2.5263480000	0.6305220000	-0.0002330000

thermodynamic data

Zero-point correction= 0.112588 (Hartree/Particle)
Thermal correction to Energy= 0.119999
Thermal correction to Enthalpy= 0.120943
Thermal correction to Gibbs Free Energy= 0.080203
Sum of electronic and zero-point Energies= -445.256926
Sum of electronic and thermal Energies= -445.249515
Sum of electronic and thermal Enthalpies= -445.248571
Sum of electronic and thermal Free Energies= -445.289312

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.300	29.210	85.746

(u)B3LYP/6-31G*	

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

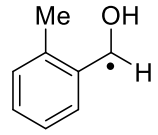
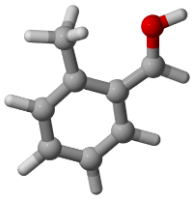
C	0.0897930000	-0.5041860000	0.0002670000
C	-0.0985580000	0.9223780000	-0.0000300000
C	-1.4472690000	1.3892430000	-0.0002080000
C	-2.5303680000	0.5263440000	-0.0001740000
C	-2.3174970000	-0.8560800000	0.0001060000
C	-1.0083490000	-1.3595030000	0.0003480000
H	-1.6137080000	2.4641800000	-0.0004130000
H	-3.5404900000	0.9265860000	-0.0003550000
C	0.9245310000	1.8850630000	-0.0002490000
H	0.6588280000	2.9392280000	-0.0003700000
H	-3.1563840000	-1.5458370000	0.0001780000
H	-0.8572550000	-2.4329050000	0.0006690000
O	1.3840200000	-0.9337010000	0.0006080000
C	1.6344440000	-2.3268220000	-0.0006560000
H	2.7209520000	-2.4334100000	-0.0013040000
H	1.2224620000	-2.8141410000	0.8936290000
H	1.2214720000	-2.8126560000	-0.8952810000
O	2.2553300000	1.5874430000	0.0003070000

thermodynamic data

Zero-point correction= 0.152907 (Hartree/Particle)
Thermal correction to Energy= 0.162347
Thermal correction to Enthalpy= 0.163291
Thermal correction to Gibbs Free Energy= 0.117974
Sum of electronic and zero-point Energies= -460.494194
Sum of electronic and thermal Energies= -460.484754
Sum of electronic and thermal Enthalpies= -460.483810
Sum of electronic and thermal Free Energies= -460.529127

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.874	35.994	95.378

(u)B3LYP/6-31G*	

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

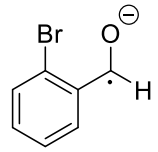
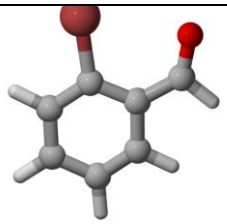
C	0.0115340000	0.8538510000	-0.0000490000
C	-0.2913570000	-0.5530110000	-0.0001630000
C	0.8019270000	-1.4735410000	0.0001120000
C	2.1174800000	-1.0483520000	0.0001170000
C	2.4060990000	0.3223530000	-0.0000190000
C	1.3502380000	1.2409010000	-0.0000240000
H	0.5803790000	-2.5387510000	0.0003170000
H	2.9216690000	-1.7796850000	0.0002920000
C	-1.0626870000	1.9161280000	0.0000020000
C	-1.5806010000	-1.1167670000	-0.0006970000
H	-1.7056800000	-2.1961820000	0.0002530000
H	3.4343910000	0.6721760000	-0.0000200000
H	1.5759860000	2.3053330000	0.0000960000
H	-0.6080150000	2.9122310000	0.0010190000
H	-1.7161100000	1.8386710000	0.8760440000
H	-1.7147390000	1.8399400000	-0.8772350000
O	-2.7247440000	-0.3672160000	0.0005030000
H	-3.4857260000	-0.9653790000	-0.0004640000

thermodynamic data

Zero-point correction= 0.148054 (Hartree/Particle)
Thermal correction to Energy= 0.156515
Thermal correction to Enthalpy= 0.157459
Thermal correction to Gibbs Free Energy= 0.114720
Sum of electronic and zero-point Energies= -385.297093
Sum of electronic and thermal Energies= -385.288633
Sum of electronic and thermal Enthalpies= -385.287689
Sum of electronic and thermal Free Energies= -385.330428

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	98.214	32.745	89.952

(u)B3LYP/6-31G*	

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

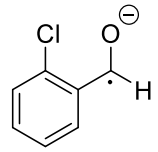
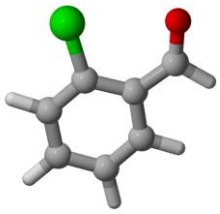
C	-0.2139680000	-0.3804370000	0.0000000000
C	-0.7761640000	0.9464310000	0.0001140000
C	-2.2179110000	0.9580830000	0.0000910000
C	-2.9918310000	-0.1802950000	-0.0000010000
C	-2.3906410000	-1.4634680000	-0.0000900000
C	-0.9850630000	-1.5282000000	-0.0000910000
H	-2.6981310000	1.9376030000	0.0001570000
H	-4.0786820000	-0.0903990000	-0.0000090000
Br	1.7077890000	-0.6506440000	-0.0000780000
C	-0.0822260000	2.1968390000	0.0002240000
H	-0.7949830000	3.0633020000	0.0001760000
H	-2.9862280000	-2.3727470000	-0.0001470000
H	-0.4833090000	-2.4929470000	-0.0001730000
O	1.1519420000	2.4292500000	0.0001580000

thermodynamic data

Zero-point correction= 0.096330 (Hartree/Particle)
Thermal correction to Energy= 0.104271
Thermal correction to Enthalpy= 0.105215
Thermal correction to Gibbs Free Energy= 0.061764
Sum of electronic and zero-point Energies= -2916.581042
Sum of electronic and thermal Energies= -2916.573101
Sum of electronic and thermal Enthalpies= -2916.572157
Sum of electronic and thermal Free Energies= -2916.615608

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.431	29.433	91.450

(u)B3LYP/6-31G*	

xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

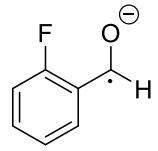
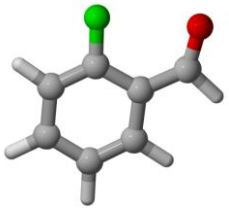
C	0.0366290000	-0.6092560000	0.0001310000
C	0.0200000000	0.8199810000	0.0001090000
C	1.3150760000	1.4371630000	-0.0001030000
C	2.4865270000	0.7078470000	-0.0001400000
C	2.4503630000	-0.6959440000	0.0000180000
C	1.2126080000	-1.3442090000	0.0001200000
H	1.3540280000	2.5235080000	-0.0002050000
H	3.4405100000	1.2276920000	-0.0002700000
Cl	-1.4799490000	-1.5419160000	-0.0000630000
C	-1.0944310000	1.6823680000	0.0002850000
H	-0.9352520000	2.7548540000	0.0002010000
H	3.3663810000	-1.2778560000	0.0000260000
H	1.1567660000	-2.4280440000	0.0001090000
O	-2.4075090000	1.3769270000	-0.0001220000
H	-2.5238610000	0.4092940000	-0.0003380000

thermodynamic data

Zero-point correction= 0.096680 (Hartree/Particle)
Thermal correction to Energy= 0.104424
Thermal correction to Enthalpy= 0.105368
Thermal correction to Gibbs Free Energy= 0.063152
Sum of electronic and zero-point Energies= -805.069843
Sum of electronic and thermal Energies= -805.062098
Sum of electronic and thermal Enthalpies= -805.061154
Sum of electronic and thermal Free Energies= -805.103370

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.527	29.171	88.851

(u)B3LYP/6-31G*	

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

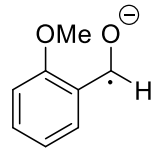
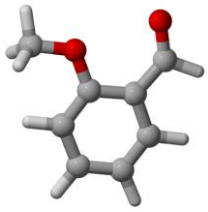
C	-0.0142180000	0.8402210000	-0.0000040000
C	0.4290690000	-0.5252100000	0.0000360000
C	-0.6511580000	-1.4809050000	0.0000330000
C	-1.9842790000	-1.1146590000	0.0000030000
C	-2.3677870000	0.2434870000	-0.0000290000
C	-1.3365660000	1.2169420000	-0.0000330000
H	-0.3800460000	-2.5373000000	0.0000600000
H	-2.7505280000	-1.8915180000	0.0000050000
F	0.9195300000	1.8356740000	-0.0000110000
C	1.7905700000	-0.9569740000	0.0000720000
H	1.8707050000	-2.0776610000	-0.0000150000
H	-3.4131990000	0.5413270000	-0.0000500000
H	-1.5634250000	2.2818040000	-0.0000570000
O	2.8458680000	-0.2718910000	-0.0000380000

thermodynamic data

Zero-point correction= 0.097979 (Hartree/Particle)
Thermal correction to Energy= 0.105347
Thermal correction to Enthalpy= 0.106291
Thermal correction to Gibbs Free Energy= 0.065463
Sum of electronic and zero-point Energies= -444.702272
Sum of electronic and thermal Energies= -444.694904
Sum of electronic and thermal Enthalpies= -444.693959
Sum of electronic and thermal Free Energies= -444.734788

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	66.106	28.319	85.931

(u)B3LYP/6-31G*	

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

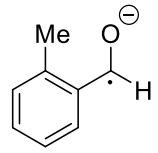
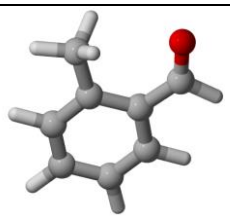
C	-0.1706140000	-0.4713210000	-0.0001650000
C	0.1269080000	0.9473860000	-0.0001560000
C	1.5309290000	1.2659060000	-0.0000830000
C	2.5279070000	0.3082740000	-0.0000410000
C	2.2052520000	-1.0620190000	-0.0000750000
C	0.8318400000	-1.4261920000	-0.0001440000
H	1.7976970000	2.3235030000	-0.0000560000
H	3.5735440000	0.6207330000	0.0000110000
C	-0.8322080000	2.0082570000	-0.0001160000
H	-0.3241390000	3.0121520000	0.0004090000
H	2.9753840000	-1.8298640000	-0.0000430000
H	0.5751650000	-2.4822380000	-0.0002180000
O	-1.5160690000	-0.7973290000	-0.0002440000
C	-1.8598690000	-2.1533830000	0.0004290000
H	-2.9542700000	-2.1938990000	0.0007170000
H	-1.4823960000	-2.6844850000	-0.8904090000
H	-1.4819120000	-2.6836850000	0.8915290000
O	-2.0889250000	1.9743730000	0.0002640000

thermodynamic data

Zero-point correction= 0.138744 (Hartree/Particle)
Thermal correction to Energy= 0.147774
Thermal correction to Enthalpy= 0.148718
Thermal correction to Gibbs Free Energy= 0.104064
Sum of electronic and zero-point Energies= -459.940738
Sum of electronic and thermal Energies= -459.931708
Sum of electronic and thermal Enthalpies= -459.930764
Sum of electronic and thermal Free Energies= -459.975418

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	92.729	34.365	93.982

(u)B3LYP/6-31G*	

xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

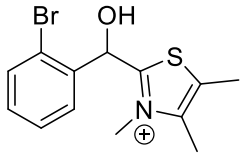
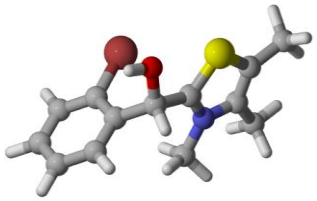
C	0.0349140000	0.8510210000	-0.0000010000
C	0.3530310000	-0.5674130000	0.0000440000
C	-0.7675440000	-1.4687990000	0.0000120000
C	-2.0773360000	-1.0344550000	-0.0000620000
C	-2.3757630000	0.3465800000	-0.0001190000
C	-1.2929920000	1.2522960000	-0.0000850000
H	-0.5540020000	-2.5390340000	0.0000490000
H	-2.8875790000	-1.7660600000	-0.0000820000
C	1.1321350000	1.8889110000	0.0000770000
C	1.6757210000	-1.1038060000	0.0000920000
H	1.6845780000	-2.2258300000	0.0000360000
H	-3.4033690000	0.7041700000	-0.0001890000
H	-1.5031550000	2.3247000000	-0.0001300000
H	0.7026250000	2.9018550000	-0.0002340000
H	1.7935990000	1.7852220000	-0.8684060000
H	1.7931040000	1.7856150000	0.8690020000
O	2.7851510000	-0.4945810000	0.0000260000

thermodynamic data

Zero-point correction= 0.134093 (Hartree/Particle)
Thermal correction to Energy= 0.142144
Thermal correction to Enthalpy= 0.143088
Thermal correction to Gibbs Free Energy= 0.100993
Sum of electronic and zero-point Energies= -384.749723
Sum of electronic and thermal Energies= -384.741673
Sum of electronic and thermal Enthalpies= -384.740729
Sum of electronic and thermal Free Energies= -384.782823

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.196	30.999	88.595

B3LYP/6-31G*	

xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8643280000	0.5205540000	0.7659430000
N	-1.2781540000	1.1710280000	-0.3210010000
C	-2.5935580000	0.8653440000	-0.7200080000
C	-3.1895900000	-0.0181920000	0.1334880000
S	-2.0934800000	-0.4689470000	1.4149830000
C	-4.5724500000	-0.5970180000	0.0943030000
C	-3.1727740000	1.4954590000	-1.9493250000
C	0.4658980000	0.6500380000	1.4847500000
H	-3.2973940000	2.5787890000	-1.8339510000
H	-4.1579270000	1.0749730000	-2.1541720000
H	-2.5480700000	1.3152030000	-2.8308960000
H	-5.1419480000	-0.3199240000	0.9882500000
H	-4.5421130000	-1.6907390000	0.0427740000
H	-5.1235150000	-0.2360690000	-0.7764200000
C	-0.4226150000	2.0768190000	-1.1106520000
H	0.3522970000	2.4990100000	-0.4755000000
H	-1.0356870000	2.8821380000	-1.5123810000
H	0.0418170000	1.5146390000	-1.9250700000
C	1.7353330000	0.5845020000	0.6461130000
C	2.0220950000	-0.4201960000	-0.2914480000
C	3.2462810000	-0.4625040000	-0.9555440000
C	4.2158030000	0.5040310000	-0.6835250000
C	3.9588130000	1.5104780000	0.2467620000
C	2.7284460000	1.5437730000	0.9009560000
H	4.7094230000	2.2632480000	0.4652420000
H	2.5320950000	2.3265630000	1.6307910000
Br	0.7377130000	-1.7694730000	-0.7197010000
H	0.4531160000	1.6417360000	1.9694440000
H	5.1692190000	0.4637300000	-1.2012520000
H	3.4374580000	-1.2489270000	-1.6772910000
O	0.4019180000	-0.3739030000	2.4650580000
H	1.2145670000	-0.3541630000	2.9959190000

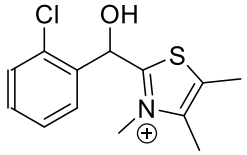
thermodynamic data

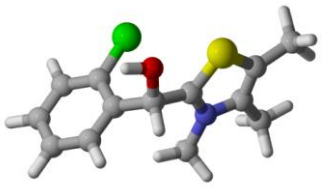
Zero-point correction= 0.256304 (Hartree/Particle)
Thermal correction to Energy= 0.274105

Thermal correction to Enthalpy= 0.275049
Thermal correction to Gibbs Free Energy= 0.208793
Sum of electronic and zero-point Energies= -3603.806243
Sum of electronic and thermal Energies= -3603.788443
Sum of electronic and thermal Enthalpies= -3603.787498
Sum of electronic and thermal Free Energies= -3603.853754

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	172.003	64.970	139.447

B3LYP/6-31G*	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7602040000	-0.1307200000	-0.7127770000
N	1.2139900000	1.0494980000	-0.2900550000
C	2.5393680000	1.0325350000	0.1856170000
C	3.0968640000	-0.2098300000	0.0881190000
S	1.9556330000	-1.3424440000	-0.5921050000
C	4.4691090000	-0.6727530000	0.4770720000
C	3.1583930000	2.2895990000	0.7144140000
C	-0.5837990000	-0.4406660000	-1.3480210000
H	3.1878850000	3.0805440000	-0.0436760000
H	4.1848920000	2.0979970000	1.0286250000
H	2.6145380000	2.6746570000	1.5846710000
H	4.9887770000	-1.1273930000	-0.3731530000
H	4.4221560000	-1.4183800000	1.2784100000
H	5.0772860000	0.1617140000	0.8318900000
C	0.4361740000	2.3020230000	-0.3223400000
H	-0.5667950000	2.1033230000	-0.6897520000
H	0.9365240000	3.0182440000	-0.9778120000
H	0.3696290000	2.7115590000	0.6873820000
C	-1.8351370000	-0.0386900000	-0.5760920000
C	-2.0967420000	-0.3818170000	0.7623410000
C	-3.3070040000	-0.0478200000	1.3685620000
C	-4.2849330000	0.6316820000	0.6414890000
C	-4.0538540000	0.9777600000	-0.6893870000
C	-2.8399100000	0.6410930000	-1.2849430000
H	-4.8122340000	1.5011010000	-1.2627050000
H	-2.6640300000	0.9034640000	-2.3260340000

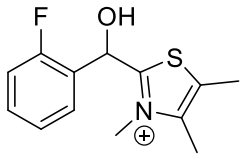
Cl	-0.9123940000	-1.2437740000	1.7311520000
H	-0.6064530000	0.1165660000	-2.3002110000
H	-5.2260590000	0.8848100000	1.1197890000
H	-3.4781880000	-0.3260350000	2.4028520000
O	-0.5094600000	-1.8336110000	-1.6029820000
H	-1.3819980000	-2.1508830000	-1.8862670000

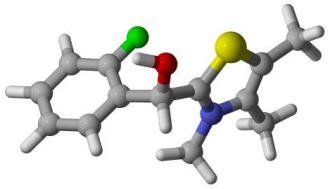
thermodynamic data

Zero-point correction= 0.256460 (Hartree/Particle)
Thermal correction to Energy= 0.273303
Thermal correction to Enthalpy= 0.274247
Thermal correction to Gibbs Free Energy= 0.211141
Sum of electronic and zero-point Energies= -1492.294352
Sum of electronic and thermal Energies= -1492.277510
Sum of electronic and thermal Enthalpies= -1492.276566
Sum of electronic and thermal Free Energies= -1492.339671

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.500	62.782	132.817

B3LYP/6-31G*





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	0.6690530000	-0.2761940000	-0.6430470000
N	1.1762420000	0.9450120000	-0.4752400000
C	2.4762950000	0.9705630000	0.0634520000
C	2.9519920000	-0.2883070000	0.2952750000
S	1.7678860000	-1.4870060000	-0.1657670000
C	4.2708080000	-0.7182520000	0.8650880000
C	3.1561550000	2.2812420000	0.3131270000
C	-0.6812000000	-0.6380520000	-1.2301260000
H	3.2222430000	2.8870360000	-0.5975930000
H	4.1727170000	2.1133760000	0.6704970000
H	2.6339060000	2.8710660000	1.0757090000
H	4.7586230000	-1.4565500000	0.2201280000
H	4.1443550000	-1.1701020000	1.8553700000

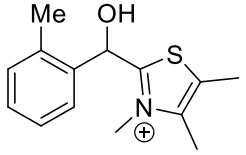
H	4.9478580000	0.1322170000	0.9687670000
C	0.4705230000	2.1859090000	-0.8450410000
H	-0.5658150000	1.9597900000	-1.0838480000
H	0.9630240000	2.6419700000	-1.7075340000
H	0.4932500000	2.8774400000	-0.0013980000
C	-1.8796800000	-0.1577500000	-0.4292110000
C	-1.9709710000	-0.3327200000	0.9565160000
C	-3.0984120000	0.0236600000	1.6811460000
C	-4.1894700000	0.5669320000	0.9996210000
C	-4.1381160000	0.7512020000	-0.3839820000
C	-2.9913430000	0.3883140000	-1.0897360000
H	-4.9881420000	1.1708150000	-0.9119340000
H	-2.9549330000	0.5230770000	-2.1685370000
F	-0.9090910000	-0.8497540000	1.6151880000
H	-0.7392560000	-0.1721190000	-2.2277890000
H	-5.0797190000	0.8460940000	1.5545170000
H	-3.1108140000	-0.1312110000	2.7547480000
O	-0.6227050000	-2.0508110000	-1.3607630000
H	-1.5275060000	-2.4008840000	-1.3912190000

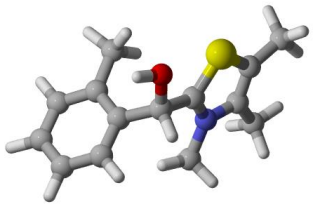
thermodynamic data

Zero-point correction= 0.258091 (Hartree/Particle)
Thermal correction to Energy= 0.275378
Thermal correction to Enthalpy= 0.276322
Thermal correction to Gibbs Free Energy= 0.212344
Sum of electronic and zero-point Energies= -1131.935898
Sum of electronic and thermal Energies= -1131.918611
Sum of electronic and thermal Enthalpies= -1131.917667
Sum of electronic and thermal Free Energies= -1131.981645

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	172.802	63.854	134.653

B3LYP/6-31G*	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

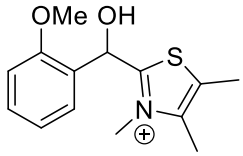
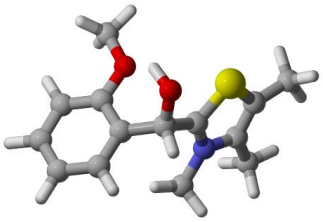
C	0.6976830000	-0.2517560000	-0.5933580000
N	1.1520000000	0.9726460000	-0.3201930000
C	2.4799670000	1.0176950000	0.1469480000
C	3.0380150000	-0.2265330000	0.2124730000
S	1.8950830000	-1.4372970000	-0.3155310000
C	4.4100440000	-0.6352710000	0.6589490000
C	3.1025010000	2.3325220000	0.5029820000
C	-0.6503810000	-0.6357170000	-1.1775590000
H	3.0901760000	3.0313530000	-0.3408900000
H	4.1435100000	2.1874810000	0.7937410000
H	2.5897090000	2.8105960000	1.3458590000
H	4.9106870000	-1.2399800000	-0.1045610000
H	4.3662250000	-1.2278160000	1.5796080000
H	5.0342640000	0.2392620000	0.8531720000
C	0.3770250000	2.2113040000	-0.5279060000
H	-0.6562190000	1.9629140000	-0.7548100000
H	0.8183510000	2.7778340000	-1.3517070000
H	0.4046580000	2.8089870000	0.3844740000
C	-1.8888500000	-0.1751130000	-0.4146370000
C	-2.1375470000	-0.5089470000	0.9373890000
C	-3.3442520000	-0.0782140000	1.5027080000
C	-4.2851320000	0.6512580000	0.7745030000
C	-4.0395970000	0.9643210000	-0.5606970000
C	-2.8460550000	0.5458480000	-1.1462770000
H	-4.7685040000	1.5178500000	-1.1443600000
H	-2.6571000000	0.7746720000	-2.1935390000
H	-0.6886000000	-0.1702520000	-2.1772170000
H	-5.2105440000	0.9634390000	1.2492590000
H	-3.5523110000	-0.3300690000	2.5391690000
C	-1.1719160000	-1.3087690000	1.7843020000
H	-1.6566910000	-1.6369990000	2.7075330000
H	-0.2951830000	-0.7167700000	2.0796140000
H	-0.8104180000	-2.1970240000	1.2589790000
O	-0.5576410000	-2.0487280000	-1.3112180000
H	-1.4352330000	-2.3931890000	-1.5436460000

thermodynamic data

Zero-point correction= 0.294429 (Hartree/Particle)
Thermal correction to Energy= 0.312306
Thermal correction to Enthalpy= 0.313250
Thermal correction to Gibbs Free Energy= 0.248419
Sum of electronic and zero-point Energies= -1071.981964
Sum of electronic and thermal Energies= -1071.964087
Sum of electronic and thermal Enthalpies= -1071.963143
Sum of electronic and thermal Free Energies= -1072.027974

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	195.975	66.706	136.450

B3LYP/6-31G*	

xyz-matrix

36
XYZ file generated by gabedit : coordinates in Angstrom

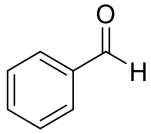
C	0.8086780000	-0.1139100000	0.7154880000
N	1.3093280000	-1.1303080000	0.0111060000
C	2.6091060000	-0.9172340000	-0.4916020000
C	3.0959940000	0.3072770000	-0.1368910000
S	1.9255420000	1.1718710000	0.8310780000
C	4.4183120000	0.9378810000	-0.4569270000
C	3.2775370000	-1.9801250000	-1.3085220000
C	-0.5204260000	-0.0025790000	1.4717430000
H	3.3496100000	-2.9281870000	-0.7639580000
H	4.2915570000	-1.6721970000	-1.5660330000
H	2.7430440000	-2.1690290000	-2.2469850000
H	4.9484130000	1.2291410000	0.4562060000
H	4.2902330000	1.8368990000	-1.0700380000
H	5.0589590000	0.2465070000	-1.0080960000
C	0.6169720000	-2.4150170000	-0.2015940000
H	-0.4132050000	-2.3339480000	0.1330480000
H	1.1336210000	-3.2004100000	0.3557590000
H	0.6249740000	-2.6554600000	-1.2658080000
C	-1.7656570000	-0.2835070000	0.6472800000
C	-2.1282720000	0.5784430000	-0.4083430000
C	-3.2911600000	0.3436780000	-1.1436890000
C	-4.1060780000	-0.7437620000	-0.8156660000
C	-3.7784120000	-1.5876640000	0.2434360000
C	-2.6132720000	-1.3460170000	0.9732480000
H	-4.4260030000	-2.4166760000	0.5088900000
H	-2.3623740000	-1.9865900000	1.8160160000
H	-0.4766970000	-0.7332590000	2.2897770000
H	-5.0110710000	-0.9165790000	-1.3902100000
H	-3.5759340000	1.0015040000	-1.9561220000
O	-1.2792360000	1.6380510000	-0.6106540000
C	-1.5946980000	2.5869140000	-1.6374340000
H	-0.8022740000	3.3349050000	-1.6021030000
H	-1.6050040000	2.1067860000	-2.6217880000
H	-2.5612680000	3.0647180000	-1.4456140000
O	-0.5280360000	1.2705430000	2.0926090000
H	-0.8941000000	1.8990930000	1.4432640000

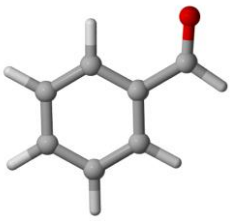
thermodynamic data

Zero-point correction= 0.300051 (Hartree/Particle)
Thermal correction to Energy= 0.318647
Thermal correction to Enthalpy= 0.319591
Thermal correction to Gibbs Free Energy= 0.252475
Sum of electronic and zero-point Energies= -1147.189568
Sum of electronic and thermal Energies= -1147.170973
Sum of electronic and thermal Enthalpies= -1147.170028
Sum of electronic and thermal Free Energies= -1147.237144

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	199.954	69.370	141.258

B3LYP/6-31++G**	**PhCHO**



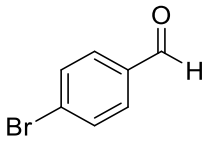


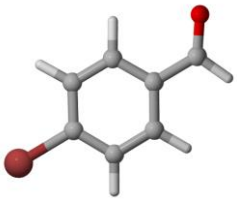
xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.0400790000	-1.1070920000	0.0000000000
C	-0.5359230000	0.2073590000	-0.0000010000
C	0.3561450000	1.2902550000	0.0000000000
C	1.7338280000	1.0658060000	0.0000000000
C	2.2216440000	-0.2443550000	0.0000000000
C	1.3345610000	-1.3297310000	0.0000000000
H	-0.0336060000	2.3058640000	0.0000000000
H	2.4235060000	1.9046640000	0.0000010000
H	3.2934410000	-0.4217530000	0.0000010000
H	1.7206780000	-2.3448820000	0.0000000000
H	-0.7467830000	-1.9311480000	-0.0000010000
C	-1.9931210000	0.4669100000	-0.0000010000
H	-2.2743190000	1.5424200000	0.0000020000
O	-2.8556560000	-0.3937590000	0.0000010000

B3LYP/6-31++G**	***p*-Br-PhCHO**



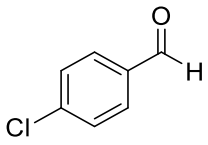


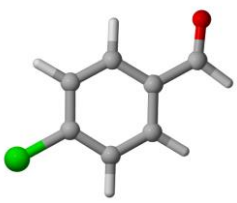
xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4900300000	-1.0501820000	-0.0000190000
C	-2.1187290000	0.2056420000	0.0000190000
C	-1.3405920000	1.3713120000	-0.0000210000
C	0.0514640000	1.2934180000	-0.0000470000
C	0.6585030000	0.0369610000	-0.0001700000
C	-0.1023900000	-1.1374770000	-0.0000450000
H	-1.8249990000	2.3449100000	0.0000030000
H	0.6591840000	2.1910780000	-0.0000350000
H	0.3927420000	-2.1020130000	-0.0000350000
H	-2.1042760000	-1.9451710000	0.0000070000
C	-3.5948110000	0.3123490000	-0.0000190000
H	-3.9884320000	1.3512840000	-0.0000340000
O	-4.3587840000	-0.6368060000	-0.0000540000
Br	2.5530160000	-0.0839360000	0.0000670000

B3LYP/6-31++G**	***p*-Cl-PhCHO**





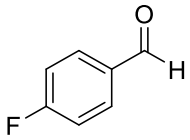
xyz-matrix

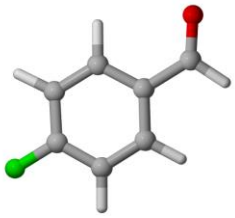
14
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8354850000	-1.0587830000	0.0000180000
C	-1.4425840000	0.2080280000	0.0000260000
C	-0.6424450000	1.3590790000	0.0000180000
C	0.7485100000	1.2591060000	0.0000040000
C	1.3297340000	-0.0103000000	-0.0000030000
C	0.5503770000	-1.1737580000	0.0000040000
H	-1.1100180000	2.3407130000	0.0000230000

H	1.3736180000	2.1448980000	-0.0000020000
H	1.0299420000	-2.1463070000	-0.0000020000
H	-1.4663900000	-1.9419870000	0.0000240000
C	-2.9167050000	0.3413320000	0.0000460000
H	-3.2908800000	1.3874930000	-0.0000460000
O	-3.6985170000	-0.5931740000	-0.0000400000
Cl	3.0766740000	-0.1522140000	-0.0000210000

B3LYP/6-31++G**	***p*-F-PhCHO**



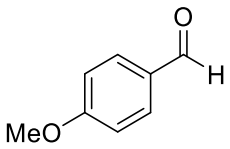


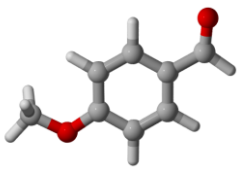
xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.4224850000	-1.0729730000	0.0000030000
C	-0.9922080000	0.2124510000	0.0000060000
C	-0.1604590000	1.3424260000	0.0000040000
C	1.2271250000	1.2044410000	0.0000010000
C	1.7538730000	-0.0827090000	-0.0000020000
C	0.9593750000	-1.2288020000	0.0000000000
H	-0.6026760000	2.3356050000	0.0000060000
H	1.8923300000	2.0607510000	-0.0000010000
H	1.4281050000	-2.2068250000	-0.0000020000
H	-1.0807350000	-1.9358310000	0.0000050000
C	-2.4607490000	0.3873540000	0.0000100000
H	-2.8046860000	1.4440430000	-0.0000110000
O	-3.2702410000	-0.5237230000	-0.0000100000
F	3.1003070000	-0.2312320000	-0.0000050000

B3LYP/6-31++G**	***p*-OMe-PhCHO**



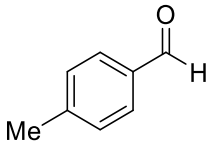


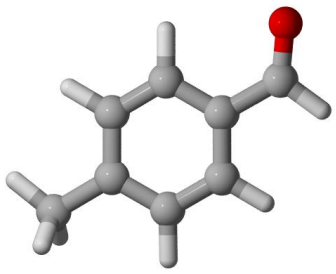
xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7350790000	-1.0036090000	-0.0000080000
C	1.4848530000	0.1821940000	-0.0000810000
C	0.8082040000	1.4156970000	-0.0000940000
C	-0.5779080000	1.4666240000	-0.0000360000
C	-1.3186470000	0.2716020000	0.0000370000
C	-0.6562120000	-0.9696660000	0.0000510000
H	1.3804550000	2.3405990000	-0.0001500000
H	-1.1131790000	2.4101930000	-0.0000450000
H	-1.2139840000	-1.8983370000	0.0001030000
H	1.2624730000	-1.9525660000	0.0000000000
C	2.9575270000	0.1504490000	-0.0001450000
H	3.4438470000	1.1503890000	-0.0001670000
O	3.6395020000	-0.8625100000	-0.0001040000
O	-2.6697310000	0.4177500000	0.0000870000
C	-3.4924340000	-0.7470000000	0.0002160000
H	-4.5194550000	-0.3813890000	0.0002800000
H	-3.3206180000	-1.3543270000	-0.8962160000
H	-3.3204720000	-1.3542310000	0.8966860000

B3LYP/6-31++G**	***p*-Me-PhCHO**





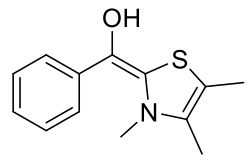
xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.4630580000	-1.0676050000	0.0001130000
C	-1.0460310000	0.2053250000	0.0001630000
C	-0.2203870000	1.3356600000	0.0001170000
C	1.1619530000	1.1970550000	0.0000390000
C	1.7541150000	-0.0728680000	-0.0000060000
C	0.9188540000	-1.1995650000	0.0000330000
H	-0.6674770000	2.3252600000	0.0001520000
H	1.7915450000	2.0809670000	0.0000110000
H	1.3627320000	-2.1894930000	0.0000000000
H	-1.1090780000	-1.9379090000	0.0001480000
C	-2.5144520000	0.3708250000	0.0002790000

H	-2.8585530000	1.4274050000	-0.0004460000
O	-3.3185460000	-0.5358330000	-0.0004240000
C	3.2557920000	-0.2155180000	-0.0000920000
H	3.6951860000	0.2623870000	-0.8808170000
H	3.5580090000	-1.2641450000	-0.0001360000
H	3.6952820000	0.2623410000	0.8806080000

B3LYP/6-31++G**	

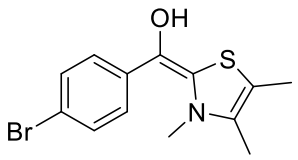
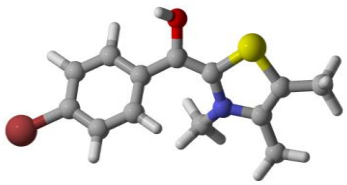
xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.5869560000	-0.5271150000	-0.0790160000
N	-1.0030820000	0.7897130000	-0.2824830000
C	-2.3898190000	0.9790670000	-0.0779180000
C	-3.0725700000	-0.1536830000	0.1761280000
S	-2.0030220000	-1.5760720000	0.1716730000
C	-4.5278450000	-0.3557800000	0.4558280000
C	-2.9438510000	2.3713650000	-0.1327310000
C	0.6713630000	-1.0440370000	-0.0902360000
H	-2.3515060000	3.0533310000	0.4850740000
H	-3.9676830000	2.3889470000	0.2380880000
H	-2.9583560000	2.7767780000	-1.1498030000
H	-4.6950350000	-0.7631350000	1.4586930000
H	-4.9689170000	-1.0601950000	-0.2577790000
H	-5.0820400000	0.5805940000	0.3778640000
C	-0.2261920000	1.6972840000	-1.1249490000
H	0.3966540000	1.1089760000	-1.8012200000
H	0.4324620000	2.3489030000	-0.5440010000
H	-0.8977850000	2.3152530000	-1.7191630000
C	1.9541740000	-0.3544630000	0.0293570000
C	3.1117730000	-0.9051120000	-0.5598380000
C	4.3544240000	-0.3013240000	-0.3994230000
C	4.4849780000	0.8632040000	0.3576250000
C	3.3530430000	1.4098200000	0.9641550000
C	2.1085120000	0.8089680000	0.8112610000
H	3.0207150000	-1.8008440000	-1.1630920000
H	5.2260880000	-0.7399570000	-0.8733130000
H	3.4445820000	2.2991900000	1.5786760000
H	1.2489660000	1.2168610000	1.3301150000
O	0.7115350000	-2.4387700000	-0.2055060000
H	1.3287500000	-2.7858050000	0.4503040000

H 5.4545500000 1.3312560000 0.4827630000

B3LYP/6-31++G**	

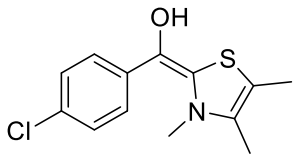
		

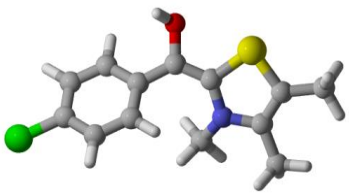
xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	2.0505110000	-0.5713740000	0.0824360000
N	2.2554690000	0.7835940000	0.3388980000
C	3.5779290000	1.2127200000	0.0777390000
C	4.4219080000	0.2222880000	-0.2697460000
S	3.6012620000	-1.3561110000	-0.2932660000
C	5.8728160000	0.2787720000	-0.6286100000
C	3.8958970000	2.6741720000	0.1810210000
C	0.8945480000	-1.2907540000	0.1207270000
H	3.1662400000	3.2738010000	-0.3717290000
H	4.8808530000	2.8802840000	-0.2354580000
H	3.8987320000	3.0302100000	1.2162670000
H	6.0479300000	-0.0448930000	-1.6601160000
H	6.4621300000	-0.3766280000	0.0216710000
H	6.2691620000	1.2894110000	-0.5225160000
C	1.3851170000	1.5118810000	1.2608060000
H	0.8799630000	0.7956330000	1.9104740000
H	0.6186110000	2.0952650000	0.7429770000
H	1.9793840000	2.1830300000	1.8796990000
C	-0.4852330000	-0.8181080000	0.0876770000
C	-1.5127210000	-1.5869420000	0.6733270000
C	-2.8450150000	-1.1963230000	0.5987080000
C	-3.1783500000	-0.0249440000	-0.0754860000
C	-2.1935030000	0.7479110000	-0.6856930000
C	-0.8646480000	0.3481040000	-0.6088400000
H	-1.2554410000	-2.4906090000	1.2128820000
H	-3.6152800000	-1.7951010000	1.0682010000
Br	-5.0149090000	0.5218150000	-0.1805240000
H	-2.4630740000	1.6412510000	-1.2349300000
H	-0.1109580000	0.9274450000	-1.1284860000
O	1.0880010000	-2.6764420000	0.1698050000
H	0.5355470000	-3.0928880000	-0.5034650000

B3LYP/6-31++G**	



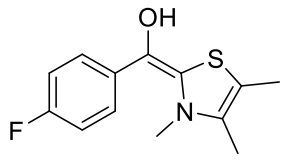
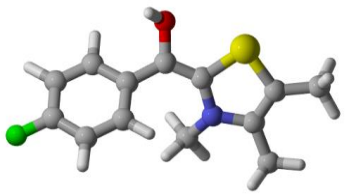


xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3607480000	-0.5672570000	0.0856290000
N	1.6233940000	0.7807550000	0.3276290000
C	2.9674350000	1.1459170000	0.0787450000
C	3.7701620000	0.1137800000	-0.2441250000
S	2.8794870000	-1.4267550000	-0.2569040000
C	5.2260410000	0.0991710000	-0.5862880000
C	3.3491930000	2.5931330000	0.1651330000
C	0.1722010000	-1.2309690000	0.1151120000
H	2.6567910000	3.2155250000	-0.4100320000
H	4.3495940000	2.7484810000	-0.2363500000
H	3.3498480000	2.9657020000	1.1945540000
H	5.3977450000	-0.2461160000	-1.6113700000
H	5.7772300000	-0.5737450000	0.0793710000
H	5.6675410000	1.0918560000	-0.4889230000
C	0.7787220000	1.5572000000	1.2342120000
H	0.2340210000	0.8713620000	1.8847330000
H	0.0457970000	2.1713620000	0.7034230000
H	1.3976840000	2.2052320000	1.8535620000
C	-1.1828890000	-0.6923690000	0.0557410000
C	-2.2550910000	-1.3999400000	0.6381590000
C	-3.5646200000	-0.9442310000	0.5390880000
C	-3.8300880000	0.2317970000	-0.1560270000
C	-2.7998330000	0.9448870000	-0.7632100000
C	-1.4941810000	0.4805840000	-0.6626180000
H	-2.0505770000	-2.3072830000	1.1937820000
H	-4.3734520000	-1.4936650000	1.0044980000
Cl	-5.4863650000	0.8163260000	-0.2832520000
H	-3.0215690000	1.8419970000	-1.3278390000
H	-0.7053490000	1.0139240000	-1.1793090000
O	0.2980590000	-2.6235060000	0.1834950000
H	-0.2639230000	-3.0215330000	-0.4930240000

B3LYP/6-31++G**	

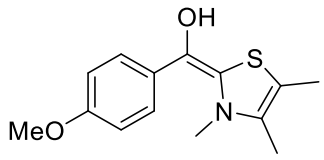
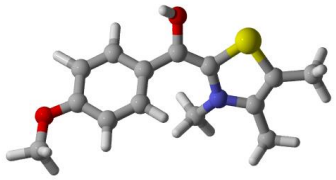
		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9765680000	-0.5512590000	0.0777770000
N	1.3065120000	0.7893410000	0.2999060000
C	2.6769320000	1.0733270000	0.0827920000
C	3.4279840000	-0.0113120000	-0.2106410000
S	2.4524510000	-1.4991100000	-0.2245190000
C	4.8900140000	-0.1123780000	-0.5190350000
C	3.1450220000	2.4970230000	0.1676960000
C	-0.2479160000	-1.1515840000	0.1062280000
H	2.4947410000	3.1609270000	-0.4134270000
H	4.1567980000	2.5893430000	-0.2296820000
H	3.1661270000	2.8732170000	1.1978920000
H	5.0654790000	-0.4929600000	-1.5329590000
H	5.3909530000	-0.7975980000	0.1762680000
H	5.3833080000	0.8590720000	-0.4360080000
C	0.4785010000	1.6199040000	1.1725070000
H	0.0014890000	0.9861520000	1.9271210000
H	-0.3118810000	2.1437990000	0.6250780000
H	1.1008510000	2.3577260000	1.6783120000
C	-1.5792260000	-0.5485020000	0.0207200000
C	-2.6833810000	-1.1745240000	0.6431650000
C	-3.9738950000	-0.6606210000	0.5220710000
C	-4.1660940000	0.4906490000	-0.2325530000
C	-3.1165970000	1.1319410000	-0.8792800000
C	-1.8316410000	0.6031880000	-0.7579060000
H	-2.5169090000	-2.0638400000	1.2425420000
H	-4.8199130000	-1.1346660000	1.0086170000
F	-5.4249220000	0.9992440000	-0.3536370000
H	-3.3119150000	2.0117940000	-1.4834110000
H	-1.0149110000	1.0673970000	-1.3015790000
O	-0.1950710000	-2.5496120000	0.1936330000
H	-0.7617880000	-2.9313930000	-0.4933770000

B3LYP/6-31++G**	

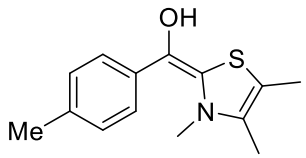
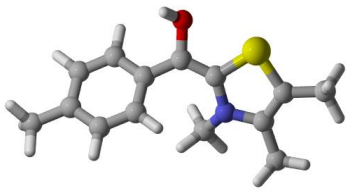
		

xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3781090000	-0.5704260000	0.0486360000
N	1.5975480000	0.7812490000	0.3469650000
C	2.9318390000	1.1949480000	0.1200460000
C	3.7656880000	0.2016740000	-0.2601680000
S	2.9237420000	-1.3643020000	-0.3483790000
C	5.2208570000	0.2513830000	-0.6106910000
C	3.2788240000	2.6461900000	0.2845380000
C	0.2129160000	-1.2751680000	0.0686710000
H	2.5582080000	3.2850480000	-0.2390150000
H	4.2677440000	2.8505340000	-0.1284710000
H	3.2958370000	2.9593100000	1.3357300000
H	5.3981160000	-0.0416130000	-1.6532260000
H	5.8001870000	-0.4335870000	0.0213240000
H	5.6307050000	1.2544920000	-0.4699530000
C	0.7253200000	1.4743160000	1.2923170000
H	0.3526040000	0.7592730000	2.0335600000
H	-0.1412780000	1.9297150000	0.8019510000
H	1.2845110000	2.2542460000	1.8090270000
C	-1.1698920000	-0.7887550000	0.0687840000
C	-2.1871170000	-1.5253260000	0.7215780000
C	-3.5142790000	-1.1206840000	0.6823140000
C	-3.8816910000	0.0404850000	-0.0163600000
C	-2.8977610000	0.7794650000	-0.6842320000
C	-1.5651220000	0.3571770000	-0.6455880000
H	-1.9170230000	-2.4174180000	1.2784060000
H	-4.2868720000	-1.6859800000	1.1940520000
H	-3.1530250000	1.6654530000	-1.2538880000
H	-0.8221110000	0.9149150000	-1.2079800000
O	0.3874590000	-2.6665570000	0.0504080000
H	-0.1953490000	-3.0467500000	-0.6235890000
O	-5.2137560000	0.3577680000	0.0087600000
C	-5.6459410000	1.5222280000	-0.6811010000
H	-6.7229050000	1.5826910000	-0.5185670000
H	-5.1670850000	2.4258530000	-0.2821660000
H	-5.4450840000	1.4491870000	-1.7576880000

B3LYP/6-31++G**	

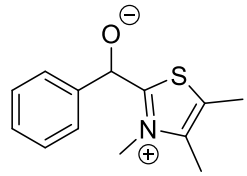
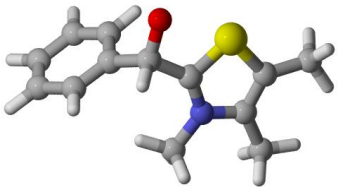
		

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.0065760000	-0.5516280000	0.0758730000
N	1.3240950000	0.7926000000	0.3005490000
C	2.6904920000	1.0898170000	0.0809690000
C	3.4522870000	0.0134830000	-0.2159960000
S	2.4925880000	-1.4849750000	-0.2292450000
C	4.9144100000	-0.0713450000	-0.5286780000
C	3.1447000000	2.5181270000	0.1659330000
C	-0.2119370000	-1.1626400000	0.1060760000
H	2.4857140000	3.1757200000	-0.4126130000
H	4.1544020000	2.6213410000	-0.2341980000
H	3.1646580000	2.8936720000	1.1964320000
H	5.0914460000	-0.4460670000	-1.5446420000
H	5.4241280000	-0.7545470000	0.1623730000
H	5.3983370000	0.9046340000	-0.4427700000
C	0.4908470000	1.6107950000	1.1796300000
H	0.0285590000	0.9698290000	1.9375190000
H	-0.3120890000	2.1209900000	0.6378060000
H	1.1060270000	2.3580100000	1.6806880000
C	-1.5488900000	-0.5723030000	0.0233640000
C	-2.6494110000	-1.2074600000	0.6430960000
C	-3.9386520000	-0.6968830000	0.5194800000
C	-4.2011210000	0.4632240000	-0.2280870000
C	-3.1141840000	1.0837240000	-0.8590570000
C	-1.8187220000	0.5776970000	-0.7473780000
H	-2.4769800000	-2.0965130000	1.2423270000
H	-4.7594460000	-1.2058970000	1.0206690000
H	-3.2853340000	1.9692570000	-1.4672020000
H	-1.0094720000	1.0558380000	-1.2912690000
O	-0.1439070000	-2.5603090000	0.1876670000
H	-0.7451480000	-2.9423860000	-0.4688250000
C	-5.6049250000	1.0084150000	-0.3504850000
H	-5.6281620000	1.9142010000	-0.9636490000
H	-6.0231110000	1.2602430000	0.6317010000
H	-6.2811610000	0.2774050000	-0.8100430000

B3LYP/6-31++G**	

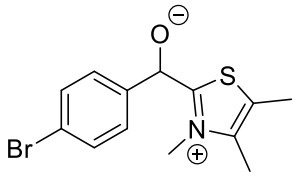
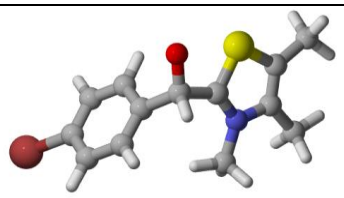
		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.5745060000	-0.3026730000	0.5507980000
N	-1.0740480000	0.9289590000	0.4110060000
C	-2.3849000000	0.9707960000	-0.1080940000
C	-2.8605480000	-0.2840570000	-0.3553870000
S	-1.6696360000	-1.5206940000	0.0756210000
C	-4.1937450000	-0.6803940000	-0.9175750000
C	-3.0552200000	2.2953790000	-0.3199450000
C	0.7354870000	-0.9371170000	1.0829460000
H	-3.0954900000	2.8860110000	0.6024350000
H	-4.0807990000	2.1454420000	-0.6593790000
H	-2.5424100000	2.8976960000	-1.0792820000
H	-4.6865670000	-1.4200870000	-0.2775660000
H	-4.0867960000	-1.1282740000	-1.9121910000
H	-4.8636820000	0.1779460000	-1.0096320000
C	-0.3269360000	2.1337300000	0.7894940000
H	0.7042640000	1.8566100000	0.9970500000
H	-0.7747780000	2.5889740000	1.6773030000
H	-0.3394520000	2.8501520000	-0.0340470000
C	1.9528760000	-0.3694030000	0.3226880000
C	2.1246990000	-0.6690430000	-1.0364110000
C	3.2409510000	-0.2022530000	-1.7303560000
C	4.2146740000	0.5594020000	-1.0706130000
C	4.0641650000	0.8423310000	0.2880960000
C	2.9367810000	0.3790410000	0.9780400000
H	4.8262580000	1.4106430000	0.8149730000
H	2.8335470000	0.5814550000	2.0427710000
O	0.5540270000	-2.2561630000	0.9618650000
H	5.0891140000	0.9134310000	-1.6094710000
H	1.3907610000	-1.3001720000	-1.5298890000
H	3.3620530000	-0.4411350000	-2.7837680000
H	0.8216170000	-0.5554460000	2.1367140000

B3LYP/6-31++G**	

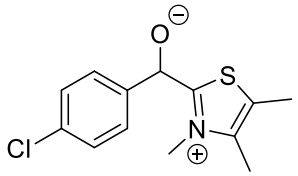
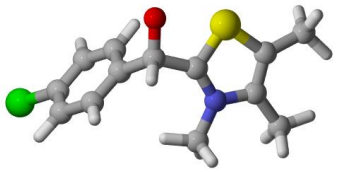
		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0173720000	-0.4747430000	0.4986680000
N	-2.3233570000	0.8186430000	0.6378080000
C	-3.4922760000	1.2174410000	-0.0435100000
C	-4.0624870000	0.1693470000	-0.7056920000
S	-3.1423750000	-1.3217710000	-0.4633830000
C	-5.2992620000	0.1667240000	-1.5548270000
C	-3.9368270000	2.6480470000	0.0239300000
C	-0.9291090000	-1.4444030000	1.0310740000
H	-4.1013180000	2.9778970000	1.0561610000
H	-4.8763960000	2.7733530000	-0.5153720000
H	-3.2044400000	3.3260540000	-0.4300410000
H	-5.9897870000	-0.6234830000	-1.2415360000
H	-5.0560480000	-0.0101180000	-2.6087630000
H	-5.8326860000	1.1180910000	-1.4910260000
C	-1.5228030000	1.7413810000	1.4507360000
H	-0.6024650000	1.2429490000	1.7460550000
H	-2.0842130000	2.0404860000	2.3400900000
H	-1.2695950000	2.6262220000	0.8636130000
C	0.4749320000	-0.9277490000	0.6584570000
C	0.8793400000	-0.9278180000	-0.6831810000
C	2.1503590000	-0.4896550000	-1.0497720000
C	3.0352540000	-0.0630160000	-0.0560290000
C	2.6742210000	-0.0872620000	1.2878360000
C	1.3886970000	-0.5196420000	1.6344380000
H	3.3826480000	0.2152640000	2.0514260000
H	1.1073680000	-0.5583050000	2.6851220000
O	-1.2463140000	-2.6359230000	0.5174120000
Br	4.7810340000	0.5279670000	-0.5491540000
H	0.1945870000	-1.3051310000	-1.4373160000
H	2.4576210000	-0.4865520000	-2.0899960000
H	-1.0054690000	-1.3622860000	2.1493700000

B3LYP/6-31++G**	

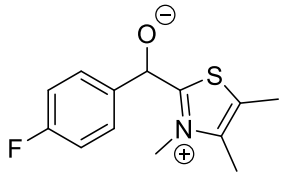
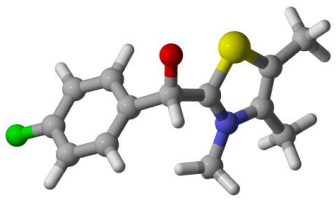
		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3456390000	-0.4121550000	0.5438400000
N	-1.7243370000	0.8691900000	0.5605980000
C	-2.9413710000	1.1267350000	-0.1048280000
C	-3.4703970000	-0.0165080000	-0.6296850000
S	-2.4530700000	-1.4192140000	-0.2731300000
C	-4.7360480000	-0.1815350000	-1.4178740000
C	-3.4732530000	2.5278120000	-0.1588600000
C	-0.1773710000	-1.2538260000	1.1223940000
H	-3.5978360000	2.9561320000	0.8421750000
H	-4.4493900000	2.5388880000	-0.6451150000
H	-2.8149630000	3.1950240000	-0.7278140000
H	-5.3750490000	-0.9553840000	-0.9792170000
H	-4.5226980000	-0.4801000000	-2.4505670000
H	-5.3130930000	0.7456060000	-1.4526190000
C	-0.9495840000	1.9158040000	1.2369770000
H	0.0166070000	1.5076360000	1.5244240000
H	-1.4841590000	2.2625860000	2.1255640000
H	-0.7887180000	2.7544110000	0.5569500000
C	1.1753470000	-0.7099380000	0.6150460000
C	1.5145780000	-0.8500810000	-0.7378480000
C	2.7460070000	-0.4096330000	-1.2198580000
C	3.6594650000	0.1638860000	-0.3301790000
C	3.3618650000	0.2899400000	1.0242650000
C	2.1151390000	-0.1499100000	1.4856660000
H	4.0916840000	0.7115430000	1.7074660000
H	1.8873220000	-0.0751860000	2.5472930000
O	-0.4472190000	-2.5119250000	0.7642050000
Cl	5.2210780000	0.7188840000	-0.9319520000
H	0.8141240000	-1.3424660000	-1.4061540000
H	3.0045640000	-0.5180040000	-2.2679740000
H	-0.2019010000	-1.0467600000	2.2266990000

B3LYP/6-31++G**	

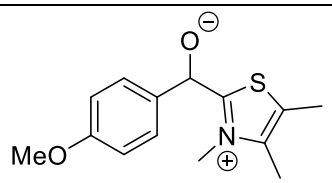
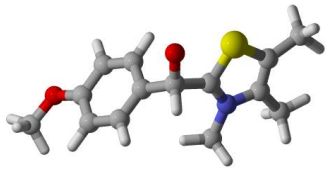
		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9586210000	-0.3573160000	-0.5614300000
N	1.3947870000	0.9035000000	-0.4841540000
C	2.6593570000	1.0473360000	0.1250760000
C	3.1649360000	-0.1608200000	0.5081180000
S	2.0645020000	-1.4813100000	0.0883310000
C	4.4663790000	-0.4508660000	1.1954630000
C	3.2574900000	2.4145190000	0.2734660000
C	-0.2791640000	-1.0921810000	-1.1405300000
H	3.3488340000	2.9267030000	-0.6911390000
H	4.2576610000	2.3413630000	0.7021710000
H	2.6616400000	3.0540760000	0.9354960000
H	5.0649180000	-1.1663640000	0.6211710000
H	4.3007470000	-0.8854120000	2.1877020000
H	5.0640860000	0.4544820000	1.3250670000
C	0.6312000000	2.0398040000	-1.0117220000
H	-0.3723350000	1.7029970000	-1.2617730000
H	1.1210100000	2.4394500000	-1.9040740000
H	0.5616390000	2.8213120000	-0.2529390000
C	-1.5757230000	-0.5374250000	-0.5125050000
C	-1.8461670000	-0.7801290000	0.8422380000
C	-3.0294630000	-0.3343830000	1.4301680000
C	-3.9496260000	0.3439790000	0.6353840000
C	-3.7345270000	0.5812400000	-0.7139960000
C	-2.5342240000	0.1319970000	-1.2802500000
H	-4.4915270000	1.0886320000	-1.3028830000
H	-2.3578940000	0.2868310000	-2.3428710000
O	-0.0498280000	-2.3879950000	-0.9108000000
F	-5.1114470000	0.7777490000	1.2034950000
H	-1.1318090000	-1.3559020000	1.4233870000
H	-3.2523730000	-0.5150860000	2.4766600000
H	-0.3030290000	-0.7869320000	-2.2221370000

B3LYP/6-31++G**	

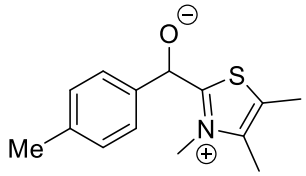
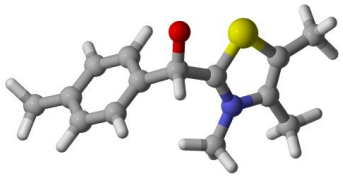
		

xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3633570000	-0.3958130000	-0.5399340000
N	1.7108090000	0.8944940000	-0.5286420000
C	2.9535400000	1.1583810000	0.0845650000
C	3.5351090000	0.0109600000	0.5396900000
S	2.5316890000	-1.4043380000	0.1851280000
C	4.8430100000	-0.1492570000	1.2567520000
C	3.4544830000	2.5698470000	0.1634950000
C	0.1867930000	-1.2427820000	-1.0863880000
H	3.5171530000	3.0367730000	-0.8260840000
H	4.4537960000	2.5882440000	0.5999510000
H	2.8107360000	3.1996710000	0.7890490000
H	5.4848610000	-0.8766020000	0.7479120000
H	4.6912980000	-0.5080110000	2.2811840000
H	5.3904140000	0.7947370000	1.3133340000
C	0.8749350000	1.9422420000	-1.1252100000
H	-0.0988240000	1.5191170000	-1.3632410000
H	1.3460900000	2.3262970000	-2.0343990000
H	0.7396300000	2.7574820000	-0.4119340000
C	-1.1518450000	-0.7311590000	-0.5191490000
C	-1.4235450000	-0.8469920000	0.8549750000
C	-2.6416120000	-0.4399730000	1.3826300000
C	-3.6377890000	0.0805570000	0.5378040000
C	-3.3967420000	0.1821530000	-0.8352730000
C	-2.1538950000	-0.2256160000	-1.3461850000
O	0.4989290000	-2.5051130000	-0.7719930000
H	-2.8558760000	-0.5292400000	2.4432090000
H	0.1655960000	-1.0099560000	-2.1864120000
O	-4.8066060000	0.4472440000	1.1533590000
C	-5.8695450000	0.9352700000	0.3479420000
H	-6.6906500000	1.1488210000	1.0338350000
H	-5.5863560000	1.8571280000	-0.1769930000
H	-6.1939500000	0.1856620000	-0.3852330000
H	-0.6747290000	-1.2945670000	1.5025590000
H	-1.9822970000	-0.1654270000	-2.4195410000
H	-4.1556960000	0.5538530000	-1.5139720000

B3LYP/6-31++G**	

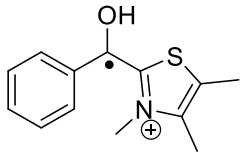
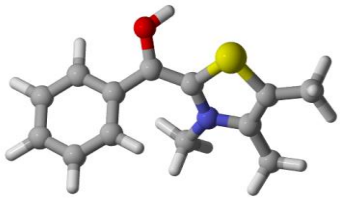
		

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9894260000	-0.3758310000	0.5501240000
N	-1.4078180000	0.8923690000	0.5025490000
C	-2.6660070000	1.0685760000	-0.1113320000
C	-3.1839080000	-0.1221820000	-0.5304350000
S	-2.1028140000	-1.4686880000	-0.1388480000
C	-4.4843700000	-0.3768060000	-1.2334890000
C	-3.2456100000	2.4470180000	-0.2262950000
C	0.2329030000	-1.1416370000	1.1161940000
H	-3.3303290000	2.9362550000	0.7507360000
H	-4.2465260000	2.3979020000	-0.6567580000
H	-2.6407750000	3.0948010000	-0.8720590000
H	-5.1037930000	-1.0858200000	-0.6732330000
H	-4.3180090000	-0.8041910000	-2.2287330000
H	-5.0617200000	0.5422470000	-1.3596710000
C	-0.6306790000	2.0025830000	1.0646020000
H	0.3712260000	1.6473230000	1.2963400000
H	-1.1117910000	2.3760780000	1.9730290000
H	-0.5576160000	2.8088710000	0.3325550000
C	1.5402740000	-0.5798230000	0.5199380000
C	1.8217700000	-0.7590490000	-0.8421730000
C	3.0164060000	-0.2960750000	-1.3890210000
C	3.9828180000	0.3454860000	-0.5932890000
C	3.7052690000	0.5058630000	0.7686390000
C	2.5000330000	0.0487730000	1.3173820000
O	-0.0126550000	-2.4281000000	0.8450780000
H	3.2129390000	-0.4442960000	-2.4490600000
H	0.2487960000	-0.8718910000	2.2073530000
H	1.1060120000	-1.2950560000	-1.4594230000
H	2.3181430000	0.1645140000	2.3846930000
H	4.4414390000	0.9815390000	1.4131780000
C	5.2928910000	0.8083340000	-1.1893730000
H	5.8181190000	1.4929750000	-0.5164270000
H	5.1393270000	1.3242700000	-2.1437790000
H	5.9613680000	-0.0396770000	-1.3844670000

(u)B3LYP/6-31++G**	

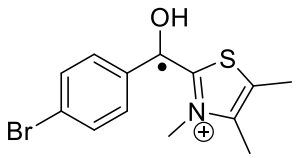
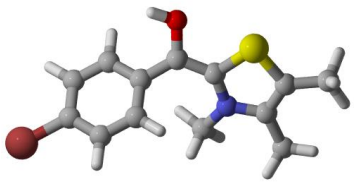
		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.5948390000	-0.5346490000	0.1390940000
N	1.0271740000	0.7390050000	0.4019140000
C	2.3865840000	0.9513340000	0.1537580000
C	3.0445740000	-0.1779450000	-0.2547950000
S	1.9385790000	-1.5273300000	-0.3775620000
C	4.4903650000	-0.3754750000	-0.5931690000
C	2.9816280000	2.3101510000	0.3679630000
C	-0.7102600000	-1.0647790000	0.2412480000
H	2.3909140000	3.0873410000	-0.1263010000
H	3.9899580000	2.3497560000	-0.0429300000
H	3.0503980000	2.5614360000	1.4325460000
H	4.6142280000	-0.7225530000	-1.6243540000
H	4.9499850000	-1.1186000000	0.0672670000
H	5.0471630000	0.5561060000	-0.4835160000
C	0.2072570000	1.7560410000	1.0847330000
H	-0.6280670000	1.2690250000	1.5820860000
H	-0.1792770000	2.4884150000	0.3727350000
H	0.8226040000	2.2595340000	1.8296620000
C	-1.9625590000	-0.3687880000	0.0078010000
C	-3.1447270000	-0.8386190000	0.6253620000
C	-4.3605460000	-0.2113780000	0.3741220000
C	-4.4249740000	0.8752630000	-0.5061070000
C	-3.2646660000	1.3316980000	-1.1446870000
C	-2.0426820000	0.7175640000	-0.8938640000
H	-3.0938000000	-1.6848180000	1.3011750000
H	-5.2612740000	-0.5705870000	0.8612040000
H	-5.3771910000	1.3567750000	-0.7048330000
H	-3.3210910000	2.1522240000	-1.8528430000
H	-1.1577710000	1.0428200000	-1.4324660000
O	-0.8436570000	-2.3991410000	0.4442140000
H	-0.0740150000	-2.7919960000	0.8856820000

(u)B3LYP/6-31++G**	

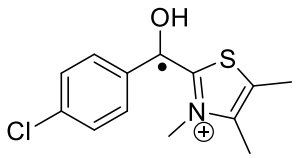
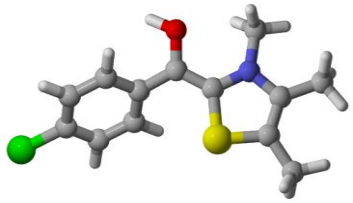
		

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	2.0625730000	-0.5615550000	0.0885710000
N	2.2748450000	0.7612660000	0.3830560000
C	3.5786970000	1.1969800000	0.1417620000
C	4.4105020000	0.1919350000	-0.2828140000
S	3.5519100000	-1.3218090000	-0.4058830000
C	5.8670810000	0.2480020000	-0.6296800000
C	3.9456920000	2.6316370000	0.3706230000
C	0.8765400000	-1.3099250000	0.1608720000
H	3.2335310000	3.3088050000	-0.1107000000
H	4.9307720000	2.8392600000	-0.0462350000
H	3.9820990000	2.8787140000	1.4379120000
H	6.0290850000	0.0508940000	-1.6950360000
H	6.4330380000	-0.4989730000	-0.0635160000
H	6.2887890000	1.2271900000	-0.3990660000
C	1.2910830000	1.6164310000	1.0698790000
H	0.5963480000	0.9898310000	1.6246730000
H	0.7337540000	2.2272930000	0.3560920000
H	1.8173310000	2.2640210000	1.7695330000
C	-0.5009720000	-0.8368740000	0.1014500000
C	-1.4954730000	-1.4665280000	0.8829570000
C	-2.8231930000	-1.0622290000	0.8004360000
C	-3.1769240000	-0.0247770000	-0.0695090000
C	-2.2112220000	0.5966940000	-0.8706820000
C	-0.8845280000	0.1931480000	-0.7839380000
H	-1.2233080000	-2.2478780000	1.5872480000
H	-3.5795220000	-1.5372990000	1.4148040000
Br	-4.9767430000	0.5179510000	-0.1933900000
H	-2.5033200000	1.3759740000	-1.5654340000
H	-0.1473040000	0.6494890000	-1.4375590000
O	1.1094380000	-2.6455580000	0.2335120000
H	0.3256270000	-3.1486900000	-0.0390030000

(u)B3LYP/6-31++G**	

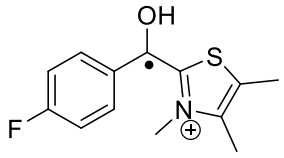
		

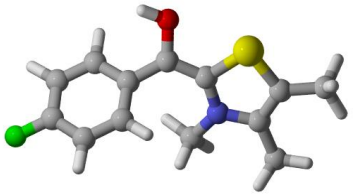
xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3057360000	0.4078250000	0.0291230000
N	-2.6065110000	0.8303380000	0.1787020000
C	-3.5594910000	-0.1766220000	0.0299150000
C	-3.0082710000	-1.4111760000	-0.2041660000
S	-1.2673900000	-1.3147190000	-0.2652770000
C	-3.6769100000	-2.7386570000	-0.3918390000
C	-5.0211520000	0.1372750000	0.1343140000
C	-0.1488650000	1.1984080000	-0.0196260000
H	-5.3044200000	0.4243610000	1.1532270000
H	-5.6127940000	-0.7373170000	-0.1335680000
H	-5.3064500000	0.9491890000	-0.5418970000
H	-3.4119640000	-3.4302430000	0.4155090000
H	-3.3795570000	-3.2015330000	-1.3385110000
H	-4.7625760000	-2.6345780000	-0.3976340000
C	-2.9762520000	2.2132500000	0.5421240000
H	-2.2768650000	2.5923290000	1.2843170000
H	-3.9757420000	2.2051610000	0.9685060000
H	-2.9533110000	2.8597410000	-0.3368840000
C	1.2160850000	0.6731180000	0.0029810000
C	2.1873370000	1.2318260000	-0.8580250000
C	3.5020590000	0.7806440000	-0.8368940000
C	3.8674070000	-0.2339820000	0.0558680000
C	2.9253720000	-0.7954780000	0.9256210000
C	1.6106450000	-0.3437930000	0.8979960000
H	1.9054310000	1.9904030000	-1.5831080000
H	4.2385020000	1.1990110000	-1.5137880000
Cl	5.5104900000	-0.7990170000	0.0881040000
H	3.2270610000	-1.5652700000	1.6270080000
H	0.8992840000	-0.7559030000	1.6059890000
O	-0.3272790000	2.5313650000	-0.1914570000
H	0.5037420000	3.0043310000	-0.0261160000

(u)B3LYP/6-31++G**	



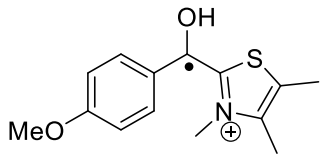


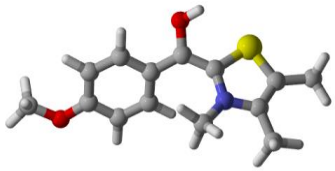
xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9957560000	-0.5403750000	0.1019270000
N	1.3354820000	0.7648700000	0.3528980000
C	2.6834710000	1.0556490000	0.1367330000
C	3.4178160000	-0.0440270000	-0.2294740000
S	2.4115860000	-1.4661580000	-0.3235830000
C	4.8828260000	-0.1532220000	-0.5233310000
C	3.1898710000	2.4523470000	0.3322180000
C	-0.2627180000	-1.1613100000	0.1553420000
H	2.5655800000	3.1825310000	-0.1916680000
H	4.2029140000	2.5441940000	-0.0583470000
H	3.2205390000	2.7299850000	1.3922000000
H	5.0575840000	-0.4786470000	-1.5544140000
H	5.3616580000	-0.8807160000	0.1406820000
H	5.3851640000	0.8047820000	-0.3828520000
C	0.4268950000	1.7487000000	0.9659220000
H	-0.3710580000	1.2261760000	1.4878000000
H	-0.0076180000	2.4065310000	0.2093510000
H	0.9878320000	2.3441330000	1.6851720000
C	-1.5861640000	-0.5552190000	0.0445410000
C	-2.6536470000	-1.0574540000	0.8243690000
C	-3.9383080000	-0.5429400000	0.6855580000
C	-4.1520830000	0.4695650000	-0.2479430000
C	-3.1296910000	0.9808370000	-1.0467940000
C	-1.8477330000	0.4639170000	-0.8977450000
H	-2.4684990000	-1.8265340000	1.5688430000
H	-4.7644100000	-0.9044330000	1.2877770000
F	-5.3903710000	0.9681740000	-0.3889310000
H	-3.3529240000	1.7494280000	-1.7785030000
H	-1.0524940000	0.8210930000	-1.5446240000
O	-0.1688650000	-2.5107940000	0.2691060000
H	-0.9915220000	-2.9401130000	-0.0147740000

(u)B3LYP/6-31++G**	



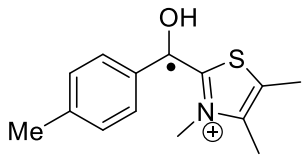
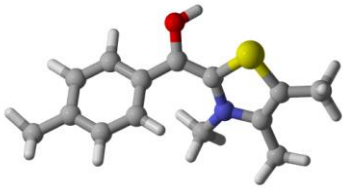


xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3770280000	-0.5627040000	-0.1437430000
N	1.7114390000	0.7349320000	-0.4376910000
C	3.0389190000	1.0705780000	-0.1470840000
C	3.7727210000	0.0173900000	0.3241990000
S	2.7808790000	-1.4205790000	0.4547450000
C	5.2149460000	-0.0444750000	0.7242940000
C	3.5225250000	2.4687040000	-0.3881500000
C	0.1262330000	-1.2047950000	-0.2693740000
H	2.8495100000	3.2063960000	0.0595570000
H	3.6068930000	2.6927830000	-1.4576240000
H	4.5083300000	2.6095350000	0.0542180000
H	5.7537960000	-0.7939460000	0.1347900000
H	5.3246630000	-0.3094410000	1.7813450000
H	5.7056660000	0.9170220000	0.5663910000
C	0.8480140000	1.6438850000	-1.2109430000
H	0.3973250000	2.4009220000	-0.5652790000
H	0.0581760000	1.0680920000	-1.6871070000
H	1.4479970000	2.1313190000	-1.9794940000
C	-1.1792720000	-0.6214810000	-0.0935820000
C	-1.3873900000	0.5242490000	0.7202810000
C	-2.6539110000	1.0292330000	0.9248840000
C	-3.7738750000	0.4066070000	0.3271230000
C	-3.5908800000	-0.7437580000	-0.4661290000
C	-2.3139610000	-1.2496660000	-0.6607130000
H	-4.4350170000	-1.2417970000	-0.9266110000
H	-2.1792610000	-2.1385260000	-1.2666390000
H	-2.8223750000	1.8888160000	1.5644760000
O	-4.9593570000	0.9784150000	0.5855060000
C	-6.1628910000	0.4050900000	0.0521820000
H	-6.9694410000	1.0410780000	0.4135360000
H	-6.1462220000	0.4156830000	-1.0424240000
H	-6.3030420000	-0.6157800000	0.4214880000
O	0.1245220000	-2.5569420000	-0.4353960000
H	0.9270450000	-2.8759560000	-0.8769660000
H	-0.5487420000	0.9836130000	1.2339230000

(u)B3LYP/6-31++G**	

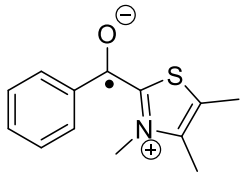
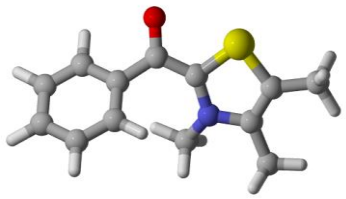
		

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.0073800000	-0.5634130000	0.1378620000
N	1.3511930000	0.7296170000	0.4362290000
C	2.6815580000	1.0550960000	0.1521110000
C	3.4084080000	-0.0038080000	-0.3204720000
S	2.4044190000	-1.4305210000	-0.4596980000
C	4.8517730000	-0.0770960000	-0.7142750000
C	3.1773730000	2.4477750000	0.3989950000
C	-0.2495500000	-1.1957550000	0.2596280000
H	2.5126300000	3.1930730000	-0.0483120000
H	4.1657850000	2.5806430000	-0.0399440000
H	3.2607760000	2.6671200000	1.4695150000
H	4.9638340000	-0.3504190000	-1.7688740000
H	5.3836700000	-0.8253710000	-0.1170100000
H	5.3473530000	0.8826850000	-0.5616150000
C	0.4869460000	1.6501530000	1.1961130000
H	-0.3062290000	1.0827740000	1.6764710000
H	0.0410880000	2.3995100000	0.5384570000
H	1.0865130000	2.1446540000	1.9601940000
C	-1.5547750000	-0.5940520000	0.0900690000
C	-2.6868480000	-1.1913400000	0.6932920000
C	-3.9518050000	-0.6556860000	0.4954550000
C	-4.1500360000	0.4759080000	-0.3176630000
C	-3.0244030000	1.0491060000	-0.9396730000
C	-1.7518120000	0.5304330000	-0.7450050000
H	-2.5581790000	-2.0688680000	1.3169620000
H	-4.8068840000	-1.1236810000	0.9746550000
C	-5.5240680000	1.0600610000	-0.5096110000
H	-3.1577550000	1.8980900000	-1.6040220000
H	-0.9128960000	0.9617340000	-1.2828770000
H	-5.6030700000	1.5993270000	-1.4572260000
H	-5.7539760000	1.7716870000	0.2938320000
H	-6.2949430000	0.2848710000	-0.4862330000
O	-0.2695140000	-2.5445710000	0.4178800000
H	0.5384970000	-2.8845290000	0.8335870000

(u)B3LYP/6-31++G**	

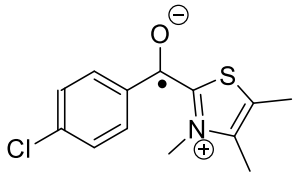
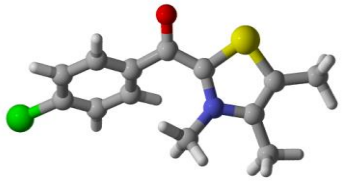
		

xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	0.5919480000	-0.5599640000	0.1282650000
N	0.9859120000	0.7594920000	0.3082790000
C	2.3605790000	0.9672830000	0.0916160000
C	3.0452480000	-0.1699440000	-0.1983850000
S	1.9813660000	-1.5807140000	-0.2015080000
C	4.5006740000	-0.3525100000	-0.5045900000
C	2.9064490000	2.3617490000	0.1892280000
C	-0.6977210000	-1.1841140000	0.1353040000
H	2.3918830000	3.0396550000	-0.5020040000
H	3.9676090000	2.3746320000	-0.0614880000
H	2.8012280000	2.7771100000	1.1981940000
H	4.6534560000	-0.7174940000	-1.5273160000
H	4.9545850000	-1.0844810000	0.1739300000
H	5.0521630000	0.5844870000	-0.3982670000
C	0.2312980000	1.7063860000	1.1386710000
H	-0.7591370000	1.3084710000	1.3364680000
H	0.1221350000	2.6667250000	0.6281570000
H	0.7461440000	1.8616300000	2.0940040000
O	-0.7442370000	-2.4394180000	0.2148710000
C	-1.9734370000	-0.4129880000	-0.0247490000
C	-3.1301290000	-0.9003800000	0.6068830000
C	-4.3579690000	-0.2637380000	0.4278490000
C	-4.4561870000	0.8561350000	-0.4054560000
C	-3.3166600000	1.3326100000	-1.0605150000
C	-2.0839570000	0.7046950000	-0.8695940000
H	-3.0465750000	-1.7878340000	1.2257680000
H	-5.2418500000	-0.6452810000	0.9313740000
H	-5.4145800000	1.3460760000	-0.5517190000
H	-3.3896690000	2.1863610000	-1.7286760000
H	-1.2075400000	1.0689340000	-1.3983840000

(u)B3LYP/6-31++G**	

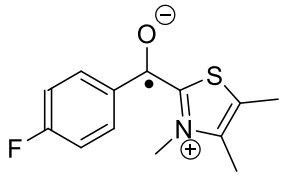
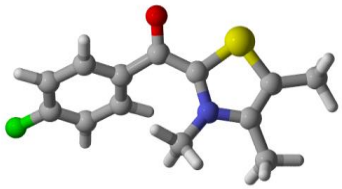
		

xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3768090000	-0.5984960000	-0.1052140000
N	1.6226180000	0.7394550000	-0.3686570000
C	2.9499270000	1.1301540000	-0.1241810000
C	3.7540770000	0.1025240000	0.2590920000
S	2.8650640000	-1.4210220000	0.3228970000
C	5.2125640000	0.1141110000	0.6029040000
C	3.3393730000	2.5683960000	-0.3039430000
C	0.1741010000	-1.3750940000	-0.1468260000
H	2.6472540000	3.2384090000	0.2176840000
H	3.3576880000	2.8655730000	-1.3594620000
H	4.3371680000	2.7433580000	0.0999990000
H	5.7732820000	-0.5743150000	-0.0405740000
H	5.3832750000	-0.1969710000	1.6404150000
H	5.6443440000	1.1094650000	0.4765080000
C	0.6985260000	1.5862840000	-1.1269510000
H	0.1089160000	2.2364870000	-0.4735580000
H	0.0134630000	0.9534810000	-1.6896480000
H	1.2613560000	2.2016380000	-1.8308290000
O	0.2781220000	-2.6300880000	-0.1826160000
C	-1.1877770000	-0.7578520000	-0.0677590000
C	-1.4822320000	0.3209580000	0.7816550000
C	-2.7849890000	0.8076590000	0.9044810000
C	-3.8049450000	0.2091060000	0.1647200000
C	-3.5447280000	-0.8782000000	-0.6729900000
C	-2.2421220000	-1.3624040000	-0.7729710000
Cl	-5.4483170000	0.8228470000	0.3030190000
H	-4.3523490000	-1.3403690000	-1.2303730000
H	-2.0256220000	-2.2251010000	-1.3945220000
H	-3.0091140000	1.6306480000	1.5746550000
H	-0.6941040000	0.7673080000	1.3814450000

(u)B3LYP/6-31++G**	

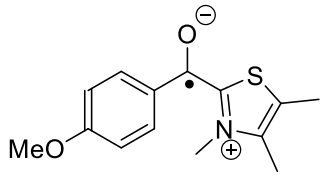
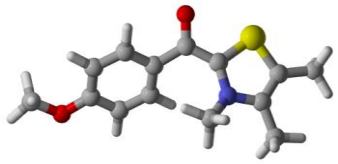
		

xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9859250000	-0.5891970000	-0.1125180000
N	1.2959810000	0.7404470000	-0.3530090000
C	2.6451020000	1.0576180000	-0.1214380000
C	3.4011520000	-0.0170900000	0.2290280000
S	2.4368650000	-1.4952150000	0.2753690000
C	4.8628160000	-0.0871690000	0.5512980000
C	3.1048940000	2.4777340000	-0.2784470000
C	-0.2560270000	-1.3017090000	-0.1434680000
H	2.4575190000	3.1706860000	0.2700850000
H	3.1192690000	2.7967850000	-1.3276430000
H	4.1175720000	2.5928270000	0.1096800000
H	5.3792190000	-0.7865820000	-0.1170140000
H	5.0315620000	-0.4326070000	1.5782300000
H	5.3431850000	0.8879810000	0.4433100000
C	0.4088760000	1.6470760000	-1.0857530000
H	-0.1308840000	2.3226510000	-0.4151100000
H	-0.3208970000	1.0611800000	-1.6427320000
H	0.9937870000	2.2375050000	-1.7931830000
O	-0.2173590000	-2.5593780000	-0.2001020000
C	-1.5829740000	-0.6155000000	-0.0334580000
C	-1.8059680000	0.4640370000	0.8372540000
C	-3.0796700000	1.0173290000	0.9884220000
C	-4.1257940000	0.4739150000	0.2533830000
C	-3.9522490000	-0.6068980000	-0.6050430000
C	-2.6770360000	-1.1550870000	-0.7324930000
F	-5.3689100000	1.0112120000	0.3886610000
H	-4.8022270000	-1.0067900000	-1.1476870000
H	-2.5121530000	-2.0179260000	-1.3692630000
H	-3.2681640000	1.8400980000	1.6698990000
H	-0.9847090000	0.8582660000	1.4288430000

(u)B3LYP/6-31++G**	

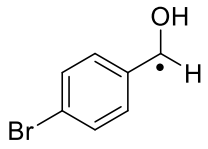
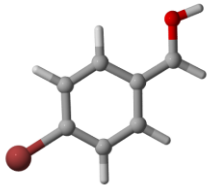
		

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3856020000	-0.5969890000	-0.1376640000
N	1.6575340000	0.7515860000	-0.3412810000
C	3.0012550000	1.0914990000	-0.0939390000
C	3.7800530000	0.0316720000	0.2458910000
S	2.8546870000	-1.4747200000	0.2556240000
C	5.2350520000	-0.0049100000	0.6021450000
C	3.4179130000	2.5279180000	-0.2163320000
C	0.1553000000	-1.3332960000	-0.1526210000
H	2.8273340000	3.1708970000	0.4470770000
H	3.2962520000	2.9064670000	-1.2377110000
H	4.4675720000	2.6460350000	0.0547800000
H	5.7748160000	-0.7186640000	-0.0314530000
H	5.3864700000	-0.3143670000	1.6433430000
H	5.7035160000	0.9735260000	0.4728770000
C	0.8638850000	1.5796600000	-1.2592330000
H	0.7090610000	2.5761960000	-0.8387330000
H	-0.1068140000	1.1198060000	-1.4175240000
H	1.3747520000	1.6698570000	-2.2259000000
O	0.2209780000	-2.5883990000	-0.2123230000
C	-1.1802680000	-0.6701730000	-0.0266590000
C	-1.4002320000	0.4744540000	0.7638400000
C	-2.6765210000	0.9973570000	0.9331050000
C	-3.7751500000	0.3871730000	0.3070990000
C	-3.5785910000	-0.7604690000	-0.4740050000
C	-2.2917050000	-1.2821690000	-0.6215920000
H	-4.4109880000	-1.2564370000	-0.9591980000
H	-2.1359700000	-2.1880250000	-1.1985840000
H	-2.8500000000	1.8691250000	1.5559570000
H	-0.5652590000	0.9470810000	1.2731440000
O	-4.9871640000	0.9793080000	0.5249250000
C	-6.1453700000	0.3952930000	-0.0596520000
H	-6.9824000000	1.0219570000	0.2505910000
H	-6.0811590000	0.3898840000	-1.1549660000
H	-6.3027580000	-0.6283120000	0.3021670000

(u)B3LYP/6-31++G**	

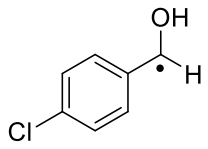
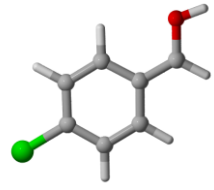
		

xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

C	1.4580500000	-1.0100990000	-0.0000680000
C	2.0942540000	0.2658480000	-0.0001120000
C	1.2616710000	1.4232210000	-0.0000740000
C	-0.1191110000	1.3118580000	0.0000940000
C	-0.7148070000	0.0431850000	0.0000330000
C	0.0745380000	-1.1126930000	-0.0001140000
H	1.7171900000	2.4100970000	-0.0000490000
H	-0.7406760000	2.2005280000	0.0001580000
H	-0.3994520000	-2.0882920000	-0.0000530000
H	2.0674900000	-1.9068710000	-0.0000740000
C	3.4930730000	0.4038400000	-0.0003770000
H	3.9853390000	1.3708500000	0.0006740000
Br	-2.6107760000	-0.1077460000	0.0000210000
O	4.2810170000	-0.7127170000	0.0002260000
H	5.2131270000	-0.4644350000	0.0004970000

(u)B3LYP/6-31++G**	

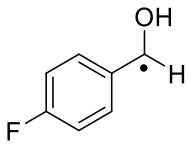
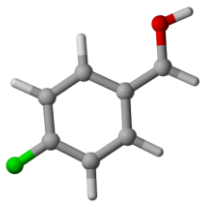
xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8026380000	-1.0220980000	-0.0000440000
C	1.4114380000	0.2674300000	-0.0000440000
C	0.5525480000	1.4057590000	0.0000030000

C	-0.8260050000	1.2664790000	0.0000150000
C	-1.3909140000	-0.0170790000	-0.0000050000
C	-0.5784570000	-1.1577800000	-0.0000140000
H	0.9870750000	2.4019430000	0.0000180000
H	-1.4681870000	2.1406400000	0.0000540000
H	-1.0323090000	-2.1431810000	0.0000200000
H	1.4324780000	-1.9045510000	-0.0000360000
C	2.8072680000	0.4366920000	-0.0003050000
H	3.2772510000	1.4147150000	0.0006510000
Cl	-3.1398660000	-0.1940830000	0.0000250000
O	3.6204780000	-0.6618300000	0.0000820000
H	4.5464900000	-0.3919210000	0.0005840000

(u)B3LYP/6-31++G**	

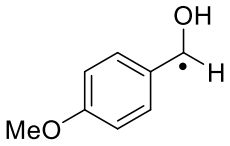
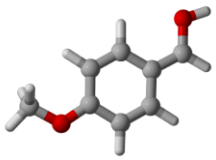
		

xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

C	0.3955910000	-1.0391750000	-0.0002510000
C	0.9567840000	0.2720070000	-0.0002070000
C	0.0602020000	1.3811640000	0.0000130000
C	-1.3143550000	1.1943410000	0.0000610000
C	-1.8149170000	-0.1082160000	0.0000150000
C	-0.9814610000	-1.2247190000	-0.0001170000
H	0.4618680000	2.3908750000	0.0000700000
H	-2.0007700000	2.0344140000	0.0001870000
H	-1.4170000000	-2.2184990000	-0.0001120000
H	1.0583830000	-1.8969120000	-0.0004210000
C	2.3482820000	0.4895660000	-0.0005960000
H	2.7857680000	1.4823840000	0.0007380000
F	-3.1651240000	-0.2923600000	0.0001610000
O	3.1978570000	-0.5835230000	0.0007620000
H	4.1142520000	-0.2826500000	-0.0015110000

(u)B3LYP/6-31++G**	

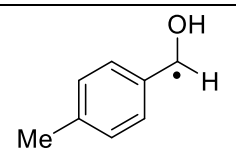
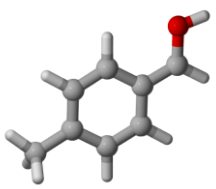
		

xyz-matrix

19
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7079050000	-0.9611480000	0.0002000000
C	-1.4537330000	0.2495300000	-0.0000020000
C	-0.7145430000	1.4716720000	-0.0001070000
C	0.6659060000	1.4763500000	0.0000040000
C	1.3842550000	0.2629690000	0.0001630000
C	0.6853340000	-0.9532440000	0.0002850000
H	-1.2512790000	2.4170770000	-0.0003000000
H	1.2229420000	2.4079310000	-0.0000650000
H	1.2152150000	-1.8988860000	0.0005030000
H	-1.2382860000	-1.9069100000	0.0003540000
C	-2.8605070000	0.2710630000	-0.0001390000
H	-3.4336540000	1.1922440000	0.0001200000
O	2.7489530000	0.3814280000	0.0003630000
C	3.5310220000	-0.8048530000	-0.0004470000
H	4.5713360000	-0.4766150000	-0.0008290000
H	3.3411390000	-1.4105880000	0.8949370000
H	3.3402480000	-1.4099520000	-0.8960670000
O	-3.5544380000	-0.9126450000	-0.0002870000
H	-4.5027530000	-0.7386040000	0.0010020000

(u)B3LYP/6-31++G**

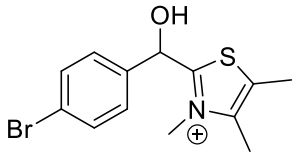
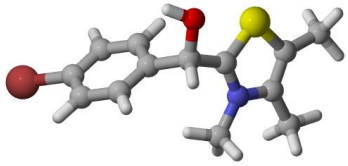
xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

C	0.4338030000	-1.0355830000	-0.0001790000

C	1.0124650000	0.2654210000	-0.0000450000
C	0.1215630000	1.3794640000	-0.0000380000
C	-1.2505080000	1.1950180000	-0.0001460000
C	-1.8224190000	-0.0952990000	-0.0002050000
C	-0.9469070000	-1.1950680000	-0.0002380000
H	0.5310780000	2.3868680000	-0.0000410000
H	-1.9026930000	2.0658140000	-0.0001750000
H	-1.3612200000	-2.2008010000	-0.0003310000
H	1.0846780000	-1.9030840000	-0.0002770000
C	2.4037610000	0.4737230000	-0.0003190000
H	2.8470690000	1.4642510000	0.0009820000
C	-3.3209710000	-0.2756810000	0.0003470000
H	-3.7807760000	0.1822960000	0.8851850000
H	-3.5946300000	-1.3349540000	-0.0049710000
H	-3.7825940000	0.1918120000	-0.8784880000
O	3.2508840000	-0.6027040000	0.0003480000
H	4.1672960000	-0.3025310000	0.0002750000

B3LYP/6-31++G**	

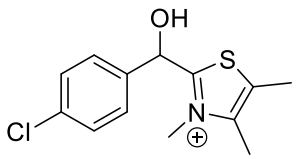
xyz-matrix

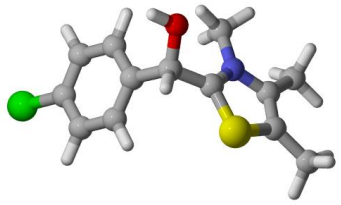
31
XYZ file generated by gabedit : coordinates in Angstrom

C	2.0508610000	-0.5667910000	0.0625360000
N	2.2519570000	0.7913330000	0.3183850000
C	3.5815640000	1.2170010000	0.0836010000
C	4.4304240000	0.2200230000	-0.2515350000
S	3.6045660000	-1.3544130000	-0.2946350000
C	5.8882210000	0.2734610000	-0.5908840000
C	3.9050890000	2.6781430000	0.1976880000
C	0.8931900000	-1.2896910000	0.1095680000
H	3.1819630000	3.2856700000	-0.3584220000
H	4.8960600000	2.8817680000	-0.2105400000

H	3.9037760000	3.0304130000	1.2363380000
H	6.0776230000	-0.0559870000	-1.6200130000
H	6.4694460000	-0.3796560000	0.0719320000
H	6.2842250000	1.2862050000	-0.4848630000
C	1.3617080000	1.5159530000	1.2239480000
H	0.9308680000	0.8109680000	1.9414340000
H	0.5359790000	2.0060050000	0.6980040000
H	1.9261110000	2.2707480000	1.7716270000
C	-0.4902390000	-0.8231070000	0.0717400000
C	-1.5122250000	-1.5762890000	0.6928820000
C	-2.8465510000	-1.1823170000	0.6251930000
C	-3.1871900000	-0.0212740000	-0.0697120000
C	-2.2080580000	0.7301310000	-0.7201270000
C	-0.8769210000	0.3253670000	-0.6548170000
H	-1.2471510000	-2.4676050000	1.2527400000
H	-3.6153420000	-1.7661970000	1.1194480000
Br	-5.0108840000	0.5211120000	-0.1701820000
H	-2.4853180000	1.6108430000	-1.2892260000
H	-0.1273230000	0.8861660000	-1.2042770000
O	1.0910610000	-2.6759740000	0.1682910000
H	0.5455530000	-3.1028510000	-0.5091670000

B3LYP/6-31++G**	





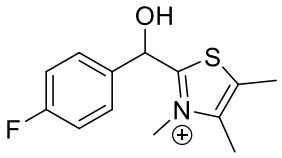
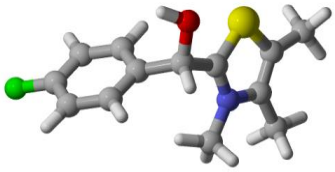
xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3654990000	-0.5652840000	0.0857340000
N	1.6315500000	0.7837460000	0.3287710000
C	2.9771120000	1.1461970000	0.0804480000
C	3.7775290000	0.1076270000	-0.2482170000
S	2.8807080000	-1.4285260000	-0.2648940000
C	5.2356270000	0.0899650000	-0.5896220000
C	3.3652410000	2.5928480000	0.1765000000
C	0.1714860000	-1.2270810000	0.1225350000
H	2.6696060000	3.2246680000	-0.3876230000
H	4.3643060000	2.7478970000	-0.2333460000
H	3.3781670000	2.9579100000	1.2105810000
H	5.4084510000	-0.2611240000	-1.6145130000
H	5.7872890000	-0.5805630000	0.0810680000
H	5.6779480000	1.0847680000	-0.4972890000

C	0.7816880000	1.5646460000	1.2262940000
H	0.2447830000	0.8813030000	1.8893170000
H	0.0394760000	2.1645070000	0.6885200000
H	1.3966170000	2.2291570000	1.8348850000
C	-1.1856130000	-0.6891920000	0.0602150000
C	-2.2587830000	-1.3967170000	0.6485330000
C	-3.5723630000	-0.9431480000	0.5464470000
C	-3.8412350000	0.2320550000	-0.1568770000
C	-2.8090630000	0.9452550000	-0.7693170000
C	-1.4994470000	0.4818160000	-0.6664740000
H	-2.0509230000	-2.3013490000	1.2110910000
H	-4.3811750000	-1.4926360000	1.0164340000
Cl	-5.4982590000	0.8128940000	-0.2869360000
H	-3.0316540000	1.8409770000	-1.3395910000
H	-0.7100890000	1.0135380000	-1.1881810000
O	0.2971690000	-2.6209910000	0.1922900000
H	-0.2580030000	-3.0240380000	-0.4920470000

B3LYP/6-31++G**	

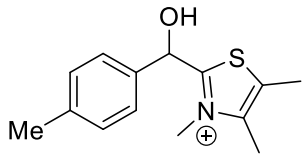
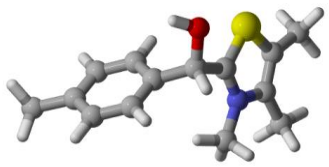
xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9765680000	-0.5512590000	0.0777770000
N	1.3065120000	0.7893410000	0.2999060000
C	2.6769320000	1.0733270000	0.0827920000
C	3.4279840000	-0.0113120000	-0.2106410000
S	2.4524510000	-1.4991100000	-0.2245190000
C	4.8900140000	-0.1123780000	-0.5190350000
C	3.1450220000	2.4970230000	0.1676960000
C	-0.2479160000	-1.1515840000	0.1062280000
H	2.4947410000	3.1609270000	-0.4134270000
H	4.1567980000	2.5893430000	-0.2296820000
H	3.1661270000	2.8732170000	1.1978920000
H	5.0654790000	-0.4929600000	-1.5329590000
H	5.3909530000	-0.7975980000	0.1762680000
H	5.3833080000	0.8590720000	-0.4360080000
C	0.4785010000	1.6199040000	1.1725070000
H	0.0014890000	0.9861520000	1.9271210000
H	-0.3118810000	2.1437990000	0.6250780000
H	1.1008510000	2.3577260000	1.6783120000

C	-1.5792260000	-0.5485020000	0.0207200000
C	-2.6833810000	-1.1745240000	0.6431650000
C	-3.9738950000	-0.6606210000	0.5220710000
C	-4.1660940000	0.4906490000	-0.2325530000
C	-3.1165970000	1.1319410000	-0.8792800000
C	-1.8316410000	0.6031880000	-0.7579060000
H	-2.5169090000	-2.0638400000	1.2425420000
H	-4.8199130000	-1.1346660000	1.0086170000
F	-5.4249220000	0.9992440000	-0.3536370000
H	-3.3119150000	2.0117940000	-1.4834110000
H	-1.0149110000	1.0673970000	-1.3015790000
O	-0.1950710000	-2.5496120000	0.1936330000
H	-0.7617880000	-2.9313930000	-0.4933770000

B3LYP/6-31++G**	

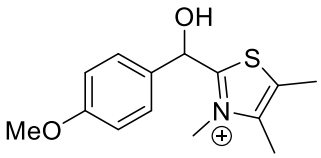
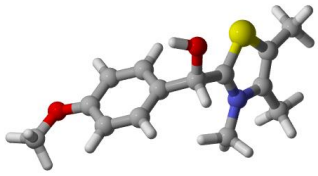
xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.0065760000	-0.5516280000	0.0758730000
N	1.3240950000	0.7926000000	0.3005490000
C	2.6904920000	1.0898170000	0.0809690000
C	3.4522870000	0.0134830000	-0.2159960000
S	2.4925880000	-1.4849750000	-0.2292450000
C	4.9144100000	-0.0713450000	-0.5286780000
C	3.1447000000	2.5181270000	0.1659330000
C	-0.2119370000	-1.1626400000	0.1060760000
H	2.4857140000	3.1757200000	-0.4126130000
H	4.1544020000	2.6213410000	-0.2341980000
H	3.1646580000	2.8936720000	1.1964320000
H	5.0914460000	-0.4460670000	-1.5446420000
H	5.4241280000	-0.7545470000	0.1623730000
H	5.3983370000	0.9046340000	-0.4427700000
C	0.4908470000	1.6107950000	1.1796300000
H	0.0285590000	0.9698290000	1.9375190000
H	-0.3120890000	2.1209900000	0.6378060000
H	1.1060270000	2.3580100000	1.6806880000
C	-1.5488900000	-0.5723030000	0.0233640000
C	-2.6494110000	-1.2074600000	0.6430960000
C	-3.9386520000	-0.6968830000	0.5194800000
C	-4.2011210000	0.4632240000	-0.2280870000

C	-3.1141840000	1.0837240000	-0.8590570000
C	-1.8187220000	0.5776970000	-0.7473780000
H	-2.4769800000	-2.0965130000	1.2423270000
H	-4.7594460000	-1.2058970000	1.0206690000
H	-3.2853340000	1.9692570000	-1.4672020000
H	-1.0094720000	1.0558380000	-1.2912690000
O	-0.1439070000	-2.5603090000	0.1876670000
H	-0.7451480000	-2.9423860000	-0.4688250000
C	-5.6049250000	1.0084150000	-0.3504850000
H	-5.6281620000	1.9142010000	-0.9636490000
H	-6.0231110000	1.2602430000	0.6317010000
H	-6.2811610000	0.2774050000	-0.8100430000

B3LYP/6-31++G**	

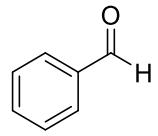
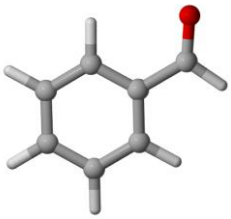
xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3781090000	-0.5704260000	0.0486360000
N	1.5975480000	0.7812490000	0.3469650000
C	2.9318390000	1.1949480000	0.1200460000
C	3.7656880000	0.2016740000	-0.2601680000
S	2.9237420000	-1.3643020000	-0.3483790000
C	5.2208570000	0.2513830000	-0.6106910000
C	3.2788240000	2.6461900000	0.2845380000
C	0.2129160000	-1.2751680000	0.0686710000
H	2.5582080000	3.2850480000	-0.2390150000
H	4.2677440000	2.8505340000	-0.1284710000
H	3.2958370000	2.9593100000	1.3357300000
H	5.3981160000	-0.0416130000	-1.6532260000
H	5.8001870000	-0.4335870000	0.0213240000
H	5.6307050000	1.2544920000	-0.4699530000
C	0.7253200000	1.4743160000	1.2923170000
H	0.3526040000	0.7592730000	2.0335600000
H	-0.1412780000	1.9297150000	0.8019510000
H	1.2845110000	2.2542460000	1.8090270000
C	-1.1698920000	-0.7887550000	0.0687840000
C	-2.1871170000	-1.5253260000	0.7215780000
C	-3.5142790000	-1.1206840000	0.6823140000
C	-3.8816910000	0.0404850000	-0.0163600000
C	-2.8977610000	0.7794650000	-0.6842320000
C	-1.5651220000	0.3571770000	-0.6455880000

H	-1.9170230000	-2.4174180000	1.2784060000
H	-4.2868720000	-1.6859800000	1.1940520000
H	-3.1530250000	1.6654530000	-1.2538880000
H	-0.8221110000	0.9149150000	-1.2079800000
O	0.3874590000	-2.6665570000	0.0504080000
H	-0.1953490000	-3.0467500000	-0.6235890000
O	-5.2137560000	0.3577680000	0.0087600000
C	-5.6459410000	1.5222280000	-0.6811010000
H	-6.7229050000	1.5826910000	-0.5185670000
H	-5.1670850000	2.4258530000	-0.2821660000
H	-5.4450840000	1.4491870000	-1.7576880000

B3LYP/6-31G*	**PhCHO**

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.0453360000	-1.1010740000	0.0000000000
C	-0.5344730000	0.2142450000	-0.0000010000
C	0.3611960000	1.2919840000	0.0000000000
C	1.7360430000	1.0606830000	0.0000000000
C	2.2172320000	-0.2508150000	0.0000000000
C	1.3265120000	-1.3311690000	0.0000000000
H	-0.0250420000	2.3095540000	0.0000000000
H	2.4303530000	1.8964430000	0.0000010000
H	3.2887810000	-0.4330830000	0.0000010000
H	1.7079640000	-2.3486820000	0.0000000000
H	-0.7592200000	-1.9193450000	-0.0000010000
C	-1.9922090000	0.4684370000	-0.0000010000
H	-2.2735080000	1.5457340000	0.0000020000
O	-2.8478900000	-0.3955460000	0.0000010000

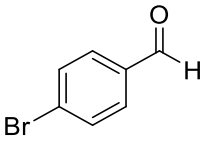
thermodynamic data

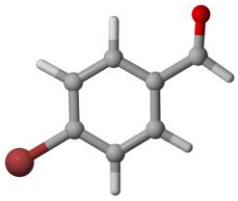
Zero-point correction= 0.110216 (Hartree/Particle)
Thermal correction to Energy= 0.116504
Thermal correction to Enthalpy= 0.117448
Thermal correction to Gibbs Free Energy= 0.079693
Sum of electronic and zero-point Energies= -345.463225
Sum of electronic and thermal Energies= -345.456937

Sum of electronic and thermal Enthalpies= -345.455993
Sum of electronic and thermal Free Energies= -345.493748

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.107	23.814	79.462

B3LYP/6-31G*	***p*-Br-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

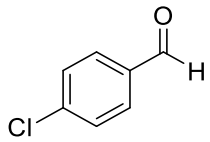
C	-1.4936660000	-1.0437940000	0.0000070000
C	-2.1196300000	0.2121490000	0.0000100000
C	-1.3399680000	1.3753300000	0.0000080000
C	0.0509910000	1.2965120000	0.0000030000
C	0.6514360000	0.0373670000	0.0000010000
C	-0.1073500000	-1.1373390000	0.0000030000
H	-1.8244190000	2.3493970000	0.0000090000
H	0.6621290000	2.1921870000	0.0000020000
H	0.3872230000	-2.1025030000	0.0000010000
H	-2.1139830000	-1.9348680000	0.0000090000
C	-3.5967050000	0.3096060000	0.0000150000
H	-3.9928880000	1.3493490000	-0.0000130000
O	-4.3508700000	-0.6440660000	-0.0000130000
Br	2.5548070000	-0.0857150000	-0.0000050000

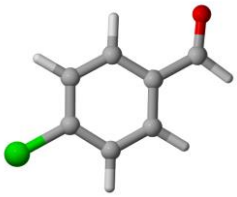
thermodynamic data

Zero-point correction= 0.100095 (Hartree/Particle)
Thermal correction to Energy= 0.107789
Thermal correction to Enthalpy= 0.108734
Thermal correction to Gibbs Free Energy= 0.066275
Sum of electronic and zero-point Energies= -2916.577421
Sum of electronic and thermal Energies= -2916.569727
Sum of electronic and thermal Enthalpies= -2916.568783
Sum of electronic and thermal Free Energies= -2916.611241

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.639	28.020	89.362

B3LYP/6-31G*	***p*-Cl-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

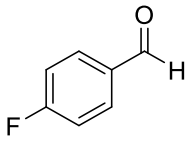
C	-0.8381430000	-1.0521020000	0.0000150000
C	-1.4412350000	0.2149600000	0.0000220000
C	-0.6401900000	1.3633920000	0.0000150000
C	0.7490230000	1.2597180000	0.0000030000
C	1.3266460000	-0.0105940000	-0.0000030000
C	0.5459230000	-1.1717070000	0.0000030000
H	-1.1067780000	2.3460420000	0.0000190000
H	1.3776470000	2.1434170000	-0.0000020000
H	1.0241580000	-2.1452580000	-0.0000020000
H	-1.4750100000	-1.9313490000	0.0000200000
C	-2.9161810000	0.3392180000	0.0000380000
H	-3.2933440000	1.3859970000	-0.0000370000
O	-3.6878340000	-0.6004010000	-0.0000320000
Cl	3.0741730000	-0.1560560000	-0.0000170000

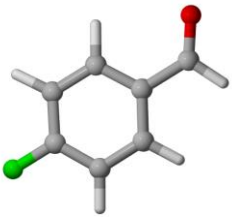
thermodynamic data

Zero-point correction= 0.100530 (Hartree/Particle)
Thermal correction to Energy= 0.108006
Thermal correction to Enthalpy= 0.108951
Thermal correction to Gibbs Free Energy= 0.067784
Sum of electronic and zero-point Energies= -805.068330
Sum of electronic and thermal Energies= -805.060853
Sum of electronic and thermal Enthalpies= -805.059909
Sum of electronic and thermal Free Energies= -805.101076

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.775	27.694	86.643

B3LYP/6-31G*	***p*-F-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

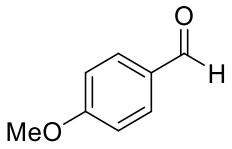
C	-0.4254180000	-1.0666190000	0.0000060000
C	-0.9911810000	0.2191540000	0.0000100000
C	-0.1569200000	1.3455280000	0.0000070000
C	1.2279850000	1.2020590000	0.0000010000
C	1.7564460000	-0.0855280000	-0.0000030000
C	0.9539400000	-1.2267100000	0.0000000000
H	-0.5972290000	2.3401630000	0.0000090000
H	1.8968880000	2.0560640000	-0.0000010000
H	1.4204280000	-2.2063060000	-0.0000030000
H	-1.0897810000	-1.9251290000	0.0000080000
C	-2.4598020000	0.3864960000	0.0000170000
H	-2.8050610000	1.4446390000	-0.0000180000
O	-3.2614770000	-0.5283970000	-0.0000170000
F	3.0929180000	-0.2365030000	-0.0000090000

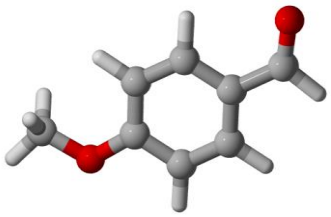
thermodynamic data

Zero-point correction= 0.102009 (Hartree/Particle)
Thermal correction to Energy= 0.109096
Thermal correction to Enthalpy= 0.110040
Thermal correction to Gibbs Free Energy= 0.070211
Sum of electronic and zero-point Energies= -444.705201
Sum of electronic and thermal Energies= -444.698114
Sum of electronic and thermal Enthalpies= -444.697170
Sum of electronic and thermal Free Energies= -444.736999

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.458	26.774	83.826

B3LYP/6-31G*	***p*-OMe-PhCHO**





xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

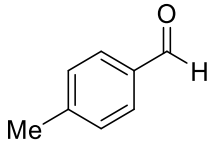
C	0.7369660000	-0.9973550000	-0.0000070000
C	1.4829970000	0.1892090000	-0.0000810000
C	0.8052130000	1.4199780000	-0.0000940000
C	-0.5795770000	1.4662660000	-0.0000360000
C	-1.3180660000	0.2701870000	0.0000380000
C	-0.6526870000	-0.9682270000	0.0000520000
H	1.3764160000	2.3461610000	-0.0001510000
H	-1.1196900000	2.4075490000	-0.0000450000
H	-1.2095760000	-1.8981030000	0.0001040000
H	1.2710270000	-1.9429080000	0.0000010000
C	2.9555030000	0.1483090000	-0.0001440000
H	3.4447550000	1.1488930000	-0.0001690000
O	3.6268260000	-0.8683710000	-0.0001050000
O	-2.6679630000	0.4162460000	0.0000870000
C	-3.4814240000	-0.7502900000	0.0002150000
H	-4.5121980000	-0.3926690000	0.0002790000
H	-3.3076700000	-1.3602410000	-0.8951210000
H	-3.3075260000	-1.3601460000	0.8955880000

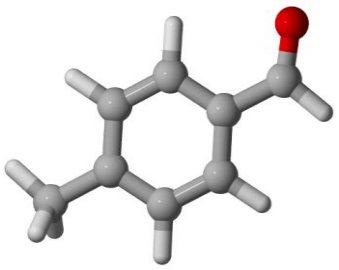
thermodynamic data

Zero-point correction= 0.143132 (Hartree/Particle)
Thermal correction to Energy= 0.151947
Thermal correction to Enthalpy= 0.152891
Thermal correction to Gibbs Free Energy= 0.109175
Sum of electronic and zero-point Energies= -459.955523
Sum of electronic and thermal Energies= -459.946709
Sum of electronic and thermal Enthalpies= -459.945765
Sum of electronic and thermal Free Energies= -459.989481

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.348	32.934	92.008

B3LYP/6-31G*	***p*-Me-PhCHO**





xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

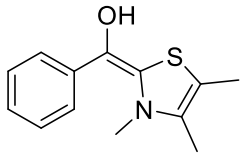
C	-0.4682970000	-1.0634900000	0.0001210000
C	-1.0471800000	0.2134010000	0.0001730000
C	-0.2178180000	1.3433650000	0.0001240000
C	1.1656220000	1.1993380000	0.0000410000
C	1.7543390000	-0.0749940000	-0.0000050000
C	0.9150280000	-1.2008090000	0.0000360000
H	-0.6635720000	2.3362120000	0.0001590000
H	1.8007690000	2.0822250000	0.0000110000
H	1.3578590000	-2.1938480000	0.0000030000
H	-1.1219750000	-1.9306260000	0.0001590000
C	-2.5162990000	0.3726680000	0.0002930000
H	-2.8664330000	1.4297140000	-0.0004650000
O	-3.3159170000	-0.5446630000	-0.0004520000
C	3.2574510000	-0.2227120000	-0.0000970000
H	3.7028580000	0.2539220000	-0.8818700000
H	3.5577860000	-1.2747750000	-0.0001410000
H	3.7029600000	0.2538770000	0.8816490000

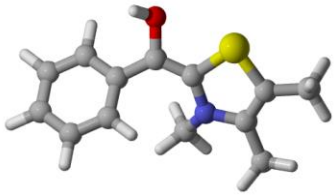
thermodynamic data

Zero-point correction= 0.137674 (Hartree/Particle)
Thermal correction to Energy= 0.144965
Thermal correction to Enthalpy= 0.145909
Thermal correction to Gibbs Free Energy= 0.105754
Sum of electronic and zero-point Energies= -384.754575
Sum of electronic and thermal Energies= -384.747284
Sum of electronic and thermal Enthalpies= -384.746339
Sum of electronic and thermal Free Energies= -384.786494

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.967	27.869	84.513

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.5880970000	-0.5133990000	-0.0732880000
N	-1.0145760000	0.8039600000	-0.2712750000
C	-2.4056010000	0.9761490000	-0.0740890000
C	-3.0765110000	-0.1667770000	0.1820540000
S	-1.9933800000	-1.5786760000	0.1785790000
C	-4.5315410000	-0.3825200000	0.4602240000
C	-2.9812520000	2.3607490000	-0.1387500000
C	0.6740350000	-1.0253970000	-0.1006340000
H	-2.3929400000	3.0612790000	0.4661970000
H	-4.0041090000	2.3677430000	0.2427600000
H	-3.0146100000	2.7575300000	-1.1619670000
H	-4.6970350000	-0.8003600000	1.4619000000
H	-4.9691110000	-1.0871220000	-0.2592950000
H	-5.0957390000	0.5515880000	0.3902020000
C	-0.2411490000	1.7028510000	-1.1246050000
H	0.2483260000	1.1206490000	-1.9132590000
H	0.5388730000	2.2352530000	-0.5701050000
H	-0.9045380000	2.4343950000	-1.5866630000
C	1.9602500000	-0.3414840000	0.0242610000
C	3.1158710000	-0.9108860000	-0.5545690000
C	4.3658810000	-0.3198980000	-0.3905450000
C	4.5046870000	0.8510390000	0.3592270000
C	3.3747340000	1.4155510000	0.9569440000
C	2.1225580000	0.8254690000	0.8028490000
H	3.0134700000	-1.8134440000	-1.1498220000
H	5.2373100000	-0.7733740000	-0.8566670000
H	3.4724490000	2.3104590000	1.5668350000
H	1.2629620000	1.2405660000	1.3210920000
O	0.7149540000	-2.4192740000	-0.2261340000
H	1.3370560000	-2.7594170000	0.4394140000
H	5.4809230000	1.3108780000	0.4856400000

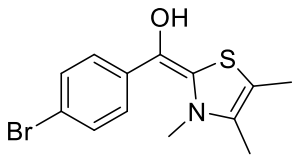
thermodynamic data

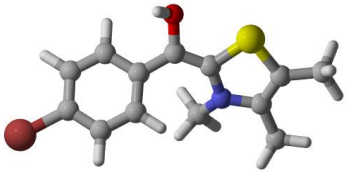
Zero-point correction= 0.253329 (Hartree/Particle)
Thermal correction to Energy= 0.269330
Thermal correction to Enthalpy= 0.270275

Thermal correction to Gibbs Free Energy= 0.210277
Sum of electronic and zero-point Energies= -1032.289180
Sum of electronic and thermal Energies= -1032.273179
Sum of electronic and thermal Enthalpies= -1032.272235
Sum of electronic and thermal Free Energies= -1032.332233

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	169.007	60.672	126.276

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	2.0508110000	-0.5572560000	0.0765140000
N	2.2724760000	0.7984430000	0.3264680000
C	3.6042840000	1.2054860000	0.0737510000
C	4.4341550000	0.1990750000	-0.2739800000
S	3.5902130000	-1.3665390000	-0.2990640000
C	5.8890000000	0.2343410000	-0.6253040000
C	3.9519840000	2.6607960000	0.1886650000
C	0.8881520000	-1.2686400000	0.1316360000
H	3.2270260000	3.2836420000	-0.3490450000
H	4.9382470000	2.8531390000	-0.2381450000
H	3.9763400000	3.0086030000	1.2296110000
H	6.0676840000	-0.1041890000	-1.6541680000
H	6.4692540000	-0.4223410000	0.0361060000
H	6.2991160000	1.2433720000	-0.5293560000
C	1.4019170000	1.5330780000	1.2407590000
H	0.9933440000	0.8382100000	1.9817790000
H	0.5590580000	2.0081310000	0.7271730000
H	1.9753750000	2.3022450000	1.7592150000
C	-0.4924830000	-0.7968510000	0.0927410000
C	-1.5169570000	-1.5758420000	0.6751610000
C	-2.8526270000	-1.1938840000	0.5978150000
C	-3.1926570000	-0.0206520000	-0.0748520000
C	-2.2110880000	0.7605120000	-0.6838220000
C	-0.8778930000	0.3679490000	-0.6076200000
H	-1.2492330000	-2.4816010000	1.2104340000
H	-3.6245810000	-1.7977540000	1.0631240000
Br	-5.0272860000	0.5130400000	-0.1797000000
H	-2.4898160000	1.6543470000	-1.2320550000

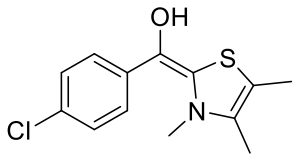
H	-0.1252810000	0.9472940000	-1.1338720000
O	1.0762980000	-2.6548370000	0.1925430000
H	0.5177620000	-3.0639400000	-0.4906660000

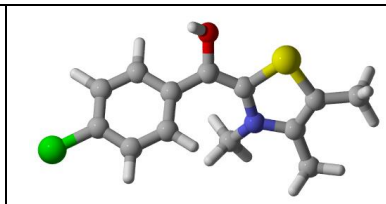
thermodynamic data

Zero-point correction= 0.243123 (Hartree/Particle)
Thermal correction to Energy= 0.260658
Thermal correction to Enthalpy= 0.261602
Thermal correction to Gibbs Free Energy= 0.196711
Sum of electronic and zero-point Energies= -3603.404924
Sum of electronic and thermal Energies= -3603.387389
Sum of electronic and thermal Enthalpies= -3603.386444
Sum of electronic and thermal Free Energies= -3603.451336

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.565	64.918	136.575

B3LYP/6-31G*





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3614190000	-0.5517490000	0.0799720000
N	1.6404530000	0.7960540000	0.3157810000
C	2.9925520000	1.1394080000	0.0748330000
C	3.7802560000	0.0923500000	-0.2501360000
S	2.8674310000	-1.4344110000	-0.2652550000
C	5.2388550000	0.0573130000	-0.5853280000
C	3.4044900000	2.5789290000	0.1758380000
C	0.1669260000	-1.2083910000	0.1277600000
H	2.7145790000	3.2268800000	-0.3781110000
H	4.4032810000	2.7211780000	-0.2413800000
H	3.4327930000	2.9386780000	1.2126690000
H	5.4129400000	-0.3037520000	-1.6073100000
H	5.7818270000	-0.6152630000	0.0915920000
H	5.6933990000	1.0480610000	-0.4991090000
C	0.7952310000	1.5783540000	1.2144180000
H	0.3630620000	0.9138280000	1.9700310000
H	-0.0306960000	2.0710800000	0.6901730000
H	1.3948770000	2.3383200000	1.7161400000

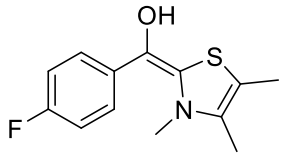
C	-1.1895250000	-0.6728070000	0.0626530000
C	-2.2584150000	-1.3928280000	0.6406020000
C	-3.5729760000	-0.9486480000	0.5385790000
C	-3.8470720000	0.2304980000	-0.1548400000
C	-2.8196510000	0.9545500000	-0.7600300000
C	-1.5086070000	0.4986270000	-0.6591280000
H	-2.0422970000	-2.3028330000	1.1917140000
H	-4.3805830000	-1.5072960000	1.0005320000
Cl	-5.5078150000	0.8016490000	-0.2834790000
H	-3.0482560000	1.8526010000	-1.3247690000
H	-0.7213470000	1.0331090000	-1.1821170000
O	0.2892540000	-2.6007580000	0.2075830000
H	-0.2777240000	-2.9920030000	-0.4791200000

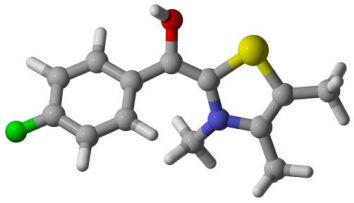
thermodynamic data

Zero-point correction= 0.243543 (Hartree/Particle)
Thermal correction to Energy= 0.260852
Thermal correction to Enthalpy= 0.261796
Thermal correction to Gibbs Free Energy= 0.198168
Sum of electronic and zero-point Energies= -1491.895679
Sum of electronic and thermal Energies= -1491.878371
Sum of electronic and thermal Enthalpies= -1491.877426
Sum of electronic and thermal Free Energies= -1491.941055

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.687	64.613	133.917

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9731510000	-0.5420710000	0.0783150000
N	1.3137820000	0.7973490000	0.2943910000
C	2.6865030000	1.0668240000	0.0751330000
C	3.4271000000	-0.0230470000	-0.2168400000
S	2.4414000000	-1.5050070000	-0.2211040000
C	4.8870770000	-0.1354760000	-0.5278370000
C	3.1689710000	2.4856060000	0.1576870000
C	-0.2513580000	-1.1370460000	0.1133900000
H	2.5225420000	3.1566780000	-0.4207730000

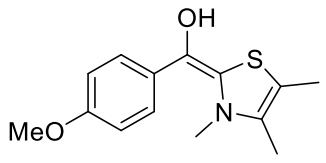
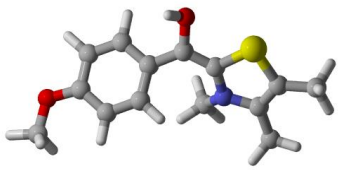
H	4.1809680000	2.5695220000	-0.2431710000
H	3.1969580000	2.8634260000	1.1881970000
H	5.0588700000	-0.5204640000	-1.5415480000
H	5.3850900000	-0.8241880000	0.1672950000
H	5.3898200000	0.8323870000	-0.4483490000
C	0.4990170000	1.6263940000	1.1792260000
H	0.0605510000	0.9980640000	1.9623980000
H	-0.3215360000	2.1213020000	0.6486900000
H	1.1222260000	2.3886820000	1.6472760000
C	-1.5816560000	-0.5349370000	0.0252550000
C	-2.6869890000	-1.1840310000	0.6183850000
C	-3.9778870000	-0.6779970000	0.4942870000
C	-4.1763770000	0.4899150000	-0.2339300000
C	-3.1208000000	1.1507060000	-0.8524730000
C	-1.8346040000	0.6305930000	-0.7308290000
H	-2.5173280000	-2.0882570000	1.1945950000
H	-4.8264610000	-1.1704660000	0.9587170000
F	-5.4274840000	0.9881400000	-0.3552760000
H	-3.3176200000	2.0428510000	-1.4386210000
H	-1.0154870000	1.1095610000	-1.2586500000
O	-0.2022240000	-2.5332940000	0.2074040000
H	-0.7852010000	-2.8999520000	-0.4794920000

thermodynamic data

Zero-point correction= 0.244981 (Hartree/Particle)
Thermal correction to Energy= 0.261881
Thermal correction to Enthalpy= 0.262825
Thermal correction to Gibbs Free Energy= 0.200537
Sum of electronic and zero-point Energies= -1131.530534
Sum of electronic and thermal Energies= -1131.513635
Sum of electronic and thermal Enthalpies= -1131.512690
Sum of electronic and thermal Free Energies= -1131.574979

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.333	63.720	131.097

B3LYP/6-31G*	

xyz-matrix

XYZ file generated by gabedit : coordinates in Angstrom

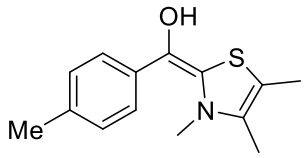
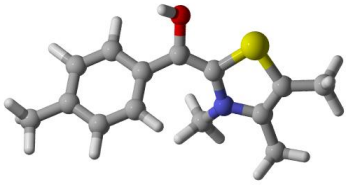
C	1.3725200000	-0.5609890000	0.0525320000
N	1.6025220000	0.7916510000	0.3407950000
C	2.9411030000	1.1892550000	0.1073550000
C	3.7634440000	0.1882170000	-0.2704170000
S	2.9104790000	-1.3732280000	-0.3418720000
C	5.2166530000	0.2245800000	-0.6278450000
C	3.3045750000	2.6372030000	0.2633130000
C	0.2066580000	-1.2608620000	0.0816720000
H	2.5836010000	3.2823130000	-0.2533510000
H	4.2912390000	2.8323910000	-0.1615140000
H	3.3365640000	2.9548480000	1.3138510000
H	5.3880700000	-0.0783280000	-1.6692580000
H	5.7944700000	-0.4611720000	0.0059550000
H	5.6368640000	1.2256680000	-0.4971830000
C	0.7572570000	1.4769230000	1.3155150000
H	0.4656620000	0.7759800000	2.1065740000
H	-0.1595660000	1.8691950000	0.8632340000
H	1.3070180000	2.3052340000	1.7628380000
C	-1.1743350000	-0.7752750000	0.0761460000
C	-2.1973440000	-1.5447870000	0.6768570000
C	-3.5247020000	-1.1476430000	0.6287200000
C	-3.8879380000	0.0388430000	-0.0267770000
C	-2.8968330000	0.8090930000	-0.6459940000
C	-1.5643970000	0.3948770000	-0.6006250000
H	-1.9289490000	-2.4590280000	1.1978550000
H	-4.3046040000	-1.7378070000	1.1006390000
H	-3.1497700000	1.7156090000	-1.1845550000
H	-0.8149800000	0.9751110000	-1.1315430000
O	0.3779650000	-2.6509130000	0.0768930000
H	-0.2181200000	-3.0208820000	-0.5965650000
O	-5.2206540000	0.3449540000	-0.0111990000
C	-5.6421250000	1.5294550000	-0.6650520000
H	-6.7233040000	1.5826450000	-0.5232040000
H	-5.1754530000	2.4222390000	-0.2269300000
H	-5.4197590000	1.5003960000	-1.7403960000

thermodynamic data

Zero-point correction= 0.285653 (Hartree/Particle)
Thermal correction to Energy= 0.303635
Thermal correction to Enthalpy= 0.304579
Thermal correction to Gibbs Free Energy= 0.239787
Sum of electronic and zero-point Energies= -1146.778730
Sum of electronic and thermal Energies= -1146.760748
Sum of electronic and thermal Enthalpies= -1146.759803
Sum of electronic and thermal Free Energies= -1146.824595

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.534	67.977	136.365

B3LYP/6-31G*	

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

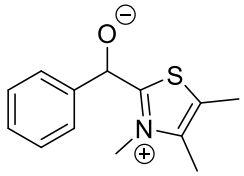
C	1.0029330000	-0.5414290000	0.0751960000
N	1.3318290000	0.8010320000	0.2937920000
C	2.7011070000	1.0831480000	0.0730460000
C	3.4519280000	0.0007310000	-0.2211860000
S	2.4805640000	-1.4907730000	-0.2260570000
C	4.9124020000	-0.0969460000	-0.5345900000
C	3.1708290000	2.5062430000	0.1563320000
C	-0.2160360000	-1.1473080000	0.1121320000
H	2.5166070000	3.1719360000	-0.4195910000
H	4.1810780000	2.6002050000	-0.2468410000
H	3.1976910000	2.8830400000	1.1872790000
H	5.0866560000	-0.4796720000	-1.5488170000
H	5.4184310000	-0.7812430000	0.1592410000
H	5.4058800000	0.8757540000	-0.4553120000
C	0.5106960000	1.6200710000	1.1818520000
H	0.0854640000	0.9867750000	1.9684800000
H	-0.3205140000	2.1004510000	0.6548720000
H	1.1258410000	2.3921280000	1.6446900000
C	-1.5517150000	-0.5582480000	0.0271280000
C	-2.6526310000	-1.2184310000	0.6164930000
C	-3.9428600000	-0.7166070000	0.4913970000
C	-4.2057090000	0.4598660000	-0.2274160000
C	-3.1187890000	1.1043410000	-0.8308160000
C	-1.8221830000	0.6064880000	-0.7195920000
H	-2.4762920000	-2.1234570000	1.1905610000
H	-4.7660740000	-1.2454360000	0.9685850000
H	-3.2924120000	2.0035780000	-1.4186070000
H	-1.0113180000	1.0996210000	-1.2481900000
O	-0.1513880000	-2.5430360000	0.2033360000
H	-0.7600240000	-2.9121790000	-0.4591930000
C	-5.6117280000	0.9981480000	-0.3502230000
H	-5.6373330000	1.9160920000	-0.9463830000
H	-6.0418130000	1.2289370000	0.6329760000
H	-6.2820540000	0.2724990000	-0.8285840000

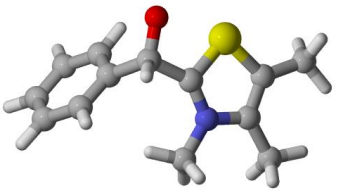
thermodynamic data

Zero-point correction= 0.280673 (Hartree/Particle)
Thermal correction to Energy= 0.297767
Thermal correction to Enthalpy= 0.298711
Thermal correction to Gibbs Free Energy= 0.236107
Sum of electronic and zero-point Energies= -1071.579657
Sum of electronic and thermal Energies= -1071.562563
Sum of electronic and thermal Enthalpies= -1071.561619
Sum of electronic and thermal Free Energies= -1071.624223

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.852	64.754	131.762

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.5691410000	-0.2406490000	0.5754200000
N	-1.0962030000	0.9691460000	0.3659270000
C	-2.3992220000	0.9489200000	-0.1756280000
C	-2.8349260000	-0.3280920000	-0.3668270000
S	-1.6180410000	-1.5146560000	0.1441480000
C	-4.1475020000	-0.7849270000	-0.9300840000
C	-3.0993510000	2.2436830000	-0.4636490000
C	0.7348150000	-0.8734230000	1.1486670000
H	-3.1676410000	2.8815500000	0.4261680000
H	-4.1168060000	2.0499050000	-0.8082390000
H	-2.5924240000	2.8213410000	-1.2470970000
H	-4.6285970000	-1.5127830000	-0.2665650000
H	-4.0133710000	-1.2726890000	-1.9034000000
H	-4.8427560000	0.0478890000	-1.0693270000
C	-0.3896620000	2.2098550000	0.6950220000
H	0.6518920000	1.9749150000	0.9058480000
H	-0.8491370000	2.6856370000	1.5669020000
H	-0.4302610000	2.8948710000	-0.1547400000
C	1.9622650000	-0.3465370000	0.3696550000
C	2.2551030000	-0.9113160000	-0.8772130000
C	3.3610900000	-0.4802720000	-1.6062750000
C	4.2048850000	0.5093720000	-1.0889710000
C	3.9385650000	1.0550210000	0.1664420000

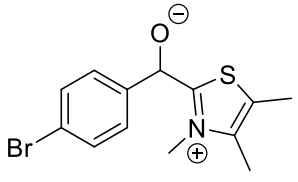
C	2.8218100000	0.6251640000	0.8913170000
H	4.6056370000	1.8022220000	0.5900890000
H	2.6359560000	1.0280220000	1.8868980000
O	0.5240670000	-2.1825550000	1.0567010000
H	5.0738360000	0.8371960000	-1.6540060000
H	1.6180250000	-1.7152340000	-1.2345450000
H	3.5778300000	-0.9240860000	-2.5752300000
H	0.8149870000	-0.4486320000	2.1885340000

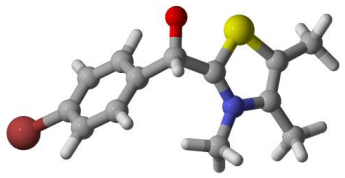
thermodynamic data

Zero-point correction= 0.252169 (Hartree/Particle)
Thermal correction to Energy= 0.268100
Thermal correction to Enthalpy= 0.269044
Thermal correction to Gibbs Free Energy= 0.208106
Sum of electronic and zero-point Energies= -1032.258438
Sum of electronic and thermal Energies= -1032.242506
Sum of electronic and thermal Enthalpies= -1032.241562
Sum of electronic and thermal Free Energies= -1032.302501

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	168.235	59.425	128.256

B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	2.0149240000	-0.3917760000	-0.5553310000
N	2.3575120000	0.8996180000	-0.5566260000
C	3.5250180000	1.1923280000	0.1808340000
C	4.0494680000	0.0664010000	0.7418200000
S	3.0919290000	-1.3694540000	0.3352500000
C	5.2686280000	-0.0583180000	1.6058510000
C	4.0131040000	2.6083350000	0.2594630000
C	0.9278230000	-1.3238510000	-1.1778300000
H	4.1818760000	3.0399250000	-0.7346540000
H	4.9603720000	2.6483160000	0.8004280000
H	3.3058270000	3.2600600000	0.7881130000
H	5.9535900000	-0.8186020000	1.2131050000

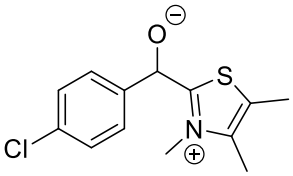
H	5.0017440000	-0.3580300000	2.6265810000
H	5.8196820000	0.8841520000	1.6702940000
C	1.6009190000	1.9221600000	-1.2843390000
H	0.6440870000	1.5022380000	-1.5878850000
H	2.1603770000	2.2496390000	-2.1659090000
H	1.4180680000	2.7789180000	-0.6324460000
C	-0.4825940000	-0.8408060000	-0.7688700000
C	-0.9651410000	-1.1907830000	0.4974190000
C	-2.2355270000	-0.8002310000	0.9124560000
C	-3.0411760000	-0.0692240000	0.0368120000
C	-2.6030790000	0.2600930000	-1.2417760000
C	-1.3199310000	-0.1332450000	-1.6356740000
H	-3.2542740000	0.7993660000	-1.9216240000
H	-0.9842340000	0.0920690000	-2.6473840000
O	1.2519530000	-2.5354920000	-0.7430970000
Br	-4.7937920000	0.4683670000	0.5971910000
H	-0.3344540000	-1.8065490000	1.1318910000
H	-2.6068850000	-1.0676010000	1.8963850000
H	1.0132490000	-1.1453780000	-2.2864200000

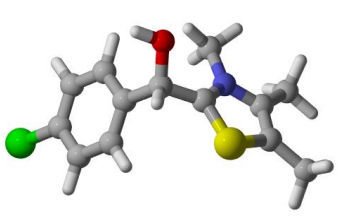
thermodynamic data

Zero-point correction= 0.242139 (Hartree/Particle)
Thermal correction to Energy= 0.259528
Thermal correction to Enthalpy= 0.260472
Thermal correction to Gibbs Free Energy= 0.194807
Sum of electronic and zero-point Energies= -3603.374487
Sum of electronic and thermal Energies= -3603.357099
Sum of electronic and thermal Enthalpies= -3603.356155
Sum of electronic and thermal Free Energies= -3603.421820

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.856	63.605	138.204

B3LYP/6-31G*	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3664160000	-0.3560080000	-0.7082590000

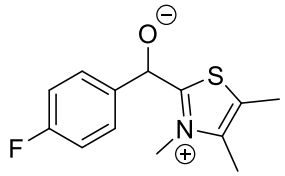
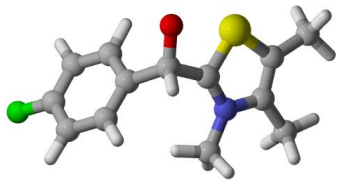
N	1.8202030000	-0.7714840000	0.4750690000
C	2.8943300000	-0.0235670000	0.9912050000
C	3.2675020000	0.9912160000	0.1559290000
S	2.2658130000	0.9806510000	-1.2733620000
C	4.3593060000	2.0075650000	0.3052600000
C	3.4959020000	-0.3867870000	2.3142330000
C	0.1724530000	-0.8806390000	-1.4944300000
H	2.7398610000	-0.4273260000	3.1054740000
H	4.2390700000	0.3564850000	2.6049700000
H	4.0020970000	-1.3585610000	2.2751940000
H	3.9773980000	3.0239620000	0.1638700000
H	5.1564510000	1.8421600000	-0.4282450000
H	4.8047760000	1.9546440000	1.3006420000
C	1.2449780000	-1.9108570000	1.2225230000
H	2.0562280000	-2.4592690000	1.6997180000
H	0.7330990000	-2.5611240000	0.5195520000
H	0.5531830000	-1.5344190000	1.9802480000
C	-1.1483900000	-0.4380260000	-0.8591750000
C	-1.5969790000	0.8763210000	-1.0468010000
C	-2.7946940000	1.3078050000	-0.4846540000
C	-3.5588730000	0.4111630000	0.2675270000
C	-3.1363840000	-0.9059270000	0.4514860000
C	-1.9298190000	-1.3243530000	-0.1096450000
H	-3.7474010000	-1.5971070000	1.0219120000
H	-1.6161080000	-2.3549750000	0.0212290000
Cl	-5.0632750000	0.9419860000	0.9721080000
H	-1.0175040000	1.5746640000	-1.6470140000
H	-3.1425320000	2.3237900000	-0.6360370000
H	0.2476700000	-0.4080720000	-2.4853420000
O	0.3329610000	-2.2825590000	-1.6048400000
H	-0.3832120000	-2.6256000000	-2.1661800000

thermodynamic data

Zero-point correction= 0.257260 (Hartree/Particle)
Thermal correction to Energy= 0.274541
Thermal correction to Enthalpy= 0.275485
Thermal correction to Gibbs Free Energy= 0.210575
Sum of electronic and zero-point Energies= -1492.292511
Sum of electronic and thermal Energies= -1492.275230
Sum of electronic and thermal Enthalpies= -1492.274286
Sum of electronic and thermal Free Energies= -1492.339196

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	172.277	64.384	136.615

B3LYP/6-31G*	

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9524290000	-0.2914770000	-0.5870930000
N	1.4148790000	0.9518290000	-0.4262810000
C	2.6760990000	1.0261120000	0.2032330000
C	3.1467460000	-0.2145590000	0.5135000000
S	2.0186470000	-1.4848180000	0.0030440000
C	4.4328440000	-0.5744280000	1.1955540000
C	3.3034130000	2.3669090000	0.4450180000
C	-0.2786140000	-1.0201170000	-1.2111260000
H	3.4160120000	2.9416240000	-0.4825710000
H	4.2981160000	2.2420160000	0.8769070000
H	2.7171960000	2.9772850000	1.1438210000
H	4.9922470000	-1.3167490000	0.6146170000
H	4.2485170000	-1.0091490000	2.1855690000
H	5.0793790000	0.2972650000	1.3308370000
C	0.6857370000	2.1354860000	-0.8891260000
H	-0.3389660000	1.8489310000	-1.1177330000
H	1.1651090000	2.5503190000	-1.7812490000
H	0.6728360000	2.8910910000	-0.1010490000
C	-1.5857740000	-0.5045390000	-0.5663610000
C	-1.9630490000	-1.0210400000	0.6795800000
C	-3.1407400000	-0.6098100000	1.2979380000
C	-3.9544390000	0.3114650000	0.6425870000
C	-3.6305220000	0.8191210000	-0.6080000000
C	-2.4383320000	0.3991570000	-1.2074760000
H	-4.3086490000	1.5090230000	-1.1005350000
H	-2.1887480000	0.7611550000	-2.2042030000
O	-0.0230890000	-2.3086870000	-1.0137470000
F	-5.1039610000	0.7092360000	1.2354390000
H	-1.3286960000	-1.7790520000	1.1291940000
H	-3.4472230000	-0.9994510000	2.2639050000
H	-0.2940610000	-0.6673360000	-2.2805950000

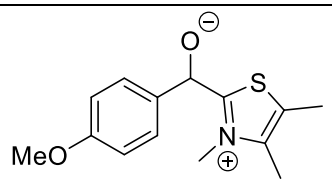
thermodynamic data

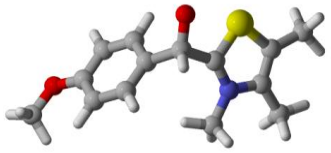
Zero-point correction= 0.243832 (Hartree/Particle)
Thermal correction to Energy= 0.260661
Thermal correction to Enthalpy= 0.261606

Thermal correction to Gibbs Free Energy=	0.198236
Sum of electronic and zero-point Energies=	-1131.500610
Sum of electronic and thermal Energies=	-1131.483781
Sum of electronic and thermal Enthalpies=	-1131.482837
Sum of electronic and thermal Free Energies=	-1131.546206

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.567	62.448	133.372

B3LYP/6-31G*	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3533660000	-0.3359340000	-0.5714950000
N	1.7090030000	0.9483450000	-0.4773180000
C	2.9458910000	1.1627320000	0.1686080000
C	3.5079310000	-0.0148200000	0.5615500000
S	2.4957940000	-1.4024660000	0.1105900000
C	4.8048440000	-0.2286380000	1.2831210000
C	3.4563140000	2.5629350000	0.3372490000
C	0.1977140000	-1.1949430000	-1.1669040000
H	3.5373960000	3.0882860000	-0.6222780000
H	4.4503230000	2.5477440000	0.7881420000
H	2.8090510000	3.1629120000	0.9895880000
H	5.4630700000	-0.9013960000	0.7207600000
H	4.6395150000	-0.6849800000	2.2665840000
H	5.3441560000	0.7098910000	1.4399710000
C	0.8911390000	2.0367290000	-1.0185730000
H	-0.0940570000	1.6441500000	-1.2645510000
H	1.3612280000	2.4543560000	-1.9143130000
H	0.7796320000	2.8227830000	-0.2685040000
C	-1.1582170000	-0.7355860000	-0.5893060000
C	-1.5179710000	-1.1453260000	0.7038030000
C	-2.7335830000	-0.7743890000	1.2579450000
C	-3.6406130000	0.0031900000	0.5174860000
C	-3.3140270000	0.3927380000	-0.7839440000
C	-2.0753200000	0.0155160000	-1.3220810000
O	0.5473790000	-2.4449870000	-0.8773840000
H	-3.0197880000	-1.0867200000	2.2581400000

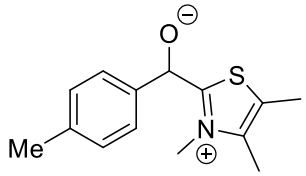
H	0.1852800000	-0.9163090000	-2.2586910000
O	-4.8132740000	0.3108180000	1.1536740000
C	-5.7827310000	1.0571180000	0.4405610000
H	-6.6271700000	1.1829070000	1.1213200000
H	-5.4020380000	2.0464910000	0.1508870000
H	-6.1202470000	0.5272050000	-0.4605010000
H	-0.8327350000	-1.7910990000	1.2452330000
H	-1.8416800000	0.2959430000	-2.3489740000
H	-4.0089170000	0.9642930000	-1.3894590000

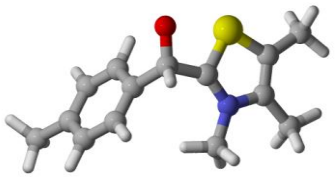
thermodynamic data

Zero-point correction= 0.284922 (Hartree/Particle)
Thermal correction to Energy= 0.303436
Thermal correction to Enthalpy= 0.304381
Thermal correction to Gibbs Free Energy= 0.237391
Sum of electronic and zero-point Energies= -1146.747815
Sum of electronic and thermal Energies= -1146.729300
Sum of electronic and thermal Enthalpies= -1146.728356
Sum of electronic and thermal Free Energies= -1146.795346

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.409	68.560	140.991

B3LYP/6-31G*	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9826160000	-0.3087150000	0.5765040000
N	-1.4256270000	0.9445010000	0.4404640000
C	-2.6822780000	1.0502660000	-0.1940570000
C	-3.1678900000	-0.1763820000	-0.5351580000
S	-2.0594960000	-1.4746240000	-0.0480800000
C	-4.4552930000	-0.5028000000	-1.2313000000
C	-3.2898510000	2.4049260000	-0.4078190000
C	0.2316030000	-1.0684970000	1.1906650000
H	-3.3956330000	2.9608430000	0.5319510000
H	-4.2857320000	2.3040240000	-0.8434090000
H	-2.6937780000	3.0221220000	-1.0922300000

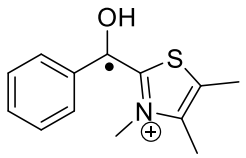
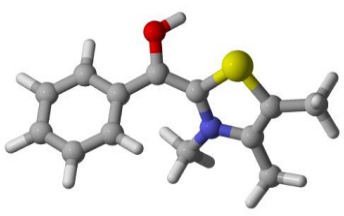
H	-5.0398130000	-1.2314040000	-0.6575110000
H	-4.2711900000	-0.9414140000	-2.2196200000
H	-5.0781910000	0.3849720000	-1.3731680000
C	-0.6801470000	2.1056300000	0.9333690000
H	0.3442200000	1.8014950000	1.1418200000
H	-1.1463130000	2.4968640000	1.8431180000
H	-0.6680600000	2.8854300000	0.1693050000
C	1.5505980000	-0.5479280000	0.5770090000
C	1.9362180000	-1.0108400000	-0.6872810000
C	3.1254670000	-0.5817670000	-1.2664520000
C	3.9839520000	0.3070830000	-0.5963770000
C	3.6082210000	0.7435410000	0.6770030000
C	2.4080140000	0.3186070000	1.2577590000
O	-0.0394320000	-2.3487770000	0.9554930000
H	3.4064430000	-0.9505680000	-2.2516580000
H	0.2382270000	-0.7468720000	2.2700970000
H	1.2984980000	-1.7382780000	-1.1812760000
H	2.1544330000	0.6457130000	2.2660780000
H	4.2668430000	1.4105070000	1.2302550000
C	5.2848830000	0.7477680000	-1.2272970000
H	5.7847700000	1.5111580000	-0.6221360000
H	5.1253680000	1.1659260000	-2.2290830000
H	5.9813860000	-0.0931900000	-1.3398600000

thermodynamic data

Zero-point correction= 0.279621 (Hartree/Particle)
Thermal correction to Energy= 0.297470
Thermal correction to Enthalpy= 0.298414
Thermal correction to Gibbs Free Energy= 0.232454
Sum of electronic and zero-point Energies= -1071.548759
Sum of electronic and thermal Energies= -1071.530910
Sum of electronic and thermal Enthalpies= -1071.529966
Sum of electronic and thermal Free Energies= -1071.595926

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.665	65.473	138.826

(u)B3LYP/6-31G*	

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

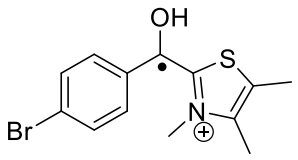
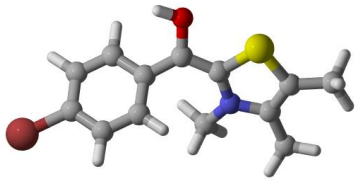
C	0.5931920000	-0.5273110000	0.1334410000
N	1.0296650000	0.7454830000	0.3931670000
C	2.3909710000	0.9506780000	0.1520510000
C	3.0456960000	-0.1811060000	-0.2502720000
S	1.9351440000	-1.5274440000	-0.3749110000
C	4.4925290000	-0.3866240000	-0.5791310000
C	2.9905710000	2.3080460000	0.3649780000
C	-0.7098150000	-1.0590480000	0.2376460000
H	2.4073340000	3.0863920000	-0.1380540000
H	4.0036490000	2.3416890000	-0.0369360000
H	3.0513190000	2.5648240000	1.4295430000
H	4.6191140000	-0.7663080000	-1.5990990000
H	4.9522360000	-1.1091320000	0.1050540000
H	5.0492470000	0.5489780000	-0.4982280000
C	0.2059130000	1.7663590000	1.0629990000
H	-0.6134580000	1.2771670000	1.5858050000
H	-0.2048570000	2.4750310000	0.3399290000
H	0.8250570000	2.2980500000	1.7853510000
C	-1.9639530000	-0.3667110000	0.0083850000
C	-3.1419360000	-0.8435880000	0.6268070000
C	-4.3598170000	-0.2220670000	0.3796430000
C	-4.4299930000	0.8670020000	-0.4955210000
C	-3.2741470000	1.3314840000	-1.1340110000
C	-2.0502900000	0.7219490000	-0.8889470000
H	-3.0847400000	-1.6910040000	1.3009450000
H	-5.2584010000	-0.5869230000	0.8672730000
H	-5.3850420000	1.3454280000	-0.6902680000
H	-3.3355740000	2.1552380000	-1.8385140000
H	-1.1667800000	1.0497140000	-1.4290730000
O	-0.8374970000	-2.3938420000	0.4334940000
H	-0.0626130000	-2.7720600000	0.8863090000

thermodynamic data

Zero-point correction= 0.254382 (Hartree/Particle)
Thermal correction to Energy= 0.270298
Thermal correction to Enthalpy= 0.271242
Thermal correction to Gibbs Free Energy= 0.210291
Sum of electronic and zero-point Energies= -1032.082441
Sum of electronic and thermal Energies= -1032.066525
Sum of electronic and thermal Enthalpies= -1032.065581
Sum of electronic and thermal Free Energies= -1032.126532

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	169.615	60.157	128.282

(u)B3LYP/6-31G*	

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	2.0648120000	-0.5527650000	0.0946920000
N	2.2959860000	0.7667440000	0.3857340000
C	3.6037150000	1.1859750000	0.1356210000
C	4.4180140000	0.1725550000	-0.2977020000
S	3.5406270000	-1.3322200000	-0.4112160000
C	5.8747190000	0.2068740000	-0.6464150000
C	3.9897370000	2.6156470000	0.3664640000
C	0.8712260000	-1.2885160000	0.1716680000
H	3.2835340000	3.3041360000	-0.1093070000
H	4.9766000000	2.8130060000	-0.0533330000
H	4.0338200000	2.8595300000	1.4350060000
H	6.0384090000	-0.0643380000	-1.6956020000
H	6.4418920000	-0.4988430000	-0.0289380000
H	6.2957480000	1.2011320000	-0.4858190000
C	1.3253740000	1.6323090000	1.0756480000
H	0.6357490000	1.0122300000	1.6452890000
H	0.7602670000	2.2383060000	0.3630600000
H	1.8629130000	2.2855010000	1.7621930000
C	-0.5026460000	-0.8074040000	0.1179730000
C	-1.4997750000	-1.4621450000	0.8752290000
C	-2.8296110000	-1.0702520000	0.7866420000
C	-3.1847040000	-0.0257520000	-0.0733350000
C	-2.2163820000	0.6251020000	-0.8467980000
C	-0.8868830000	0.2359940000	-0.7515030000
H	-1.2251060000	-2.2542100000	1.5669310000
H	-3.5882630000	-1.5629580000	1.3844300000
Br	-4.9939220000	0.5083120000	-0.1990340000
H	-2.5105480000	1.4143810000	-1.5296790000
H	-0.1471790000	0.7102250000	-1.3898750000
O	1.0931890000	-2.6244300000	0.2454990000
H	0.2964090000	-3.1110060000	-0.0319470000

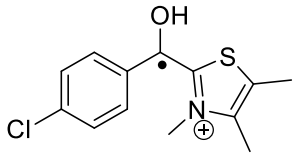
thermodynamic data

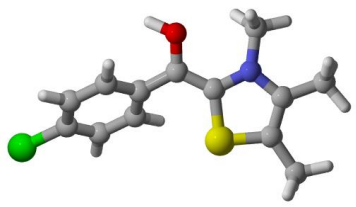
Zero-point correction= 0.244437 (Hartree/Particle)
Thermal correction to Energy= 0.261734
Thermal correction to Enthalpy= 0.262678
Thermal correction to Gibbs Free Energy= 0.197162

Sum of electronic and zero-point Energies= -3603.198976
Sum of electronic and thermal Energies= -3603.181678
Sum of electronic and thermal Enthalpies= -3603.180734
Sum of electronic and thermal Free Energies= -3603.246250

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.241	64.126	137.890

(u)B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3048370000	0.4040380000	0.0301750000
N	-2.6036850000	0.8330270000	0.1765700000
C	-3.5614990000	-0.1687250000	0.0289560000
C	-3.0178360000	-1.4051450000	-0.2038270000
S	-1.2759430000	-1.3191800000	-0.2627670000
C	-3.6923690000	-2.7301100000	-0.3881520000
C	-5.0219470000	0.1527610000	0.1337100000
C	-0.1450650000	1.1900730000	-0.0128680000
H	-5.3017240000	0.4519480000	1.1508890000
H	-5.6193240000	-0.7222510000	-0.1233020000
H	-5.3063410000	0.9597260000	-0.5500320000
H	-3.4475520000	-3.4144160000	0.4326780000
H	-3.3794760000	-3.2071210000	-1.3234890000
H	-4.7779690000	-2.6198270000	-0.4170340000
C	-2.9666920000	2.2207000000	0.5239840000
H	-2.2740710000	2.6000400000	1.2729420000
H	-3.9729640000	2.2240780000	0.9357110000
H	-2.9252180000	2.8598110000	-0.3602290000
C	1.2176210000	0.6634720000	0.0080790000
C	2.1948690000	1.2567840000	-0.8215680000
C	3.5094520000	0.8098080000	-0.8045460000
C	3.8693260000	-0.2355000000	0.0533420000
C	2.9216780000	-0.8309070000	0.8928790000
C	1.6071510000	-0.3824130000	0.8704740000

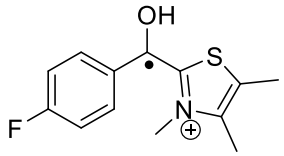
H	1.9150570000	2.0401650000	-1.5211550000
H	4.2515750000	1.2549240000	-1.4581050000
Cl	5.5133410000	-0.7968760000	0.0797220000
H	3.2202590000	-1.6247200000	1.5686590000
H	0.8911450000	-0.8183790000	1.5596190000
O	-0.3175320000	2.5234210000	-0.1778860000
H	0.5218320000	2.9822280000	0.0050930000

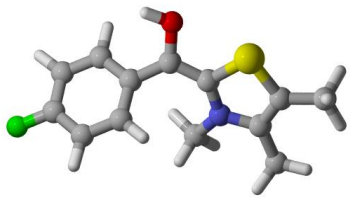
thermodynamic data

Zero-point correction= 0.244877 (Hartree/Particle)
Thermal correction to Energy= 0.262032
Thermal correction to Enthalpy= 0.262976
Thermal correction to Gibbs Free Energy= 0.198164
Sum of electronic and zero-point Energies= -1491.691303
Sum of electronic and thermal Energies= -1491.674148
Sum of electronic and thermal Enthalpies= -1491.673204
Sum of electronic and thermal Free Energies= -1491.738016

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.427	63.845	136.408

(u)B3LYP/6-31G*	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9940440000	-0.5343480000	0.0991580000
N	1.3417070000	0.7680640000	0.3511370000
C	2.6914380000	1.0506930000	0.1347150000
C	3.4179620000	-0.0514230000	-0.2334510000
S	2.4039450000	-1.4692440000	-0.3260050000
C	4.8821540000	-0.1708860000	-0.5272650000
C	3.2064860000	2.4444630000	0.3311010000
C	-0.2657580000	-1.1503750000	0.1578290000
H	2.5887520000	3.1793220000	-0.1957440000
H	4.2227540000	2.5297730000	-0.0549210000

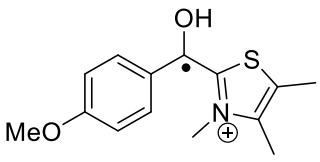
H	3.2351240000	2.7234470000	1.3915840000
H	5.0541440000	-0.5346750000	-1.5465500000
H	5.3635320000	-0.8743360000	0.1617520000
H	5.3861330000	0.7920580000	-0.4246210000
C	0.4365150000	1.7497480000	0.9702490000
H	-0.3284280000	1.2229350000	1.5375540000
H	-0.0433780000	2.3764730000	0.2142510000
H	1.0114400000	2.3774500000	1.6501920000
C	-1.5866510000	-0.5442810000	0.0467850000
C	-2.6588340000	-1.0722830000	0.8024440000
C	-3.9434630000	-0.5639350000	0.6623860000
C	-4.1598030000	0.4695600000	-0.2486640000
C	-3.1291460000	1.0041630000	-1.0231200000
C	-1.8468410000	0.4936560000	-0.8750380000
H	-2.4736570000	-1.8576830000	1.5302000000
H	-4.7732800000	-0.9450630000	1.2475460000
F	-5.3916740000	0.9599390000	-0.3891050000
H	-3.3511960000	1.7880640000	-1.7391100000
H	-1.0477830000	0.8675240000	-1.5081770000
O	-0.1746940000	-2.4982610000	0.2782140000
H	-1.0052260000	-2.9157010000	-0.0123690000

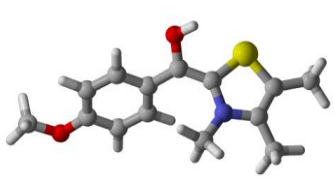
thermodynamic data

Zero-point correction=	0.246163 (Hartree/Particle)
Thermal correction to Energy=	0.262980
Thermal correction to Enthalpy=	0.263924
Thermal correction to Gibbs Free Energy=	0.200222
Sum of electronic and zero-point Energies=	-1131.327059
Sum of electronic and thermal Energies=	-1131.310242
Sum of electronic and thermal Enthalpies=	-1131.309298
Sum of electronic and thermal Free Energies=	-1131.373000

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	165.022	62.998	134.073

(u)B3LYP/6-31G*	





xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3737810000	-0.5534330000	-0.1379800000
N	1.7149440000	0.7435580000	-0.4265730000
C	3.0465110000	1.0681350000	-0.1443070000
C	3.7757710000	0.0091480000	0.3169140000
S	2.7758920000	-1.4241510000	0.4469570000
C	5.2208500000	-0.0657210000	0.7038570000
C	3.5374470000	2.4647460000	-0.3811050000
C	0.1241940000	-1.1951240000	-0.2647470000
H	2.8729540000	3.2048630000	0.0772010000
H	3.6135740000	2.6958010000	-1.4505310000
H	4.5292500000	2.5968480000	0.0525730000
H	5.7585200000	-0.7867240000	0.0773210000
H	5.3387500000	-0.3789420000	1.7473520000
H	5.7089890000	0.9040490000	0.5879260000
C	0.8473340000	1.6606300000	-1.1828810000
H	0.3770220000	2.3932330000	-0.5223120000
H	0.0717540000	1.0844600000	-1.6831440000
H	1.4478240000	2.1783220000	-1.9314870000
C	-1.1819730000	-0.6147170000	-0.0911470000
C	-1.3952510000	0.5315390000	0.7196650000
C	-2.6626290000	1.0323760000	0.9191860000
C	-3.7795060000	0.4044860000	0.3218480000
C	-3.5903860000	-0.7472160000	-0.4673730000
C	-2.3131540000	-1.2480140000	-0.6588100000
H	-4.4331090000	-1.2484240000	-0.9280160000
H	-2.1731640000	-2.1370660000	-1.2635830000
H	-2.8371390000	1.8935790000	1.5553460000
O	-4.9649740000	0.9739300000	0.5766420000
C	-6.1610850000	0.3918570000	0.0439300000
H	-6.9739000000	1.0239480000	0.4000280000
H	-6.1434160000	0.3957000000	-1.0513680000
H	-6.2972430000	-0.6294750000	0.4153240000
O	0.1270350000	-2.5467100000	-0.4243990000
H	0.9302190000	-2.8505760000	-0.8830040000
H	-0.5576810000	0.9919960000	1.2348370000

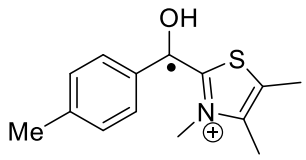
thermodynamic data

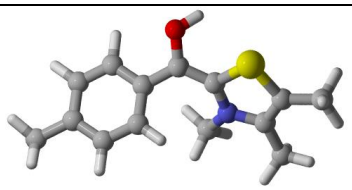
Zero-point correction= 0.287304 (Hartree/Particle)
Thermal correction to Energy= 0.305848
Thermal correction to Enthalpy= 0.306793
Thermal correction to Gibbs Free Energy= 0.239839
Sum of electronic and zero-point Energies= -1146.579807
Sum of electronic and thermal Energies= -1146.561263
Sum of electronic and thermal Enthalpies= -1146.560318
Sum of electronic and thermal Free Energies= -1146.627272

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	191.923	69.381	140.915

(u)B3LYP/6-31G*	





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

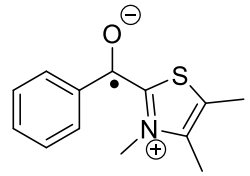
C	1.0050300000	-0.5554010000	0.1332210000
N	1.3538420000	0.7372230000	0.4268710000
C	2.6872610000	1.0539790000	0.1498340000
C	3.4106110000	-0.0091580000	-0.3148700000
S	2.4005940000	-1.4323290000	-0.4541550000
C	4.8564120000	-0.0929460000	-0.6971990000
C	3.1890800000	2.4453050000	0.3941150000
C	-0.2501400000	-1.1883860000	0.2569150000
H	2.5310280000	3.1931640000	-0.0606880000
H	4.1822580000	2.5714870000	-0.0381070000
H	3.2664830000	2.6693540000	1.4649420000
H	4.9756290000	-0.4188710000	-1.7365410000
H	5.3901860000	-0.8080000000	-0.0605940000
H	5.3469610000	0.8767480000	-0.5918490000
C	0.4839700000	1.6647340000	1.1692730000
H	-0.2913930000	1.0959340000	1.6779910000
H	0.0136980000	2.3853440000	0.4958520000
H	1.0844020000	2.1939090000	1.9095040000
C	-1.5564590000	-0.5899160000	0.0896610000
C	-2.6844080000	-1.1917130000	0.6944570000
C	-3.9502200000	-0.6614590000	0.4987230000
C	-4.1528520000	0.4700790000	-0.3115870000
C	-3.0318070000	1.0484090000	-0.9343050000
C	-1.7583430000	0.5343590000	-0.7434580000
H	-2.5504330000	-2.0686300000	1.3182270000
H	-4.8037010000	-1.1322220000	0.9787850000
C	-5.5294080000	1.0499510000	-0.4995570000
H	-3.1703110000	1.8988960000	-1.5961510000
H	-0.9205590000	0.9659270000	-1.2836070000
H	-5.6106670000	1.5978060000	-1.4429280000
H	-5.7655090000	1.7539380000	0.3098580000
H	-6.2977530000	0.2709010000	-0.4839950000
O	-0.2656040000	-2.5366730000	0.4086390000
H	0.5457570000	-2.8626120000	0.8372340000

thermodynamic data

Zero-point correction= 0.281893 (Hartree/Particle)
Thermal correction to Energy= 0.299699
Thermal correction to Enthalpy= 0.300643
Thermal correction to Gibbs Free Energy= 0.234965
Sum of electronic and zero-point Energies= -1071.376103
Sum of electronic and thermal Energies= -1071.358297
Sum of electronic and thermal Enthalpies= -1071.357353
Sum of electronic and thermal Free Energies= -1071.423031

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.064	66.214	138.231

(u)B3LYP/6-31G*	

xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	0.5884660000	-0.5399060000	0.1208410000
N	1.0008630000	0.7761270000	0.2882730000
C	2.3803180000	0.9588490000	0.0749270000
C	3.0481840000	-0.1897320000	-0.1980890000
S	1.9649520000	-1.5873230000	-0.1851070000
C	4.5013040000	-0.3961020000	-0.4971730000
C	2.9455980000	2.3461970000	0.1594170000
C	-0.7019400000	-1.1616990000	0.1303670000
H	2.4400280000	3.0256660000	-0.5381120000
H	4.0077710000	2.3433980000	-0.0911030000
H	2.8455110000	2.7743180000	1.1646340000
H	4.6528800000	-0.7776200000	-1.5148130000
H	4.9435820000	-1.1265980000	0.1918030000
H	5.0674080000	0.5343660000	-0.4017140000
C	0.2677690000	1.7294530000	1.1286360000
H	-0.7330100000	1.3513930000	1.3163180000
H	0.1843480000	2.6993150000	0.6299260000
H	0.7813620000	1.8629710000	2.0886470000
O	-0.7420130000	-2.4141580000	0.2092980000
C	-1.9822360000	-0.3970080000	-0.0220680000

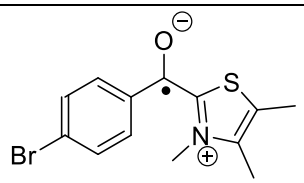
C	-3.1420780000	-0.9387990000	0.5553680000
C	-4.3765480000	-0.3177430000	0.3840100000
C	-4.4788940000	0.8428750000	-0.3884540000
C	-3.3371430000	1.3750660000	-0.9907440000
C	-2.0977130000	0.7611520000	-0.8083410000
H	-3.0512790000	-1.8576390000	1.1256550000
H	-5.2636850000	-0.7426940000	0.8466020000
H	-5.4438020000	1.3231660000	-0.5281790000
H	-3.4128720000	2.2633190000	-1.6129400000
H	-1.2179380000	1.1685590000	-1.2994770000

thermodynamic data

Zero-point correction= 0.241534 (Hartree/Particle)
Thermal correction to Energy= 0.257314
Thermal correction to Enthalpy= 0.258258
Thermal correction to Gibbs Free Energy= 0.197303
Sum of electronic and zero-point Energies= -1031.701793
Sum of electronic and thermal Energies= -1031.686013
Sum of electronic and thermal Enthalpies= -1031.685069
Sum of electronic and thermal Free Energies= -1031.746024

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.467	58.781	128.292

(u)B3LYP/6-31G*		

xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0629920000	0.5896760000	0.0884340000
N	-2.2605430000	-0.7550870000	0.3577460000
C	-3.5738760000	-1.1925170000	0.1153410000
C	-4.4129750000	-0.1975240000	-0.2717250000
S	-3.5806190000	1.3589060000	-0.3390420000
C	-5.8691790000	-0.2639440000	-0.6166790000
C	-3.9113080000	-2.6432280000	0.2990230000
C	-0.8999490000	1.4230040000	0.1352890000
H	-3.1941470000	-3.2901820000	-0.2195740000
H	-4.9024100000	-2.8566020000	-0.1051520000

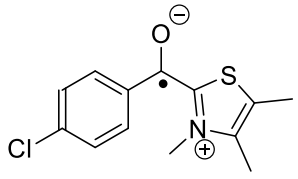
H	-3.9196900000	-2.9396610000	1.3558210000
H	-6.0516650000	0.0445330000	-1.6537130000
H	-6.4573320000	0.4014490000	0.0278530000
H	-6.2643600000	-1.2758120000	-0.4942360000
C	-1.3112210000	-1.5542560000	1.1338160000
H	-0.6791870000	-0.8860530000	1.7188330000
H	-0.6661950000	-2.1651390000	0.4942070000
H	-1.8564930000	-2.2070360000	1.8181240000
O	-1.0682430000	2.6680520000	0.1537150000
C	0.4927080000	0.8753440000	0.0872320000
C	1.5027020000	1.5693290000	0.7730990000
C	2.8298970000	1.1561070000	0.7068420000
C	3.1590890000	0.0506430000	-0.0787470000
C	2.1852810000	-0.6348490000	-0.8019390000
C	0.8571560000	-0.2176840000	-0.7144130000
H	1.2284200000	2.4447610000	1.3529270000
H	3.6036440000	1.6868180000	1.2511580000
Br	4.9811910000	-0.5233480000	-0.1785760000
H	2.4629930000	-1.4719070000	-1.4335880000
H	0.1023920000	-0.7298890000	-1.3051970000

thermodynamic data

Zero-point correction= 0.231588 (Hartree/Particle)
Thermal correction to Energy= 0.248738
Thermal correction to Enthalpy= 0.249682
Thermal correction to Gibbs Free Energy= 0.184391
Sum of electronic and zero-point Energies= -3602.817149
Sum of electronic and thermal Energies= -3602.799999
Sum of electronic and thermal Enthalpies= -3602.799055
Sum of electronic and thermal Free Energies= -3602.864347

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.085	62.896	137.417

(u)B3LYP/6-31G*		

xyz-matrix

XYZ file generated by gabedit : coordinates in Angstrom

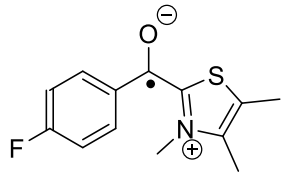
C	1.3727440000	-0.5842400000	-0.0956040000
N	1.6301550000	0.7532750000	-0.3500560000
C	2.9647140000	1.1261610000	-0.1151480000
C	3.7601430000	0.0881900000	0.2508090000
S	2.8569830000	-1.4288060000	0.3059010000
C	5.2206660000	0.0816750000	0.5832920000
C	3.3679470000	2.5618170000	-0.2838970000
C	0.1704330000	-1.3604100000	-0.1383300000
H	2.6875220000	3.2347230000	0.2509720000
H	3.3789090000	2.8715660000	-1.3368480000
H	4.3723430000	2.7233200000	0.1115080000
H	5.7715870000	-0.6009940000	-0.0759070000
H	5.3972260000	-0.2501070000	1.6141630000
H	5.6620540000	1.0756020000	0.4719770000
C	0.7120890000	1.6053770000	-1.1071350000
H	0.0981970000	2.2332330000	-0.4535140000
H	0.0479680000	0.9750400000	-1.6988450000
H	1.2812970000	2.2448770000	-1.7844160000
O	0.2781470000	-2.6115610000	-0.1769030000
C	-1.1929830000	-0.7464450000	-0.0613200000
C	-1.4898800000	0.3548470000	0.7565440000
C	-2.7937300000	0.8361690000	0.8714190000
C	-3.8131730000	0.2064130000	0.1592410000
C	-3.5514760000	-0.9063460000	-0.6424530000
C	-2.2475220000	-1.3829600000	-0.7355880000
Cl	-5.4598310000	0.8145150000	0.2866330000
H	-4.3606090000	-1.3924620000	-1.1774510000
H	-2.0263490000	-2.2648180000	-1.3281530000
H	-3.0204160000	1.6792760000	1.5156800000
H	-0.7004270000	0.8229550000	1.3383120000

thermodynamic data

Zero-point correction= 0.231924 (Hartree/Particle)
Thermal correction to Energy= 0.248895
Thermal correction to Enthalpy= 0.249840
Thermal correction to Gibbs Free Energy= 0.185615
Sum of electronic and zero-point Energies= -1491.308077
Sum of electronic and thermal Energies= -1491.291106
Sum of electronic and thermal Enthalpies= -1491.290161
Sum of electronic and thermal Free Energies= -1491.354386

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.184	62.621	135.173

(u)B3LYP/6-31G*	

xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9822280000	-0.5746010000	-0.1001820000
N	1.3035590000	0.7536220000	-0.3351360000
C	2.6586740000	1.0536390000	-0.1137360000
C	3.4054240000	-0.0294710000	0.2225680000
S	2.4279640000	-1.5005990000	0.2635340000
C	4.8679490000	-0.1158280000	0.5341350000
C	3.1331090000	2.4696410000	-0.2634060000
C	-0.2589370000	-1.2877000000	-0.1347910000
H	2.4959140000	3.1669270000	0.2930950000
H	3.1454530000	2.7976570000	-1.3108720000
H	4.1500200000	2.5721500000	0.1195630000
H	5.3759510000	-0.8085720000	-0.1487190000
H	5.0410760000	-0.4812270000	1.5541990000
H	5.3571630000	0.8574400000	0.4406870000
C	0.4205690000	1.6617470000	-1.0681230000
H	-0.1697070000	2.2942890000	-0.3975670000
H	-0.2669540000	1.0750650000	-1.6782420000
H	1.0155990000	2.2975390000	-1.7262070000
O	-0.2147370000	-2.5415500000	-0.1939270000
C	-1.5877360000	-0.6051560000	-0.0295490000
C	-1.8152340000	0.4953060000	0.8121670000
C	-3.0909340000	1.0416800000	0.9532990000
C	-4.1411290000	0.4712990000	0.2437270000
C	-3.9585990000	-0.6344300000	-0.5818960000
C	-2.6820660000	-1.1751300000	-0.7018240000
F	-5.3778880000	0.9988730000	0.3686350000
H	-4.8096970000	-1.0572950000	-1.1060260000
H	-2.5119370000	-2.0561280000	-1.3120890000
H	-3.2828490000	1.8829960000	1.6114830000
H	-0.9933830000	0.9099550000	1.3894650000

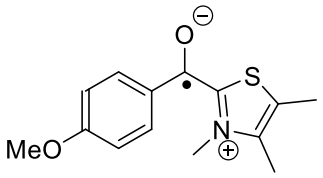
thermodynamic data

Zero-point correction= 0.233338 (Hartree/Particle)
Thermal correction to Energy= 0.249938
Thermal correction to Enthalpy= 0.250883
Thermal correction to Gibbs Free Energy= 0.187876
Sum of electronic and zero-point Energies= -1130.943747
Sum of electronic and thermal Energies= -1130.927146

Sum of electronic and thermal Enthalpies= -1130.926202
Sum of electronic and thermal Free Energies= -1130.989209

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.839	61.736	132.609

(u)B3LYP/6-31G*		

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3853280000	-0.5811050000	-0.1045950000
N	1.6718150000	0.7568390000	-0.3362340000
C	3.0193810000	1.0901990000	-0.1190200000
C	3.7961010000	0.0257000000	0.2079320000
S	2.8578840000	-1.4720890000	0.2445150000
C	5.2612430000	-0.0226300000	0.5149850000
C	3.4534440000	2.5198460000	-0.2617150000
C	0.1599090000	-1.3232230000	-0.1249690000
H	2.8016130000	3.1943710000	0.3059630000
H	3.4459960000	2.8565750000	-1.3064180000
H	4.4706380000	2.6483020000	0.1127520000
H	5.7843100000	-0.7050290000	-0.1670560000
H	5.4474400000	-0.3799140000	1.5357620000
H	5.7255780000	0.9623120000	0.4161890000
C	0.7708080000	1.6410330000	-1.0772500000
H	0.2081900000	2.3055760000	-0.4137340000
H	0.0588370000	1.0343450000	-1.6362750000
H	1.3464270000	2.2441380000	-1.7829610000
O	0.2363030000	-2.5752630000	-0.1892360000
C	-1.1796830000	-0.6689050000	-0.0048650000
C	-1.4231060000	0.4435320000	0.8211620000
C	-2.7033570000	0.9595110000	0.9726880000
C	-3.7835790000	0.3711880000	0.2978940000
C	-3.5641690000	-0.7519650000	-0.5113730000
C	-2.2749590000	-1.2658550000	-0.6423700000
H	-4.3846920000	-1.2337110000	-1.0312020000
H	-2.1014160000	-2.1538900000	-1.2420740000
H	-2.8978580000	1.8083680000	1.6211780000
H	-0.6029330000	0.8897020000	1.3775990000

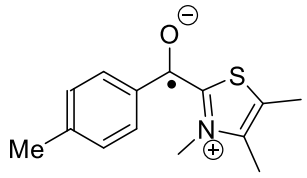
O	-4.9994370000	0.9575190000	0.5018090000
C	-6.1340320000	0.3889000000	-0.1324100000
H	-6.9845460000	1.0033230000	0.1688350000
H	-6.0397650000	0.4122310000	-1.2262580000
H	-6.3015650000	-0.6465540000	0.1919420000

thermodynamic data

Zero-point correction= 0.274184 (Hartree/Particle)
Thermal correction to Energy= 0.292703
Thermal correction to Enthalpy= 0.293647
Thermal correction to Gibbs Free Energy= 0.225730
Sum of electronic and zero-point Energies= -1146.192458
Sum of electronic and thermal Energies= -1146.173939
Sum of electronic and thermal Enthalpies= -1146.172995
Sum of electronic and thermal Free Energies= -1146.240911

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	183.674	67.965	142.942

(u)B3LYP/6-31G*		

xyz-matrix

33
XYZ file generated by gabedit : coordinates in Angstrom

C	1.0066860000	-0.5698260000	0.1237940000
N	1.3193860000	0.7710980000	0.3141420000
C	2.6752490000	1.0649990000	0.0722850000
C	3.4219420000	-0.0207930000	-0.2485750000
S	2.4511340000	-1.4992220000	-0.2449370000
C	4.8772470000	-0.1060560000	-0.5923680000
C	3.1349950000	2.4890160000	0.1828540000
C	-0.2327340000	-1.2885210000	0.1476590000
H	2.5660090000	3.1448750000	-0.4880160000
H	4.1894320000	2.5740820000	-0.0855570000
H	3.0213550000	2.8824170000	1.2006270000
H	5.0279990000	-0.4413520000	-1.6263550000
H	5.3923550000	-0.8233470000	0.0588380000
H	5.3748890000	0.8609460000	-0.4794390000

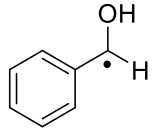
C	0.5477140000	1.6333730000	1.2165320000
H	-0.4359610000	1.2018460000	1.3774190000
H	0.4224330000	2.6283840000	0.7806920000
H	1.0571140000	1.7267550000	2.1839640000
O	-0.1760680000	-2.5415410000	0.1980500000
C	-1.5683270000	-0.6185130000	0.0412600000
C	-2.6771250000	-1.2601190000	0.6158070000
C	-3.9558710000	-0.7307100000	0.4779530000
C	-4.1817530000	0.4439750000	-0.2554900000
C	-3.0780120000	1.0651140000	-0.8537410000
C	-1.7918100000	0.5471190000	-0.7079810000
H	-2.5132670000	-2.1872650000	1.1556630000
H	-4.7989630000	-1.2413970000	0.9387970000
C	-5.5696800000	1.0260900000	-0.3839620000
H	-3.2288340000	1.9604230000	-1.4534720000
H	-0.9588510000	1.0373670000	-1.2052150000
H	-5.6692170000	1.6300380000	-1.2921360000
H	-5.8103060000	1.6769780000	0.4678330000
H	-6.3326060000	0.2405590000	-0.4142130000

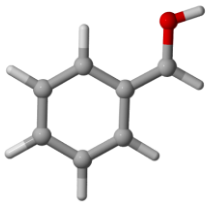
thermodynamic data

Zero-point correction= 0.269070 (Hartree/Particle)
Thermal correction to Energy= 0.286725
Thermal correction to Enthalpy= 0.287669
Thermal correction to Gibbs Free Energy= 0.222027
Sum of electronic and zero-point Energies= -1070.992468
Sum of electronic and thermal Energies= -1070.974813
Sum of electronic and thermal Enthalpies= -1070.973869
Sum of electronic and thermal Free Energies= -1071.039511

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.923	64.806	138.156

(u)B3LYP/6-31G*	





xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

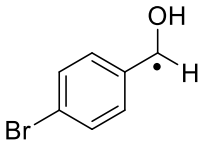
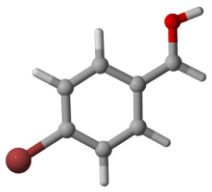
C	0.0179760000	-1.0825690000	-0.0000370000
C	0.4937910000	0.2604410000	-0.0000420000
C	-0.4715880000	1.3082460000	0.0000020000
C	-1.8279070000	1.0250140000	0.0000390000
C	-2.2798340000	-0.3030050000	0.0000350000
C	-1.3435940000	-1.3465430000	0.0000200000
H	-0.1309890000	2.3415090000	0.0000300000
H	-2.5456550000	1.8416680000	0.0001090000
H	-3.3441360000	-0.5199470000	0.0000570000
H	-1.6864720000	-2.3784860000	0.0000960000
H	0.7370420000	-1.8949460000	0.0000190000
C	1.8660890000	0.5678850000	-0.0005580000
H	2.2308240000	1.5909590000	0.0013470000
O	2.7913670000	-0.4381010000	0.0001090000
H	3.6788610000	-0.0527620000	0.0007190000

thermodynamic data

Zero-point correction= 0.119916 (Hartree/Particle)
Thermal correction to Energy= 0.126899
Thermal correction to Enthalpy= 0.127844
Thermal correction to Gibbs Free Energy= 0.088320
Sum of electronic and zero-point Energies= -346.010987
Sum of electronic and thermal Energies= -346.004004
Sum of electronic and thermal Enthalpies= -346.003060
Sum of electronic and thermal Free Energies= -346.042584

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.631	27.043	83.185

(u)B3LYP/6-31G*		

xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

C	1.4580870000	-1.0103430000	-0.0000440000
C	2.0958000000	0.2644450000	0.0000010000

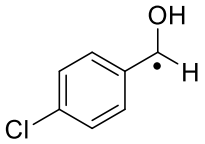
C	1.2632050000	1.4207040000	0.0000020000
C	-0.1168130000	1.3123530000	-0.0000050000
C	-0.7091600000	0.0432850000	-0.0000120000
C	0.0764140000	-1.1148780000	-0.0000190000
H	1.7213270000	2.4069240000	0.0000380000
H	-0.7390930000	2.2009540000	0.0000440000
H	-0.3993190000	-2.0900370000	0.0000270000
H	2.0687390000	-1.9067520000	-0.0000150000
C	3.4936600000	0.4006980000	-0.0004620000
H	3.9811400000	1.3711090000	0.0012460000
Br	-2.6139980000	-0.1070130000	0.0000120000
O	4.2844740000	-0.7114290000	0.0001990000
H	5.2141610000	-0.4428900000	-0.0001270000

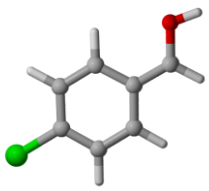
thermodynamic data

Zero-point correction= 0.109964 (Hartree/Particle)
Thermal correction to Energy= 0.118363
Thermal correction to Enthalpy= 0.119307
Thermal correction to Gibbs Free Energy= 0.075031
Sum of electronic and zero-point Energies= -2917.126870
Sum of electronic and thermal Energies= -2917.118471
Sum of electronic and thermal Enthalpies= -2917.117527
Sum of electronic and thermal Free Energies= -2917.161803

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.274	31.184	93.186

(u)B3LYP/6-31G*





xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8009520000	-1.0220290000	-0.0000610000
C	1.4106690000	0.2662790000	-0.0000190000
C	0.5527600000	1.4037660000	0.0000130000
C	-0.8244510000	1.2655180000	0.0000180000

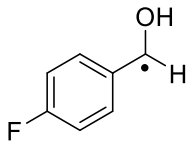
C	-1.3894900000	-0.0165570000	-0.0000040000
C	-0.5779510000	-1.1573480000	-0.0000240000
H	0.9893420000	2.3996580000	0.0000600000
H	-1.4670350000	2.1398320000	0.0000840000
H	-1.0332640000	-2.1424650000	0.0000220000
H	1.4314090000	-1.9045660000	-0.0000400000
C	2.8053120000	0.4333670000	-0.0005300000
H	3.2711210000	1.4143370000	0.0012090000
Cl	-3.1392990000	-0.1931560000	0.0000220000
O	3.6206900000	-0.6611430000	0.0002800000
H	4.5441740000	-0.3719810000	-0.0003100000

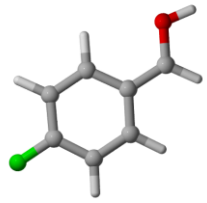
thermodynamic data

Zero-point correction= 0.110346 (Hartree/Particle)
Thermal correction to Energy= 0.118538
Thermal correction to Enthalpy= 0.119482
Thermal correction to Gibbs Free Energy= 0.076483
Sum of electronic and zero-point Energies= -805.617653
Sum of electronic and thermal Energies= -805.609462
Sum of electronic and thermal Enthalpies= -805.608517
Sum of electronic and thermal Free Energies= -805.651516

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.384	30.893	90.498

(u)B3LYP/6-31G*





xyz-matrix

15
XYZ file generated by gabedit : coordinates in Angstrom

C	0.3930970000	-1.0387350000	-0.0002730000
C	0.9563120000	0.2708120000	-0.0002030000
C	0.0601790000	1.3786940000	0.0000040000
C	-1.3126670000	1.1921820000	0.0000830000
C	-1.8198530000	-0.1080860000	0.0000260000
C	-0.9815710000	-1.2224180000	-0.0001360000
H	0.4637130000	2.3883420000	0.0000620000

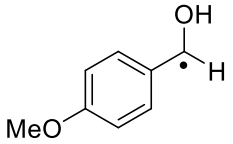
H	-1.9991180000	2.0329120000	0.0002070000
H	-1.4184480000	-2.2161920000	-0.0001550000
H	1.0560570000	-1.8969330000	-0.0004720000
C	2.3466810000	0.4860090000	-0.0006680000
H	2.7798250000	1.4817460000	0.0007010000
F	-3.1599450000	-0.2904840000	0.0001740000
O	3.1990530000	-0.5830190000	0.0008170000
H	4.1119830000	-0.2621140000	-0.0014350000

thermodynamic data

Zero-point correction= 0.111612 (Hartree/Particle)
Thermal correction to Energy= 0.119461
Thermal correction to Enthalpy= 0.120406
Thermal correction to Gibbs Free Energy= 0.078653
Sum of electronic and zero-point Energies= -445.252240
Sum of electronic and thermal Energies= -445.244390
Sum of electronic and thermal Enthalpies= -445.243446
Sum of electronic and thermal Free Energies= -445.285198

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.963	30.117	87.875

(u)B3LYP/6-31G*	

xyz-matrix

19
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7050680000	-0.9607850000	-0.0001090000
C	-1.4518850000	0.2488110000	-0.0000020000
C	-0.7131950000	1.4695400000	0.0000320000
C	0.6660310000	1.4739310000	-0.0000060000
C	1.3852310000	0.2623740000	-0.0000790000
C	0.6853660000	-0.9530530000	-0.0001490000
H	-1.2513680000	2.4148300000	0.0000900000
H	1.2247130000	2.4050660000	0.0000160000
H	1.2169120000	-1.8985020000	-0.0002490000
H	-1.2363000000	-1.9066040000	-0.0001770000
C	-2.8572260000	0.2684430000	0.0000470000
H	-3.4258560000	1.1935650000	0.0000960000
O	2.7484210000	0.3830160000	-0.0001420000

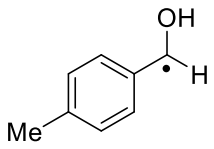
C	3.5230480000	-0.8032560000	0.0002180000
H	4.5664430000	-0.4815970000	0.0004230000
H	3.3318700000	-1.4118400000	0.8945600000
H	3.3323150000	-1.4120960000	-0.8940480000
O	-3.5547060000	-0.9108390000	0.0000970000
H	-4.5022610000	-0.7162690000	-0.0000640000

thermodynamic data

Zero-point correction= 0.152593 (Hartree/Particle)
Thermal correction to Energy= 0.162217
Thermal correction to Enthalpy= 0.163161
Thermal correction to Gibbs Free Energy= 0.117360
Sum of electronic and zero-point Energies= -460.500198
Sum of electronic and thermal Energies= -460.490574
Sum of electronic and thermal Enthalpies= -460.489630
Sum of electronic and thermal Free Energies= -460.535431

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.793	36.327	96.396

(u)B3LYP/6-31G*		

xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

C	0.4315920000	-1.0356000000	0.0000450000
C	1.0116420000	0.2640130000	-0.0000580000
C	0.1220200000	1.3774070000	0.0000470000
C	-1.2485140000	1.1943590000	0.0001890000
C	-1.8207090000	-0.0940110000	0.0002090000
C	-0.9466980000	-1.1937740000	0.0002010000
H	0.5338090000	2.3845340000	0.0001070000
H	-1.9009240000	2.0656430000	0.0003440000
H	-1.3631500000	-2.1992480000	0.0003680000
H	1.0825680000	-1.9035970000	0.0001280000
C	2.4017500000	0.4698560000	-0.0004870000
H	2.8406550000	1.4633540000	0.0007690000
C	-3.3189760000	-0.2743870000	-0.0002600000
H	-3.7837460000	0.1930000000	0.8780990000

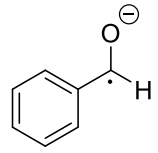
H	-3.5935400000	-1.3342970000	0.0053120000
H	-3.7820240000	0.1830570000	-0.8848060000
O	3.2511810000	-0.6021700000	0.0000860000
H	4.1642630000	-0.2822640000	-0.0003280000

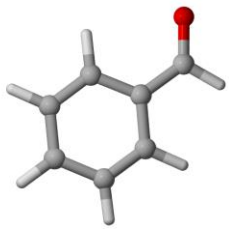
thermodynamic data

Zero-point correction= 0.147300 (Hartree/Particle)
Thermal correction to Energy= 0.155328
Thermal correction to Enthalpy= 0.156273
Thermal correction to Gibbs Free Energy= 0.114236
Sum of electronic and zero-point Energies= -385.301530
Sum of electronic and thermal Energies= -385.293502
Sum of electronic and thermal Enthalpies= -385.292558
Sum of electronic and thermal Free Energies= -385.334594

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	97.470	31.104	88.473

(u)B3LYP/6-31G*	





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

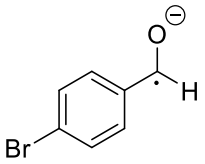
C	-0.0372660000	-1.1035660000	-0.0000070000
C	-0.5747440000	0.2315570000	-0.0000110000
C	0.3858750000	1.2982340000	-0.0000060000
C	1.7465820000	1.0545660000	0.0000020000
C	2.2553770000	-0.2660360000	0.0000050000
C	1.3254840000	-1.3314880000	0.0000010000
H	0.0178110000	2.3261040000	-0.0000080000
H	2.4408280000	1.8975070000	0.0000050000
H	3.3271660000	-0.4545600000	0.0000110000
H	1.6936450000	-2.3599860000	0.0000030000
H	-0.7479080000	-1.9264710000	-0.0000100000
C	-1.9804150000	0.4715120000	-0.0000170000
H	-2.2534740000	1.5596000000	0.0000190000
O	-2.9004280000	-0.3963580000	0.0000230000

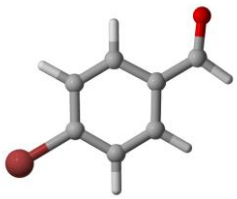
thermodynamic data

Zero-point correction= 0.106206 (Hartree/Particle)
Thermal correction to Energy= 0.112667
Thermal correction to Enthalpy= 0.113611
Thermal correction to Gibbs Free Energy= 0.075076
Sum of electronic and zero-point Energies= -345.461275
Sum of electronic and thermal Energies= -345.454813
Sum of electronic and thermal Enthalpies= -345.453869
Sum of electronic and thermal Free Energies= -345.492404

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	70.700	25.212	81.104

(u)B3LYP/6-31G*	





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.5023910000	-1.0465240000	-0.0002080000
C	-2.1782750000	0.2243210000	-0.0002780000
C	-1.3407220000	1.3892750000	-0.0002000000
C	0.0378100000	1.3056000000	-0.0000800000
C	0.6539360000	0.0365140000	-0.0000230000
C	-0.1251790000	-1.1379170000	-0.0000870000
H	-1.8147680000	2.3716720000	-0.0002440000
H	0.6498620000	2.2042780000	-0.0000330000
H	0.3653750000	-2.1087600000	-0.0000440000
H	-2.1187750000	-1.9415880000	-0.0002650000
C	-3.6017800000	0.3095610000	-0.0003770000
H	-3.9939170000	1.3591020000	0.0002720000
O	-4.4146460000	-0.6548550000	0.0003380000
Br	2.5876850000	-0.0894530000	0.0001470000

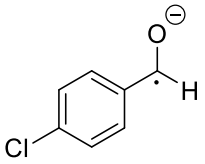
thermodynamic data

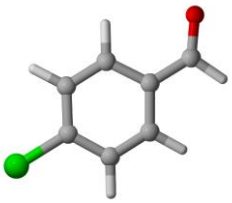
Zero-point correction= 0.096384 (Hartree/Particle)
Thermal correction to Energy= 0.104508
Thermal correction to Enthalpy= 0.105452

Thermal correction to Gibbs Free Energy= 0.061222
Sum of electronic and zero-point Energies= -2916.589547
Sum of electronic and thermal Energies= -2916.581423
Sum of electronic and thermal Enthalpies= -2916.580479
Sum of electronic and thermal Free Energies= -2916.624709

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.580	29.453	93.090

(u)B3LYP/6-31G*	





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8404080000	-1.0555510000	-0.0000510000
C	-1.4931270000	0.2275110000	-0.0000710000
C	-0.6334350000	1.3762630000	-0.0000470000
C	0.7434080000	1.2665760000	-0.0000110000
C	1.3373180000	-0.0133030000	0.0000040000
C	0.5351780000	-1.1721510000	-0.0000150000
H	-1.0890480000	2.3673230000	-0.0000590000
H	1.3725340000	2.1538910000	0.0000030000
H	1.0082580000	-2.1521150000	-0.0000030000
H	-1.4732180000	-1.9390100000	-0.0000700000
C	-2.9147050000	0.3393860000	-0.0001000000
H	-3.2864090000	1.3967540000	0.0000820000
O	-3.7465920000	-0.6091390000	0.0001190000
Cl	3.1197200000	-0.1627120000	0.0000500000

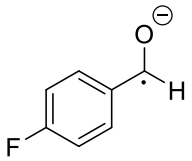
thermodynamic data

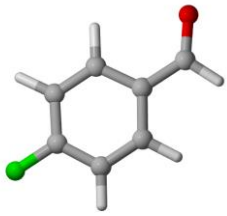
Zero-point correction= 0.096789 (Hartree/Particle)
Thermal correction to Energy= 0.104651
Thermal correction to Enthalpy= 0.105596
Thermal correction to Gibbs Free Energy= 0.062993
Sum of electronic and zero-point Energies= -805.079243
Sum of electronic and thermal Energies= -805.071381

Sum of electronic and thermal Enthalpies= -805.070437
Sum of electronic and thermal Free Energies= -805.113040

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.670	29.159	89.666

(u)B3LYP/6-31G*	





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

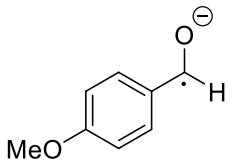
C	-0.4256790000	-1.0683390000	-0.0000020000
C	-1.0395200000	0.2355580000	-0.0000020000
C	-0.1439520000	1.3578570000	-0.0000010000
C	1.2314560000	1.2018960000	0.0000010000
C	1.7768730000	-0.0918120000	0.0000010000
C	0.9498170000	-1.2230900000	0.0000000000
H	-0.5694350000	2.3621730000	-0.0000010000
H	1.9006230000	2.0607250000	0.0000010000
H	1.4081730000	-2.2112320000	0.0000000000
H	-1.0865230000	-1.9306430000	-0.0000020000
C	-2.4570980000	0.3888860000	-0.0000020000
H	-2.7975290000	1.4572740000	0.0000090000
O	-3.3186330000	-0.5381420000	0.0000000000
F	3.1491530000	-0.2487670000	0.0000020000

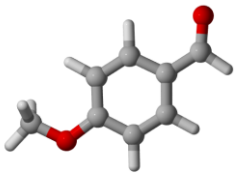
thermodynamic data

Zero-point correction= 0.097977 (Hartree/Particle)
Thermal correction to Energy= 0.105367
Thermal correction to Enthalpy= 0.106312
Thermal correction to Gibbs Free Energy= 0.065398
Sum of electronic and zero-point Energies= -444.705211
Sum of electronic and thermal Energies= -444.697820
Sum of electronic and thermal Enthalpies= -444.696876
Sum of electronic and thermal Free Energies= -444.737790

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	66.119	28.304	86.111

(u)B3LYP/6-31G*	





xyz-matrix

18
XYZ file generated by gabedit : coordinates in Angstrom

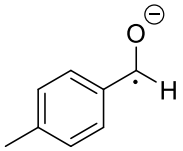
C	0.7369660000	-0.9973550000	-0.0000070000
C	1.4829970000	0.1892090000	-0.0000810000
C	0.8052130000	1.4199780000	-0.0000940000
C	-0.5795770000	1.4662660000	-0.0000360000
C	-1.3180660000	0.2701870000	0.0000380000
C	-0.6526870000	-0.9682270000	0.0000520000
H	1.3764160000	2.3461610000	-0.0001510000
H	-1.1196900000	2.4075490000	-0.0000450000
H	-1.2095760000	-1.8981030000	0.0001040000
H	1.2710270000	-1.9429080000	0.0000010000
C	2.9555030000	0.1483090000	-0.0001440000
H	3.4447550000	1.1488930000	-0.0001690000
O	3.6268260000	-0.8683710000	-0.0001050000
O	-2.6679630000	0.4162460000	0.0000870000
C	-3.4814240000	-0.7502900000	0.0002150000
H	-4.5121980000	-0.3926690000	0.0002790000
H	-3.3076700000	-1.3602410000	-0.8951210000
H	-3.3075260000	-1.3601460000	0.8955880000

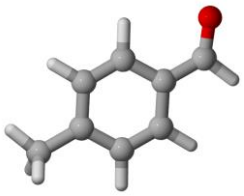
thermodynamic data

Zero-point correction= 0.138728 (Hartree/Particle)
Thermal correction to Energy= 0.147866
Thermal correction to Enthalpy= 0.148810
Thermal correction to Gibbs Free Energy= 0.103514
Sum of electronic and zero-point Energies= -459.946558
Sum of electronic and thermal Energies= -459.937420
Sum of electronic and thermal Enthalpies= -459.936476
Sum of electronic and thermal Free Energies= -459.981773

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	92.787	34.328	95.334

(u)B3LYP/6-31G*	





xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

C	0.4604970000	-1.0677660000	-0.0000060000
C	1.0915020000	0.2248300000	-0.0000050000
C	0.2042560000	1.3508880000	-0.0000010000
C	-1.1676400000	1.2030280000	0.0000030000
C	-1.7839960000	-0.0788280000	0.0000030000
C	-0.9160600000	-1.1961850000	-0.0000010000
H	0.6393760000	2.3522750000	-0.0000020000
H	-1.8010890000	2.0933910000	0.0000060000
H	-1.3562970000	-2.1968760000	-0.0000020000
H	1.1070500000	-1.9416920000	-0.0000090000
C	2.5098050000	0.3737170000	-0.0000040000
H	2.8516960000	1.4423840000	0.0000120000
C	-3.2827500000	-0.2292310000	0.0000040000
H	-3.7663820000	0.2310630000	0.8804380000
H	-3.5715230000	-1.2890520000	0.0000210000
H	-3.7663810000	0.2310340000	-0.8804460000
O	3.1642480000	-0.3285460000	0.0000010000

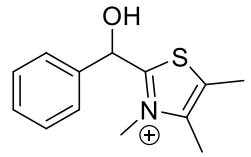
thermodynamic data

Zero-point correction= 0.133602 (Hartree/Particle)
Thermal correction to Energy= 0.141057
Thermal correction to Enthalpy= 0.142002
Thermal correction to Gibbs Free Energy= 0.101024
Sum of electronic and zero-point Energies= -384.751386
Sum of electronic and thermal Energies= -384.743931
Sum of electronic and thermal Enthalpies= -384.742987
Sum of electronic and thermal Free Energies= -384.783965

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin

Total	88.515	28.953	86.245

B3LYP/6-31G*	

xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

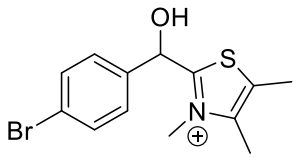
C	0.5906170000	-0.3236060000	-0.5743180000
N	1.1081360000	0.8988980000	-0.4498370000
C	2.3995740000	0.9365490000	0.1088620000
C	2.8566420000	-0.3137690000	0.4135390000
S	1.6686200000	-1.5221820000	-0.0169070000
C	4.1597480000	-0.7296900000	1.0281790000
C	3.0936700000	2.2496420000	0.3014090000
C	-0.7581420000	-0.7013580000	-1.1536930000
H	3.1650390000	2.8131510000	-0.6355130000
H	4.1088240000	2.0867790000	0.6651170000
H	2.5785980000	2.8780150000	1.0377370000
H	4.6606720000	-1.4888140000	0.4182750000
H	4.0084750000	-1.1502720000	2.0286940000
H	4.8367160000	0.1218780000	1.1224870000
C	0.4144600000	2.1239830000	-0.8902840000
H	-0.6479900000	1.9188550000	-1.0001020000
H	0.8354780000	2.4627680000	-1.8406990000
H	0.5438680000	2.8989650000	-0.1345940000
C	-1.9343200000	-0.2455340000	-0.3012040000
C	-2.0231430000	-0.6122370000	1.0502880000
C	-3.1361570000	-0.2404000000	1.8016940000
C	-4.1671230000	0.4973520000	1.2117830000
C	-4.0873210000	0.8580090000	-0.1337710000
C	-2.9744460000	0.4853080000	-0.8902480000
H	-4.8915930000	1.4204770000	-0.5981260000
H	-2.9231280000	0.7514670000	-1.9441030000
H	-5.0332240000	0.7847370000	1.8002760000
H	-1.2302610000	-1.1955150000	1.5117740000
H	-3.2018690000	-0.5279670000	2.8467280000
H	-0.8391870000	-0.2317760000	-2.1473840000
O	-0.6810030000	-2.1137600000	-1.2857300000
H	-1.5816180000	-2.4755440000	-1.2587600000

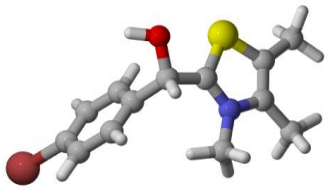
thermodynamic data

Zero-point correction= 0.266292 (Hartree/Particle)
Thermal correction to Energy= 0.282729
Thermal correction to Enthalpy= 0.283674
Thermal correction to Gibbs Free Energy= 0.221275
Sum of electronic and zero-point Energies= -1032.695545
Sum of electronic and thermal Energies= -1032.679108
Sum of electronic and thermal Enthalpies= -1032.678164
Sum of electronic and thermal Free Energies= -1032.740562

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	177.415	60.911	131.328

B3LYP/6-31G*	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0392000000	-0.5506330000	0.4538120000
N	-2.3885590000	0.7055140000	0.7338530000
C	-3.5154820000	1.1723790000	0.0317330000
C	-4.0204530000	0.2202980000	-0.8073280000
S	-3.0860630000	-1.2524330000	-0.6956760000
C	-5.1905660000	0.2975470000	-1.7422040000
C	-4.0130780000	2.5671750000	0.2554720000
C	-0.8973000000	-1.3473940000	1.0537800000
H	-4.2241140000	2.7591180000	1.3132520000
H	-4.9382620000	2.7278150000	-0.2991660000
H	-3.2908570000	3.3169440000	-0.0889560000
H	-5.8494810000	-0.5687680000	-1.6244410000
H	-4.8603680000	0.3278600000	-2.7868230000
H	-5.7837200000	1.1945220000	-1.5520780000
C	-1.6891460000	1.5440370000	1.7258150000
H	-0.7056080000	1.1254300000	1.9263580000
H	-2.2760300000	1.5895290000	2.6471290000
H	-1.5651110000	2.5482660000	1.3200810000
C	0.4777030000	-0.8367300000	0.6487530000
C	0.8257670000	-0.7036020000	-0.7041890000
C	2.1041040000	-0.2905050000	-1.0672730000
C	3.0451640000	-0.0096430000	-0.0718600000

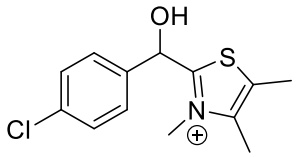
C	2.7206880000	-0.1468230000	1.2780390000
C	1.4372530000	-0.5628600000	1.6320410000
H	3.4626890000	0.0606940000	2.0410320000
H	1.1917790000	-0.6857070000	2.6848470000
Br	4.7858600000	0.5586180000	-0.5655330000
H	0.1024590000	-0.9320760000	-1.4825950000
H	2.3741780000	-0.1886110000	-2.1125490000
H	-0.9868740000	-1.2874060000	2.1505890000
O	-1.1515220000	-2.6731570000	0.6119660000
H	-0.3194210000	-3.1731300000	0.6355750000

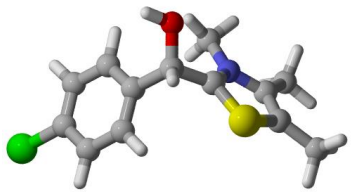
thermodynamic data

Zero-point correction= 0.256135 (Hartree/Particle)
Thermal correction to Energy= 0.273971
Thermal correction to Enthalpy= 0.274915
Thermal correction to Gibbs Free Energy= 0.207924
Sum of electronic and zero-point Energies= -3603.806197
Sum of electronic and thermal Energies= -3603.788361
Sum of electronic and thermal Enthalpies= -3603.787417
Sum of electronic and thermal Free Energies= -3603.854408

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.919	65.041	140.995

B3LYP/6-31G*	





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	1.3664160000	-0.3560080000	-0.7082590000
N	1.8202030000	-0.7714840000	0.4750690000
C	2.8943300000	-0.0235670000	0.9912050000
C	3.2675020000	0.9912160000	0.1559290000
S	2.2658130000	0.9806510000	-1.2733620000
C	4.3593060000	2.0075650000	0.3052600000
C	3.4959020000	-0.3867870000	2.3142330000
C	0.1724530000	-0.8806390000	-1.4944300000
H	2.7398610000	-0.4273260000	3.1054740000
H	4.2390700000	0.3564850000	2.6049700000
H	4.0020970000	-1.3585610000	2.2751940000

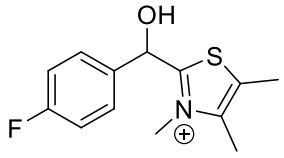
H	3.9773980000	3.0239620000	0.1638700000
H	5.1564510000	1.8421600000	-0.4282450000
H	4.8047760000	1.9546440000	1.3006420000
C	1.2449780000	-1.9108570000	1.2225230000
H	2.0562280000	-2.4592690000	1.6997180000
H	0.7330990000	-2.5611240000	0.5195520000
H	0.5531830000	-1.5344190000	1.9802480000
C	-1.1483900000	-0.4380260000	-0.8591750000
C	-1.5969790000	0.8763210000	-1.0468010000
C	-2.7946940000	1.3078050000	-0.4846540000
C	-3.5588730000	0.4111630000	0.2675270000
C	-3.1363840000	-0.9059270000	0.4514860000
C	-1.9298190000	-1.3243530000	-0.1096450000
H	-3.7474010000	-1.5971070000	1.0219120000
H	-1.6161080000	-2.3549750000	0.0212290000
Cl	-5.0632750000	0.9419860000	0.9721080000
H	-1.0175040000	1.5746640000	-1.6470140000
H	-3.1425320000	2.3237900000	-0.6360370000
H	0.2476700000	-0.4080720000	-2.4853420000
O	0.3329610000	-2.2825590000	-1.6048400000
H	-0.3832120000	-2.6256000000	-2.1661800000

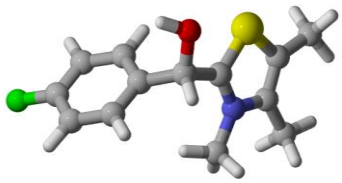
thermodynamic data

Zero-point correction= 0.257260 (Hartree/Particle)
Thermal correction to Energy= 0.274541
Thermal correction to Enthalpy= 0.275485
Thermal correction to Gibbs Free Energy= 0.210575
Sum of electronic and zero-point Energies= -1492.292511
Sum of electronic and thermal Energies= -1492.275230
Sum of electronic and thermal Enthalpies= -1492.274286
Sum of electronic and thermal Free Energies= -1492.339196

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	172.277	64.384	136.615

B3LYP/6-31G*		





xyz-matrix

32
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9741840000	-0.3962410000	-0.5693270000

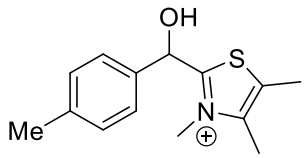
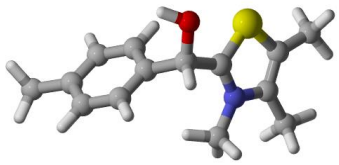
N	1.4326110000	0.8555780000	-0.5373580000
C	2.6724000000	1.0112760000	0.1112810000
C	3.1494530000	-0.1776660000	0.5848310000
S	2.0476190000	-1.4781140000	0.1965370000
C	4.4112690000	-0.4661820000	1.3419920000
C	3.3004250000	2.3673440000	0.2111100000
C	-0.3056980000	-0.8945220000	-1.2120470000
H	3.4145240000	2.8348630000	-0.7730250000
H	4.2937190000	2.2885390000	0.6545340000
H	2.7122180000	3.0433100000	0.8432000000
H	4.9843950000	-1.2684900000	0.8656440000
H	4.1927000000	-0.7756560000	2.3702370000
H	5.0504910000	0.4179430000	1.3881210000
C	0.7311550000	1.9936200000	-1.1609130000
H	-0.3189820000	1.7425450000	-1.2929260000
H	1.1902420000	2.2250380000	-2.1259090000
H	0.8033950000	2.8598930000	-0.5035610000
C	-1.5670400000	-0.4148540000	-0.5102320000
C	-1.7612530000	-0.6528970000	0.8603930000
C	-2.9432730000	-0.2673650000	1.4839020000
C	-3.9312160000	0.3564240000	0.7225960000
C	-3.7728430000	0.5978950000	-0.6384870000
C	-2.5840860000	0.2040570000	-1.2509780000
H	-4.5715520000	1.0740780000	-1.1966890000
H	-2.4566450000	0.3704400000	-2.3183910000
F	-5.0667130000	0.7307140000	1.3205900000
H	-0.9916000000	-1.1510730000	1.4439370000
H	-3.1145640000	-0.4435870000	2.5403890000
H	-0.3208770000	-0.5294670000	-2.2518810000
O	-0.1573950000	-2.3072080000	-1.1900600000
H	-1.0389270000	-2.7116970000	-1.2363320000

thermodynamic data

Zero-point correction= 0.258230 (Hartree/Particle)
Thermal correction to Energy= 0.275378
Thermal correction to Enthalpy= 0.276322
Thermal correction to Gibbs Free Energy= 0.212218
Sum of electronic and zero-point Energies= -1131.934019
Sum of electronic and thermal Energies= -1131.916871
Sum of electronic and thermal Enthalpies= -1131.915927
Sum of electronic and thermal Free Energies= -1131.980031

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	172.802	63.753	134.920

B3LYP/6-31G*	

xyz-matrix

35
XYZ file generated by gabedit : coordinates in Angstrom

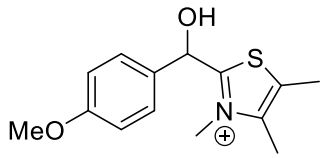
C	1.0066550000	-0.4111900000	-0.5593460000
N	1.4547290000	0.8445320000	-0.5544430000
C	2.6851700000	1.0272330000	0.1052830000
C	3.1651440000	-0.1446840000	0.6160100000
S	2.0782140000	-1.4642780000	0.2481010000
C	4.4199530000	-0.4033150000	1.3952410000
C	3.3011560000	2.3906060000	0.1761660000
C	-0.2607860000	-0.9365840000	-1.2036480000
H	3.4222820000	2.8327250000	-0.8188060000
H	4.2900790000	2.3319120000	0.6323040000
H	2.7003630000	3.0781990000	0.7833590000
H	5.0151980000	-1.1989170000	0.9348330000
H	4.1910570000	-0.7083150000	2.4225420000
H	5.0421060000	0.4927760000	1.4441790000
C	0.7488950000	1.9588830000	-1.2145580000
H	-0.2989630000	1.6960720000	-1.3435170000
H	1.2111520000	2.1652820000	-2.1837740000
H	0.8119270000	2.8444560000	-0.5825120000
C	-1.5324750000	-0.4466590000	-0.5296760000
C	-1.7432760000	-0.6421050000	0.8441840000
C	-2.9389800000	-0.2426800000	1.4321290000
C	-3.9592760000	0.3581430000	0.6754160000
C	-3.7392070000	0.5462610000	-0.6951030000
C	-2.5446240000	0.1461660000	-1.2943050000
H	-3.0876000000	-0.4000450000	2.4973100000
H	-0.2657100000	-0.6004390000	-2.2531500000
H	-0.9766220000	-1.1129660000	1.4547740000
H	-2.4072770000	0.2867760000	-2.3647110000
H	-4.5139680000	1.0037050000	-1.3043970000
C	-5.2620930000	0.7615540000	1.3201320000
H	-5.7996940000	1.4972300000	0.7151550000
H	-5.1010840000	1.1876110000	2.3157850000
H	-5.9199360000	-0.1083360000	1.4428680000
O	-0.1047730000	-2.3484960000	-1.1458340000
H	-0.9871780000	-2.7528160000	-1.1216500000

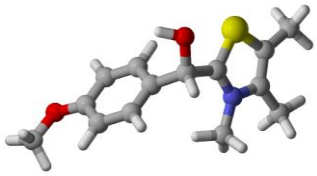
thermodynamic data

Zero-point correction= 0.294015 (Hartree/Particle)
Thermal correction to Energy= 0.312217
Thermal correction to Enthalpy= 0.313162
Thermal correction to Gibbs Free Energy= 0.246451
Sum of electronic and zero-point Energies= -1071.987886
Sum of electronic and thermal Energies= -1071.969684
Sum of electronic and thermal Enthalpies= -1071.968740
Sum of electronic and thermal Free Energies= -1072.035451

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	195.919	66.874	140.404

B3LYP/6-31G*	





xyz-matrix

36
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3830540000	-0.4431490000	0.5405400000
N	-1.7688560000	0.8317220000	0.6018250000
C	-2.9776450000	1.1131990000	-0.0626900000
C	-3.5069430000	-0.0024400000	-0.6454980000
S	-2.4924060000	-1.3939340000	-0.3393660000
C	-4.7600140000	-0.1521180000	-1.4554750000
C	-3.5231420000	2.5081230000	-0.0652590000
C	-0.1509010000	-1.0663640000	1.1662180000
H	-3.6436290000	2.8986320000	0.9512440000
H	-4.5032690000	2.5259330000	-0.5432440000
H	-2.8756110000	3.1975460000	-0.6200900000
H	-5.3890520000	-0.9596190000	-1.0664350000
H	-4.5292370000	-0.3821340000	-2.5017960000
H	-5.3493640000	0.7670130000	-1.4377900000
C	-1.0176330000	1.8682600000	1.3340290000
H	0.0120420000	1.5408610000	1.4631370000
H	-1.4856030000	2.0449730000	2.3063890000
H	-1.0219440000	2.7899380000	0.7523650000
C	1.1490290000	-0.6007800000	0.5384460000
C	1.3560570000	-0.6778100000	-0.8526440000
C	2.5720040000	-0.3167220000	-1.4059770000
C	3.6247340000	0.1303610000	-0.5821900000
C	3.4316610000	0.2067630000	0.8054090000

C	2.2006750000	-0.1608230000	1.3499710000
H	2.7445040000	-0.3744050000	-2.4756360000
H	-0.1448840000	-0.7922180000	2.2335320000
O	4.7651790000	0.4545890000	-1.2223600000
C	5.8909180000	0.8937340000	-0.4604030000
H	6.6809770000	1.0812480000	-1.1874110000
H	5.6651570000	1.8194660000	0.0819620000
H	6.2171170000	0.1197500000	0.2440400000
H	0.5622350000	-1.0316950000	-1.5058430000
H	2.0691410000	-0.1136980000	2.4292240000
H	4.2271390000	0.5371290000	1.4624070000
O	-0.3770390000	-2.4652530000	1.0295030000
H	0.4851780000	-2.9039210000	0.9470190000

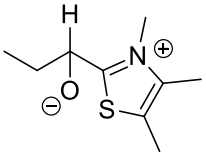
thermodynamic data

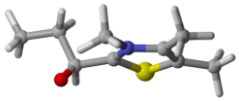
Zero-point correction= 0.299188 (Hartree/Particle)
Thermal correction to Energy= 0.318161
Thermal correction to Enthalpy= 0.319105
Thermal correction to Gibbs Free Energy= 0.250952
Sum of electronic and zero-point Energies= -1147.189170
Sum of electronic and thermal Energies= -1147.170197
Sum of electronic and thermal Enthalpies= -1147.169253
Sum of electronic and thermal Free Energies= -1147.237406

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	199.649	70.056	143.439

Computerchemie aliphatische Aldehyde (Acetaldehyd und Propionaldehyd):

B3LYP/6-31G*	**Aliphatisch2**





xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

C	1.8670200000	-0.3545670000	-0.4697270000

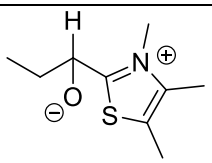
H	1.9763790000	-1.4175060000	-0.8304670000
O	2.1581690000	0.5722660000	-1.3664600000
C	2.6710260000	-0.2993780000	0.8710900000
C	0.3369020000	-0.2803990000	-0.1349740000
N	-0.3785850000	0.8419060000	0.0047220000
C	-1.7703290000	0.6730270000	0.1200680000
C	-2.1441510000	-0.6337210000	0.0565820000
S	-0.7214900000	-1.6432000000	-0.1529080000
C	0.2813280000	2.1622720000	-0.0024650000
H	0.4518670000	2.4971340000	1.0246670000
H	-0.3583730000	2.8771030000	-0.5220880000
H	1.2292270000	1.9961750000	-0.5454270000
C	-2.6524700000	1.8731810000	0.2850010000
H	-3.6826110000	1.5649570000	0.4725120000
H	-2.6527550000	2.5040840000	-0.6120690000
H	-2.3299980000	2.4956980000	1.1271680000
C	-3.5119820000	-1.2432570000	0.1148550000
H	-3.7575810000	-1.7606610000	-0.8202290000
H	-4.2758940000	-0.4794140000	0.2815790000
H	-3.5897640000	-1.9752630000	0.9271880000
C	4.1684960000	-0.3710960000	0.5701510000
H	4.7713350000	-0.2237750000	1.4739510000
H	4.4232190000	0.3995450000	-0.1628590000
H	4.4359990000	-1.3450380000	0.1402800000
H	2.3655190000	-1.1163630000	1.5431290000
H	2.4469860000	0.6466770000	1.3843320000

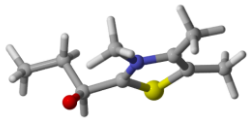
thermodynamic data

Zero-point correction= 0.227961 (Hartree/Particle)
Thermal correction to Energy= 0.241852
Thermal correction to Enthalpy= 0.242796
Thermal correction to Gibbs Free Energy= 0.187477
Sum of electronic and zero-point Energies= -879.861647
Sum of electronic and thermal Energies= -879.847756
Sum of electronic and thermal Enthalpies= -879.846812
Sum of electronic and thermal Free Energies= -879.902131

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	151.764	50.620	116.428

M062X/6-31++G**	**Aliphatisch2**





xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

C	1.8696490000	-0.2878930000	-0.5238390000
H	2.0048840000	-1.3107020000	-0.9700670000
O	2.2592730000	0.7161360000	-1.2908070000
C	2.5450960000	-0.3563790000	0.8796210000
C	0.3364020000	-0.2428370000	-0.2569360000
N	-0.3809670000	0.8540140000	-0.0569310000
C	-1.7576050000	0.6527400000	0.1252760000
C	-2.0979730000	-0.6586210000	0.0539220000
S	-0.6774970000	-1.6184550000	-0.2543640000
C	0.2370420000	2.1920520000	-0.0001760000
H	-0.3873670000	2.8863510000	-0.5633120000
H	1.2281170000	2.0815150000	-0.4658360000

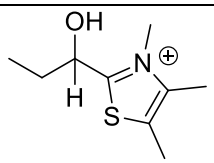
H	0.3016650000	2.5086590000	1.0437660000
C	-2.6479280000	1.8317730000	0.3537500000
H	-3.6598390000	1.5008120000	0.5854400000
H	-2.6946360000	2.4707340000	-0.5334030000
H	-2.2898840000	2.4395970000	1.1895950000
C	-3.4444430000	-1.3011260000	0.1765220000
H	-3.6997860000	-1.8511230000	-0.7334790000
H	-4.2175900000	-0.5492440000	0.3410470000
H	-3.4702000000	-2.0025640000	1.0150970000
C	4.0543130000	-0.4711710000	0.7020030000
H	4.5766070000	-0.4361360000	1.6627610000
H	4.4030550000	0.3474710000	0.0683490000
H	4.3114710000	-1.4143380000	0.2068190000
H	2.1537180000	-1.2025790000	1.4637290000
H	2.3050140000	0.5684130000	1.4234410000

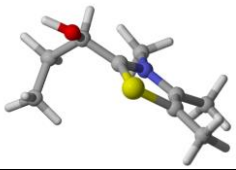
thermodynamic data

Zero-point correction= 0.228687 (Hartree/Particle)
Thermal correction to Energy= 0.242546
Thermal correction to Enthalpy= 0.243490
Thermal correction to Gibbs Free Energy= 0.188148
Sum of electronic and zero-point Energies= -879.634519
Sum of electronic and thermal Energies= -879.620660
Sum of electronic and thermal Enthalpies= -879.619716
Sum of electronic and thermal Free Energies= -879.675058

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	152.200	50.445	116.477

B3LYP/6-31G*	**aliphatischpr**





xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.9130240000	0.1865760000	0.7128970000
H	-2.0212640000	0.9072170000	1.5405490000
O	-2.3025170000	-1.1073330000	1.1349420000
C	-2.7376530000	0.6963030000	-0.4956970000
C	-0.4405220000	0.0350560000	0.4127010000
S	0.2641170000	-1.5053190000	0.2189610000
C	1.8277460000	-0.7977670000	-0.1113550000
C	1.7596130000	0.5647420000	-0.0494900000
C	2.8616910000	1.5585540000	-0.2534290000
H	2.6039090000	2.3007650000	-1.0169110000
H	3.7682890000	1.0497890000	-0.5831370000
H	3.1052250000	2.0930640000	0.6725800000
C	3.0072340000	-1.6821990000	-0.3855890000
H	3.8787840000	-1.0916910000	-0.6752030000
H	2.7950360000	-2.3859120000	-1.1972280000
H	3.2773020000	-2.2654800000	0.5018870000
N	0.4586180000	1.0087840000	0.2575100000
C	0.1468030000	2.4442380000	0.3923240000
H	0.9244830000	2.9229530000	0.9879290000
H	-0.8088140000	2.5665190000	0.8975720000
H	0.1020180000	2.9101090000	-0.5952460000

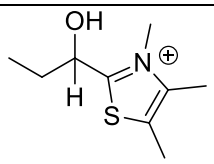
C	-2.6965140000	-0.2046750000	-1.7326610000
H	-2.4137920000	1.7132330000	-0.7488420000
H	-3.7709970000	0.7983160000	-0.1367990000
H	-1.6974590000	-0.2415530000	-2.1812100000
H	-3.3838120000	0.1758900000	-2.4935460000
H	-2.9967500000	-1.2287750000	-1.4920560000
H	-3.2704800000	-1.1471320000	1.1959610000

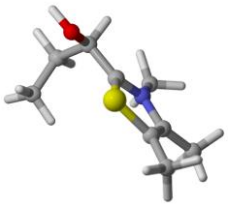
thermodynamic data

Zero-point correction= 0.242282 (Hartree/Particle)
Thermal correction to Energy= 0.256778
Thermal correction to Enthalpy= 0.257722
Thermal correction to Gibbs Free Energy= 0.201068
Sum of electronic and zero-point Energies= -880.294106
Sum of electronic and thermal Energies= -880.279610
Sum of electronic and thermal Enthalpies= -880.278666
Sum of electronic and thermal Free Energies= -880.335320

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.130	52.310	119.238

M062X /6-31++G**	**aliphatischpr**





xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.9408300000	0.0951370000	0.7145360000
H	-2.0831480000	0.7294820000	1.6032660000
O	-2.3330220000	-1.2301730000	0.9849550000

C	-2.6934820000	0.6963770000	-0.4858970000
C	-0.4620520000	-0.0226300000	0.4471910000
S	0.2819690000	-1.5245560000	0.2069190000
C	1.8064220000	-0.7683820000	-0.1103870000
C	1.7005710000	0.5853890000	-0.0129920000
C	2.7828700000	1.5996590000	-0.1912180000
H	2.5021140000	2.3663190000	-0.9189760000
H	3.6845920000	1.1058050000	-0.5540490000
H	3.0329390000	2.0910470000	0.7543900000
C	3.0327760000	-1.5783880000	-0.4088930000
H	3.5715390000	-1.1559350000	-1.2602580000
H	2.7743900000	-2.6089060000	-0.6579600000
H	3.7036670000	-1.5968550000	0.4543570000
N	0.3974860000	0.9794920000	0.3094300000
C	0.0381650000	2.3961360000	0.4675400000
H	0.8408250000	2.9038640000	1.0005000000
H	-0.8786130000	2.4762650000	1.0480760000
H	-0.1015070000	2.8526190000	-0.5147340000
C	-2.4412660000	-0.0444690000	-1.7962310000
H	-2.4366110000	1.7567110000	-0.5849370000
H	-3.7592160000	0.6705180000	-0.2290830000
H	-1.4100800000	0.0876910000	-2.1420520000
H	-3.1008430000	0.3352290000	-2.5785680000
H	-2.6290480000	-1.1157680000	-1.6856730000
H	-3.2797800000	-1.2732320000	1.1674600000

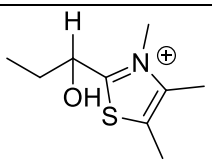
thermodynamic data

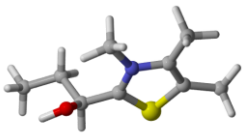
Zero-point correction= 0.243394 (Hartree/Particle)
Thermal correction to Energy= 0.257649

Thermal correction to Enthalpy= 0.258593
Thermal correction to Gibbs Free Energy= 0.202709
Sum of electronic and zero-point Energies= -880.065902
Sum of electronic and thermal Energies= -880.051647
Sum of electronic and thermal Enthalpies= -880.050703
Sum of electronic and thermal Free Energies= -880.106586

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.677	52.024	117.617

B3LYP/6-31G*	**Aliphatisch2pr**





xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

C	1.8041610000	-0.3875090000	-0.4163020000
H	1.9797880000	-1.4054600000	-0.7970240000
O	2.2035170000	0.5710080000	-1.3843170000
C	2.5428580000	-0.2504070000	0.9348590000
C	0.3030690000	-0.2538810000	-0.2538150000
N	-0.4012190000	0.8612540000	-0.0546430000
C	-1.7828740000	0.6633590000	0.1246880000
C	-2.1289840000	-0.6567760000	0.0613940000
S	-0.7096910000	-1.6280800000	-0.2395020000
C	0.1846690000	2.2200680000	-0.0094780000
H	0.1339350000	2.5981490000	1.0144180000
H	-0.3902620000	2.8703230000	-0.6701680000
H	1.2110230000	2.1707050000	-0.3603010000
C	-2.6853760000	1.8383560000	0.3437950000

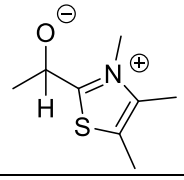
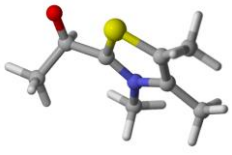
H	-3.7040880000	1.4994370000	0.5347850000
H	-2.7161090000	2.4931880000	-0.5348560000
H	-2.3689110000	2.4390740000	1.2033690000
C	-3.4745720000	-1.3056690000	0.1854280000
H	-3.7912670000	-1.7433830000	-0.7679170000
H	-4.2302250000	-0.5775260000	0.4868170000
H	-3.4625590000	-2.1039150000	0.9348000000
C	4.0563030000	-0.4456140000	0.7879060000
H	4.5377690000	-0.4011630000	1.7688720000
H	4.5126300000	0.3393260000	0.1739890000
H	4.2969470000	-1.4195470000	0.3456920000
H	2.1381640000	-1.0000560000	1.6260220000
H	2.3309920000	0.7345550000	1.3674020000
H	3.1420990000	0.4271570000	-1.5876830000

thermodynamic data

Zero-point correction= 0.242562 (Hartree/Particle)
Thermal correction to Energy= 0.256979
Thermal correction to Enthalpy= 0.257923
Thermal correction to Gibbs Free Energy= 0.201435
Sum of electronic and zero-point Energies= -880.294049
Sum of electronic and thermal Energies= -880.279632
Sum of electronic and thermal Enthalpies= -880.278687
Sum of electronic and thermal Free Energies= -880.335175

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.256	52.241	118.888

B3LYP/6-31G*	**Acetaldehydhaus**

xyz-matrix

24

XYZ file generated by gabedit : coordinates in Angstrom

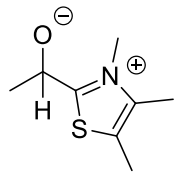
C	-2.2529980000	-0.0586670000	0.3266180000
H	-2.5130950000	0.5418870000	1.2466110000
O	-2.4792350000	-1.3677190000	0.3972140000
C	-2.9599220000	0.6450730000	-0.8695600000
C	-0.7268400000	0.0691340000	0.1870380000
S	-0.0704210000	-1.4980500000	0.0690270000
C	1.5547270000	-0.7900810000	-0.0832850000
C	1.5175590000	0.5703270000	-0.0094000000
C	2.6451050000	1.5578930000	-0.0689490000
H	2.5088910000	2.2899930000	-0.8746110000
H	3.5875910000	1.0391850000	-0.2535900000
H	2.7567450000	2.1156560000	0.8698810000
C	2.7530140000	-1.6762260000	-0.2468970000
H	3.6820020000	-1.1012550000	-0.2998660000
H	2.6798390000	-2.2760250000	-1.1620520000
H	2.8431750000	-2.3765170000	0.5921790000
N	0.1949300000	1.0364940000	0.1537820000
C	-0.1547210000	2.4529770000	0.2762550000
H	0.5239150000	2.9419860000	0.9784730000
H	-1.1739830000	2.5277540000	0.6541110000
H	-0.0912490000	2.9522730000	-0.6952370000
H	-2.7829010000	1.7293980000	-0.9281750000
H	-4.0335290000	0.4732370000	-0.7494700000
H	-2.6468240000	0.1749270000	-1.8077870000

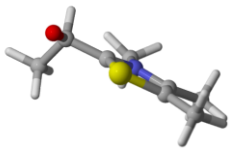
thermodynamic data

Zero-point correction= 0.198944 (Hartree/Particle)
Thermal correction to Energy= 0.211840
Thermal correction to Enthalpy= 0.212784
Thermal correction to Gibbs Free Energy= 0.159920
Sum of electronic and zero-point Energies= -840.572901
Sum of electronic and thermal Energies= -840.560005
Sum of electronic and thermal Enthalpies= -840.559061
Sum of electronic and thermal Free Energies= -840.611925

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	132.932	46.210	111.262

M062X /6-31++G**	**acetaldehydhaus**





xyz-matrix

24

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.2620090000	-0.0594970000	0.3189770000
H	-2.5114770000	0.6016300000	1.1956380000
O	-2.5688020000	-1.3407030000	0.4512400000
C	-2.8642210000	0.6132830000	-0.9431260000
C	-0.7287700000	0.0143870000	0.1992880000
S	-0.0045530000	-1.5115020000	0.0630710000
C	1.5733960000	-0.7685140000	-0.0829870000
C	1.4913830000	0.5852640000	-0.0003020000
C	2.5803540000	1.6098530000	-0.0521740000
H	2.3805030000	2.3678200000	-0.8159660000
H	3.5290690000	1.1332000000	-0.2978880000
H	2.7017750000	2.1192070000	0.9096300000

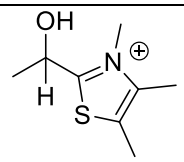
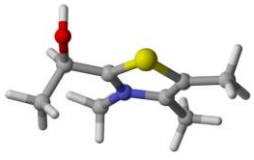
C	2.7971680000	-1.6148750000	-0.2548000000
H	3.7027500000	-1.0058350000	-0.2598470000
H	2.7576390000	-2.1721020000	-1.1951830000
H	2.8854630000	-2.3397390000	0.5593470000
N	0.1607200000	1.0009270000	0.1673390000
C	-0.2298650000	2.4038840000	0.2940740000
H	0.4612770000	2.9126440000	0.9671590000
H	-1.2357620000	2.4444430000	0.7101080000
H	-0.2183510000	2.8896850000	-0.6846040000
H	-2.5946240000	1.6705040000	-1.0712850000
H	-3.9500620000	0.5337040000	-0.8554230000
H	-2.5545950000	0.0452950000	-1.8258250000

thermodynamic data

Zero-point correction= 0.199785 (Hartree/Particle)
Thermal correction to Energy= 0.212582
Thermal correction to Enthalpy= 0.213527
Thermal correction to Gibbs Free Energy= 0.160936
Sum of electronic and zero-point Energies= -840.363442
Sum of electronic and thermal Energies= -840.350645
Sum of electronic and thermal Enthalpies= -840.349701
Sum of electronic and thermal Free Energies= -840.402291

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	133.397	45.991	110.686

B3LYP/6-31G*	**acetaldehydhauspr**

xyz-matrix

25

XYZ file generated by gabedit : coordinates in Angstrom

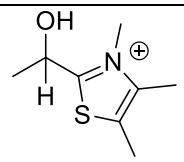
C	-2.2186740000	0.1022690000	0.2586050000
H	-2.4886260000	0.7970380000	1.0668390000
O	-2.7252000000	-1.1952420000	0.5076210000
C	-2.8252610000	0.5840750000	-1.0651920000
C	-0.7023520000	0.0036750000	0.1784140000
S	0.0466110000	-1.5202830000	0.0128580000
C	1.6297100000	-0.7815870000	-0.0846130000
C	1.5306190000	0.5767420000	0.0170850000
C	2.6306000000	1.5930220000	-0.0074070000
H	2.4768300000	2.3394400000	-0.7947390000
H	3.5870210000	1.1057980000	-0.2000690000
H	2.7183580000	2.1213430000	0.9493170000
C	2.8479580000	-1.6407020000	-0.2453070000
H	3.7494310000	-1.0292940000	-0.3201790000
H	2.7826730000	-2.2542510000	-1.1502560000
H	2.9711630000	-2.3154640000	0.6089720000
N	0.1925820000	0.9923770000	0.1688320000
C	-0.1612040000	2.4185260000	0.2978770000
H	0.4641880000	2.8750600000	1.0662370000
H	-1.2057220000	2.5145980000	0.5862720000
H	0.0000340000	2.9264890000	-0.6560570000
H	-2.4484570000	1.5687430000	-1.3575050000
H	-3.9103490000	0.6419230000	-0.9488090000
H	-2.5989970000	-0.1330810000	-1.8592700000
H	-2.7781730000	-1.3546310000	1.4639620000

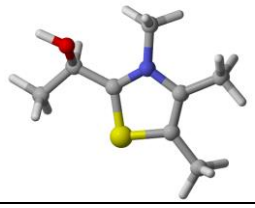
thermodynamic data

Zero-point correction= 0.213513 (Hartree/Particle)
Thermal correction to Energy= 0.226715
Thermal correction to Enthalpy= 0.227660
Thermal correction to Gibbs Free Energy= 0.173867
Sum of electronic and zero-point Energies= -841.008412
Sum of electronic and thermal Energies= -840.995209
Sum of electronic and thermal Enthalpies= -840.994265
Sum of electronic and thermal Free Energies= -841.048058

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	142.266	47.504	113.217

M062X /6-31++G**	**acetaldehydhauspr**





xyz-matrix

25

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.1993580000	0.0481040000	-0.2635480000
H	-2.4275950000	0.5310810000	-1.2283540000
O	-2.5304590000	0.9042730000	0.8120370000
C	-2.9138980000	-1.2937330000	-0.1959250000
C	-0.6966900000	-0.0902770000	-0.1831490000
S	0.1338460000	-1.5596340000	-0.0370350000
C	1.6595070000	-0.7545960000	0.0522370000
C	1.4852190000	0.5950790000	-0.0236050000
C	2.5497500000	1.6416560000	0.0290820000
H	2.6620840000	2.1505760000	-0.9332770000
H	3.5041930000	1.1741010000	0.2728010000

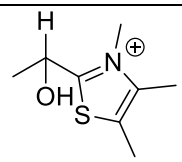
H	2.3359730000	2.3904950000	0.7967810000
C	2.9457800000	-1.5121980000	0.1949910000
H	3.6276210000	-1.2663180000	-0.6229140000
H	2.7750990000	-2.5895890000	0.1766110000
H	3.4322370000	-1.2659920000	1.1427710000
N	0.1410640000	0.9394480000	-0.1656010000
C	-0.2932410000	2.3444890000	-0.2549540000
H	-0.3910820000	2.7542160000	0.7512300000
H	-1.2582000000	2.3934300000	-0.7528490000
H	0.4483350000	2.8976840000	-0.8283300000
H	-2.6255180000	-1.9419020000	-1.0282250000
H	-3.9921250000	-1.1318070000	-0.2705060000
H	-2.7078670000	-1.7946280000	0.7539580000
H	-3.4908850000	0.9713340000	0.8950190000

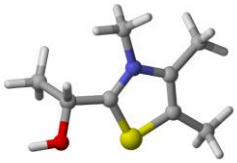
thermodynamic data

Zero-point correction= 0.214455 (Hartree/Particle)
Thermal correction to Energy= 0.226624
Thermal correction to Enthalpy= 0.227568
Thermal correction to Gibbs Free Energy= 0.176890
Sum of electronic and zero-point Energies= -840.797705
Sum of electronic and thermal Energies= -840.785537
Sum of electronic and thermal Enthalpies= -840.784593
Sum of electronic and thermal Free Energies= -840.835271

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	142.209	45.233	106.661

B3LYP /6-31G*	**Acetaldehyd2pr**





xyz-matrix

25

XYZ file generated by gabedit : coordinates in Angstrom

C	2.2058910000	0.1033660000	-0.2682950000
H	2.4538880000	0.8175640000	-1.0700990000
O	2.6143820000	-1.2027540000	-0.6287040000
C	2.8385260000	0.5695480000	1.0529970000
C	0.7017630000	-0.0048870000	-0.1697270000
S	-0.0547970000	-1.5245730000	-0.0141900000
C	-1.6315630000	-0.7764950000	0.0886450000
C	-1.5255260000	0.5814700000	-0.0117580000
N	-0.1860320000	0.9903370000	-0.1628160000
C	0.1736830000	2.4147860000	-0.2925580000
C	-2.8556420000	-1.6291040000	0.2402870000
H	3.9262420000	0.6240430000	0.9326710000
H	2.6083450000	-0.1383980000	1.8544990000
H	2.4925030000	1.5644950000	1.3496240000
H	0.0570860000	2.9158370000	0.6716820000
H	-0.4803840000	2.8823110000	-1.0293070000
H	1.2044530000	2.5056920000	-0.6281980000
H	-3.0012770000	-2.2693490000	-0.6368680000
H	-3.7491250000	-1.0122010000	0.3553180000
H	-2.7805100000	-2.2774110000	1.1197060000
C	-2.6212940000	1.6023770000	0.0113560000

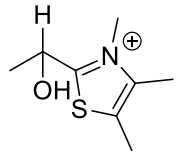
H	-2.7181870000	2.1174970000	-0.9517570000
H	-2.4567610000	2.3590270000	0.7865460000
H	-3.5771430000	1.1208720000	0.2206850000
H	3.5697660000	-1.2935080000	-0.4837900000

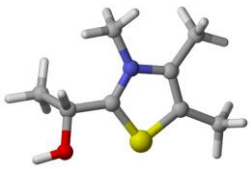
thermodynamic data

Zero-point correction= 0.213378 (Hartree/Particle)
Thermal correction to Energy= 0.226660
Thermal correction to Enthalpy= 0.227604
Thermal correction to Gibbs Free Energy= 0.173612
Sum of electronic and zero-point Energies= -841.009023
Sum of electronic and thermal Energies= -840.995741
Sum of electronic and thermal Enthalpies= -840.994797
Sum of electronic and thermal Free Energies= -841.048789

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	142.231	47.586	113.636

M062X /6-31++G**	**Acetaldehyd2pr**





xyz-matrix

25

XYZ file generated by gabedit : coordinates in Angstrom

C	2.2020720000	0.0851170000	-0.2737170000
H	2.4517760000	0.7605630000	-1.1058920000
O	2.6204040000	-1.2271380000	-0.5626520000
C	2.7921870000	0.6070850000	1.0376100000
C	0.7010190000	-0.0279150000	-0.1857300000
S	-0.0674340000	-1.5278010000	-0.0214410000

C	-1.6195620000	-0.7696220000	0.0895890000
C	-1.5019100000	0.5827100000	-0.0137240000
N	-0.1684660000	0.9748240000	-0.1719100000
C	0.2026260000	2.3915930000	-0.2967190000
C	-2.8751590000	-1.5748880000	0.2444600000
H	3.8793930000	0.6792890000	0.9447170000
H	2.5519410000	-0.0821620000	1.8510110000
H	2.4153140000	1.6015700000	1.2900830000
H	0.1218010000	2.8776700000	0.6777870000
H	-0.4726070000	2.8698100000	-1.0056950000
H	1.2223100000	2.4729500000	-0.6664250000
H	-3.4623320000	-1.5571340000	-0.6776950000
H	-3.4878040000	-1.1747210000	1.0559850000
H	-2.6498810000	-2.6159910000	0.4808190000
C	-2.5978730000	1.5973080000	0.0081260000
H	-2.7193140000	2.0784310000	-0.9674980000
H	-2.4171550000	2.3725090000	0.7581480000
H	-3.5398540000	1.1060830000	0.2533630000
H	3.5809950000	-1.2990340000	-0.5004410000

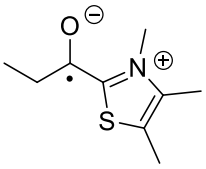
thermodynamic data

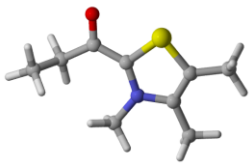
Zero-point correction= 0.214424 (Hartree/Particle)
Thermal correction to Energy= 0.227523
Thermal correction to Enthalpy= 0.228467
Thermal correction to Gibbs Free Energy= 0.175307
Sum of electronic and zero-point Energies= -840.797468
Sum of electronic and thermal Energies= -840.784369
Sum of electronic and thermal Enthalpies= -840.783425
Sum of electronic and thermal Free Energies= -840.836585

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	142.773	47.395	111.885

Radikale

B3LYP/6-31G*	**aliphatischradde**





xyz-matrix

26

XYZ file generated by gabedit : coordinates in Angstrom

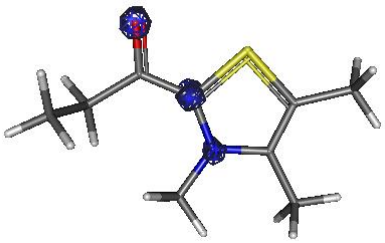
C	-1.7821360000	-0.6428220000	0.2545060000
O	-2.0647660000	-1.8601490000	0.1477450000
C	-2.9256670000	0.3337100000	0.5216140000
C	-0.4050850000	-0.2823450000	0.1200730000
S	0.7202480000	-1.6227630000	-0.0413540000
C	2.0873240000	-0.5056050000	-0.0679440000
C	1.6767120000	0.7865380000	0.0123610000
C	2.5517050000	2.0061190000	0.0149830000
H	2.4064980000	2.6243640000	-0.8804960000
H	3.6028010000	1.7140390000	0.0379280000
H	2.3667380000	2.6401170000	0.8906790000
C	3.4752340000	-1.0588180000	-0.1748160000
H	4.2285930000	-0.2665080000	-0.1737220000
H	3.6021910000	-1.6354350000	-1.1001040000
H	3.7008630000	-1.7342760000	0.6601440000
N	0.2817460000	0.9260030000	0.0968930000
C	-0.3852190000	2.2204700000	0.0667700000
H	-0.7502710000	2.5133970000	1.0583050000

H	-1.2294170000	2.1893940000	-0.6264850000
H	0.3115880000	2.9814140000	-0.2822900000
C	-3.7987380000	0.5443220000	-0.7266620000
H	-2.5889230000	1.2929700000	0.9233790000
H	-3.5339490000	-0.1396020000	1.3011130000
H	-3.2479860000	1.0575930000	-1.5251770000
H	-4.6870380000	1.1415100000	-0.4912940000
H	-4.1245330000	-0.4250140000	-1.1158390000

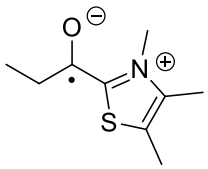
thermodynamic data

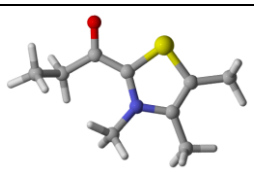
Zero-point correction= 0.217557 (Hartree/Particle)
Thermal correction to Energy= 0.231530
Thermal correction to Enthalpy= 0.232474
Thermal correction to Gibbs Free Energy= 0.175490
Sum of electronic and zero-point Energies= -879.300432
Sum of electronic and thermal Energies= -879.286460
Sum of electronic and thermal Enthalpies= -879.285516
Sum of electronic and thermal Free Energies= -879.342500

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	145.287	50.126	119.932



M062X /6-31++G**	**aliphatischradde**





xyz-matrix

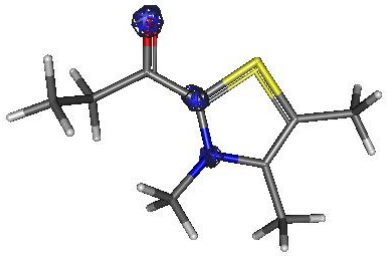
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.7657280000	-0.6748500000	0.2122590000
O	-2.0795910000	-1.8704520000	0.0385320000
C	-2.8569080000	0.3073630000	0.6077770000
C	-0.3905440000	-0.3195920000	0.0692140000
S	0.7593960000	-1.6218150000	-0.0819840000
C	2.0921270000	-0.4828730000	-0.0387200000
C	1.6525460000	0.7949420000	0.0394430000
C	2.4840660000	2.0397870000	0.0880400000
H	2.4369300000	2.6006040000	-0.8515900000
H	3.5282940000	1.7857440000	0.2683420000
H	2.1563820000	2.7015700000	0.8956820000
C	3.4950970000	-0.9993670000	-0.0960850000
H	4.2201120000	-0.1839780000	-0.0701890000
H	3.6622010000	-1.5661210000	-1.0178280000
H	3.7040570000	-1.6663040000	0.7463520000
N	0.2580890000	0.9005230000	0.0710150000
C	-0.4273090000	2.1695960000	-0.1215140000
H	0.2289620000	2.8586570000	-0.6533880000
H	-0.7207290000	2.6245480000	0.8299970000
H	-1.3171500000	2.0071010000	-0.7317090000
C	-3.8141400000	0.5786950000	-0.5571510000
H	-2.4595520000	1.2370720000	1.0210730000
H	-3.4077550000	-0.1900390000	1.4127650000
H	-3.3121380000	1.0997760000	-1.3800650000
H	-4.6634580000	1.1883500000	-0.2367690000
H	-4.1916360000	-0.3701940000	-0.9458710000

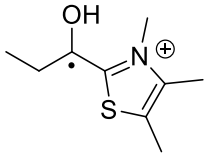
thermodynamic data

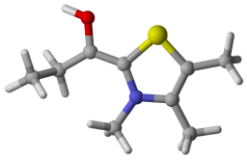
Zero-point correction=	0.218116 (Hartree/Particle)
Thermal correction to Energy=	0.232082
Thermal correction to Enthalpy=	0.233026
Thermal correction to Gibbs Free Energy=	0.176469
Sum of electronic and zero-point Energies=	-879.070449
Sum of electronic and thermal Energies=	-879.056484
Sum of electronic and thermal Enthalpies=	-879.055539
Sum of electronic and thermal Free Energies=	-879.112096

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	145.633	50.077	119.033



M062X /6-31++G**	**aliphatischradpr**





xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.7280010000	-0.5584170000	0.2287130000
O	-2.0141870000	-1.8554690000	0.0409930000
C	-2.8632470000	0.3594310000	0.5588470000
C	-0.3668910000	-0.2910330000	0.0912880000
S	0.7566700000	-1.6058310000	-0.0453600000
C	2.0933580000	-0.5116640000	-0.0637160000
C	1.6735300000	0.7865770000	0.0138950000

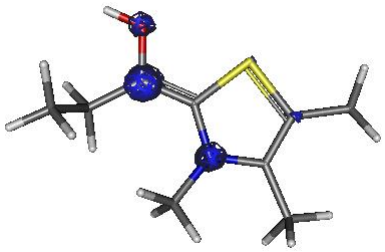
C	2.5518190000	1.9964090000	0.0355490000
H	2.4829250000	2.5640680000	-0.8980610000
H	3.5896870000	1.6897690000	0.1638090000
H	2.2954590000	2.6588310000	0.8668190000
C	3.4998570000	-1.0222900000	-0.1382510000
H	4.1129180000	-0.3770890000	-0.7705360000
H	3.5282260000	-2.0268950000	-0.5643880000
H	3.9511550000	-1.0664050000	0.8578110000
N	0.2937330000	0.9073230000	0.0729150000
C	-0.3731830000	2.2101160000	0.0219310000
H	0.2978510000	2.9279020000	-0.4448280000
H	-0.6268810000	2.5572290000	1.0266620000
H	-1.2702220000	2.1328400000	-0.5914590000
C	-3.7505830000	0.6675580000	-0.6604270000
H	-2.5013440000	1.2767980000	1.0211940000
H	-3.4611860000	-0.1436640000	1.3308060000
H	-3.1947900000	1.2026200000	-1.4350620000
H	-4.5982720000	1.2840140000	-0.3561450000
H	-4.1432330000	-0.2481970000	-1.1100900000
H	-2.9316040000	-2.0661550000	0.2639180000

thermodynamic data

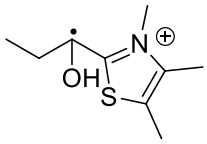
Zero-point correction= 0.230995 (Hartree/Particle)
Thermal correction to Energy= 0.245110
Thermal correction to Enthalpy= 0.246054
Thermal correction to Gibbs Free Energy= 0.189628
Sum of electronic and zero-point Energies= -879.446925
Sum of electronic and thermal Energies= -879.432809
Sum of electronic and thermal Enthalpies= -879.431865
Sum of electronic and thermal Free Energies= -879.488292

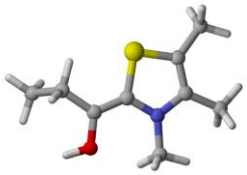
E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	153.809	51.581	118.760



B3LYP/6-31G*	**Aliphatischradpr2**





xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

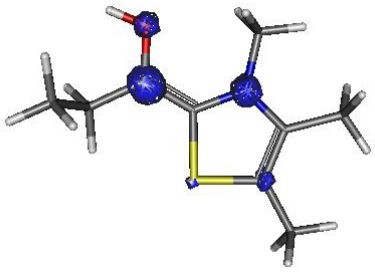
C	1.7781630000	0.3108900000	0.2694660000
O	2.2212360000	1.5829350000	0.2255410000
C	2.8005720000	-0.7795920000	0.4169870000
C	0.4091340000	0.0882850000	0.1532120000
N	-0.6034000000	1.0156700000	0.0077800000
C	-1.8779480000	0.4638860000	-0.0789130000
C	-1.8834800000	-0.9066540000	-0.0050970000
S	-0.2642410000	-1.5273980000	0.1775930000
C	-0.3591210000	2.4700890000	-0.0451940000
H	-1.3104560000	2.9813850000	-0.1606760000
H	0.2864350000	2.7079990000	-0.8912350000
H	0.1208860000	2.8003740000	0.8767610000
C	-3.0834810000	1.3407860000	-0.2371520000
H	-3.9872680000	0.7333470000	-0.2840330000

H	-3.0365320000	1.9300000000	-1.1599690000
H	-3.1951860000	2.0314380000	0.6062980000
C	-3.0310830000	-1.8674730000	-0.0645270000
H	-2.9582620000	-2.5148310000	-0.9462460000
H	-3.9858300000	-1.3411150000	-0.1144450000
H	-3.0514730000	-2.5126190000	0.8209760000
C	3.7401840000	-0.8957380000	-0.8033430000
H	4.4852930000	-1.6742200000	-0.6188380000
H	4.2812450000	0.0368310000	-0.9994660000
H	3.1828550000	-1.1591680000	-1.7070030000
H	2.3138970000	-1.7414640000	0.5995820000
H	3.3895190000	-0.5656570000	1.3214440000
H	3.1889870000	1.6060290000	0.3239360000

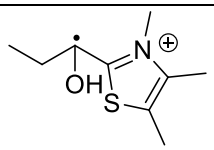
thermodynamic data

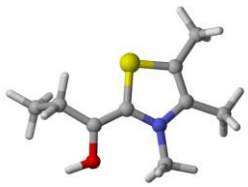
Zero-point correction= 0.229928 (Hartree/Particle)
Thermal correction to Energy= 0.244392
Thermal correction to Enthalpy= 0.245336
Thermal correction to Gibbs Free Energy= 0.186778
Sum of electronic and zero-point Energies= -879.685788
Sum of electronic and thermal Energies= -879.671325
Sum of electronic and thermal Enthalpies= -879.670380
Sum of electronic and thermal Free Energies= -879.728938

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	153.358	51.834	123.246



M062X /6-31++G**	**Aliphatischradpr2**





xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

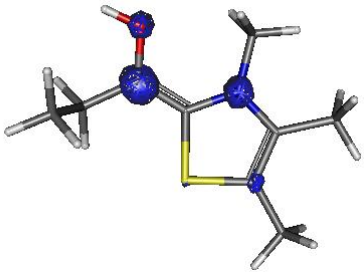
C	1.7887710000	0.3640030000	0.2932540000
O	2.2106180000	1.6306380000	0.1882090000
C	2.8127910000	-0.7159140000	0.4474950000
C	0.4267000000	0.1155260000	0.1787620000
N	-0.5896770000	1.0217700000	0.0074870000
C	-1.8442760000	0.4454380000	-0.0854460000
C	-1.8214450000	-0.9183010000	0.0092710000
S	-0.2090170000	-1.4998570000	0.2208760000
C	-0.3753740000	2.4754190000	-0.0518080000
H	-1.3417730000	2.9614470000	-0.1487630000
H	0.2480270000	2.7237330000	-0.9104120000
H	0.1131130000	2.8127920000	0.8620700000
C	-3.0755670000	1.2720890000	-0.2699100000
H	-3.9448980000	0.6170510000	-0.3260470000
H	-3.0329940000	1.8536890000	-1.1954390000
H	-3.2274550000	1.9585140000	0.5683870000
C	-2.9839950000	-1.8626750000	-0.0490580000
H	-2.6556050000	-2.8980000000	0.0545570000
H	-3.5071290000	-1.7720660000	-1.0050130000
H	-3.6925390000	-1.6544690000	0.7573800000
C	3.5176010000	-1.0325520000	-0.8838300000

H	4.2862620000	-1.7907110000	-0.7244080000
H	4.0002080000	-0.1463810000	-1.3048910000
H	2.8046970000	-1.4139840000	-1.6189280000
H	2.3535330000	-1.6195330000	0.8564910000
H	3.5441920000	-0.3839840000	1.1957200000
H	3.1681920000	1.6939120000	0.3148160000

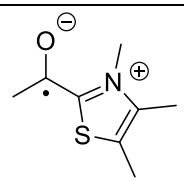
thermodynamic data

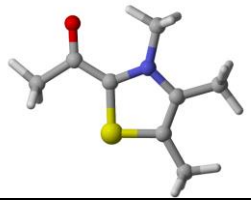
Zero-point correction= 0.230935 (Hartree/Particle)
Thermal correction to Energy= 0.245205
Thermal correction to Enthalpy= 0.246149
Thermal correction to Gibbs Free Energy= 0.188557
Sum of electronic and zero-point Energies= -879.451155
Sum of electronic and thermal Energies= -879.436885
Sum of electronic and thermal Enthalpies= -879.435941
Sum of electronic and thermal Free Energies= -879.493533

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	153.869	51.596	121.213



B3LYP/6-31G*	**acetaldehydhausradde**





xyz-matrix

23

XYZ file generated by gabedit : coordinates in Angstrom

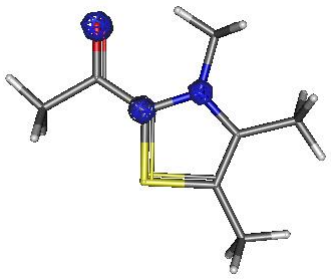
C	-2.2252730000	0.0181130000	0.0001000000
O	-2.8650540000	1.0958670000	0.0004280000
C	-2.9782540000	-1.3084580000	0.0000640000
C	-0.7969650000	-0.0562700000	-0.0001530000
S	0.0778370000	-1.5891270000	-0.0002230000
C	1.6349790000	-0.7516890000	-0.0000340000
C	1.4536160000	0.5955310000	0.0000330000
C	2.5248470000	1.6457350000	0.0002440000
H	2.4574470000	2.2921870000	-0.8830360000
H	3.5142820000	1.1857740000	0.0002400000
H	2.4573330000	2.2919000000	0.8837260000
C	2.8971420000	-1.5561690000	0.0001920000
H	3.7793420000	-0.9104430000	-0.0005440000
H	2.9606220000	-2.2048950000	-0.8830450000
H	2.9611540000	-2.2036670000	0.8842990000
N	0.1167830000	0.9912960000	-0.0000700000
C	-0.2770160000	2.4025480000	-0.0004150000
H	0.1133010000	2.9058690000	0.8911130000
H	-1.3650900000	2.4381470000	-0.0004950000
H	0.1135780000	2.9055130000	-0.8920120000
H	-2.7428160000	-1.9152040000	-0.8844720000
H	-4.0472570000	-1.0859740000	0.0000980000
H	-2.7427980000	-1.9152310000	0.8845810000

thermodynamic data

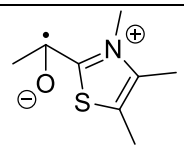
Zero-point correction= 0.188241 (Hartree/Particle)
Thermal correction to Energy= 0.201080
Thermal correction to Enthalpy= 0.202025
Thermal correction to Gibbs Free Energy= 0.148395
Sum of electronic and zero-point Energies= -840.024591

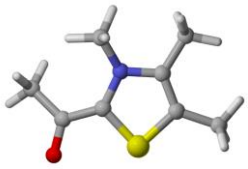
Sum of electronic and thermal Energies= -840.011751
Sum of electronic and thermal Enthalpies= -840.010807
Sum of electronic and thermal Free Energies= -840.064437

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	126.180	45.575	112.873



M062X /6-31++G**	**Acetaldehydhausradde2**





xyz-matrix

23

XYZ file generated by gabedit : coordinates in Angstrom

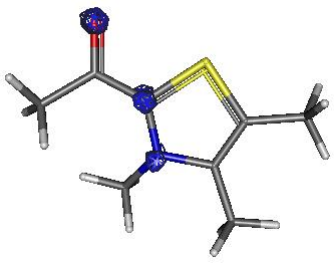
C	2.1864520000	-0.3526000000	0.0452670000
O	2.6558040000	-1.4898470000	-0.1374340000
C	3.1102850000	0.7895020000	0.4277230000
C	0.7714730000	-0.1767520000	-0.0498360000
S	-0.2163590000	-1.6118070000	-0.1174250000
C	-1.6702770000	-0.6381790000	0.0283370000
C	-1.3835920000	0.6809910000	0.0963540000
N	-0.0091500000	0.9660250000	0.0458670000
C	0.4148560000	2.2434230000	-0.5231650000

C	-2.9994140000	-1.3231650000	0.0813850000
H	3.4304280000	1.3581360000	-0.4522990000
H	3.9982110000	0.3400430000	0.8746350000
H	2.6529710000	1.4757350000	1.1467940000
H	-0.0722350000	3.0617570000	0.0087520000
H	0.1536030000	2.2944180000	-1.5878490000
H	1.4886940000	2.3613610000	-0.4213140000
H	-3.1304690000	-1.9736740000	-0.7891720000
H	-3.8187470000	-0.6022890000	0.0865910000
H	-3.0870740000	-1.9456810000	0.9775120000
C	-2.3499720000	1.8170720000	0.2289330000
H	-2.3428950000	2.4637350000	-0.6546270000
H	-2.1087160000	2.4325970000	1.1017410000
H	-3.3632900000	1.4376350000	0.3564410000

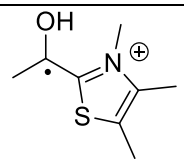
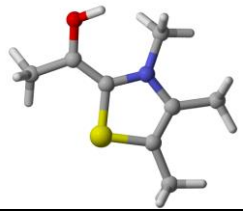
thermodynamic data

Zero-point correction= 0.189322 (Hartree/Particle)
Thermal correction to Energy= 0.201948
Thermal correction to Enthalpy= 0.202892
Thermal correction to Gibbs Free Energy= 0.149606
Sum of electronic and zero-point Energies= -839.803488
Sum of electronic and thermal Energies= -839.790862
Sum of electronic and thermal Enthalpies= -839.789918
Sum of electronic and thermal Free Energies= -839.843204

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	126.724	45.217	112.150



B3LYP/6-31G*	**acetaldehydhausradpr**

xyz-matrix

24

XYZ file generated by gabedit : coordinates in Angstrom

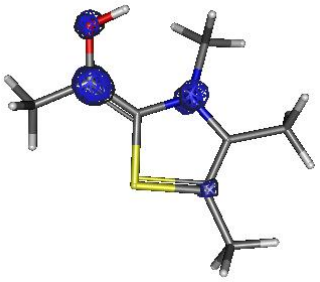
C	-2.1429470000	-0.1112860000	0.0306540000
O	-2.9166810000	0.9670620000	0.2453090000
C	-2.9581320000	-1.3525730000	-0.1388520000
C	-0.7492830000	-0.1007160000	-0.0197680000
S	0.1631580000	-1.5954800000	-0.0116110000
C	1.6774830000	-0.7302860000	0.0270890000
C	1.4705940000	0.6254540000	0.0175070000
C	2.5285110000	1.6869800000	0.0361460000
H	2.5835530000	2.2253770000	-0.9179760000
H	3.5072850000	1.2398090000	0.2107730000
H	2.3533690000	2.4176750000	0.8331330000
C	2.9609720000	-1.5022480000	0.0516270000
H	3.8214200000	-0.8364680000	0.1392200000
H	3.0835540000	-2.0885610000	-0.8664860000
H	2.9875840000	-2.1983740000	0.8972670000
N	0.1220030000	0.9742460000	-0.0255280000
C	-0.3220240000	2.3654180000	-0.2002130000
H	-0.6303850000	2.8059850000	0.7561180000
H	-1.1325920000	2.4055810000	-0.9304300000

H	0.5016940000	2.9606330000	-0.5884360000
H	-2.4099140000	-2.1604200000	-0.6274190000
H	-3.8398750000	-1.1142590000	-0.7428350000
H	-3.3187100000	-1.7064160000	0.8358190000
H	-2.4291260000	1.7364430000	0.5781060000

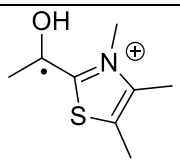
thermodynamic data

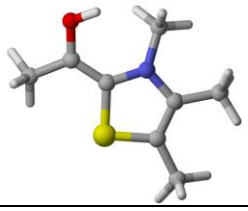
Zero-point correction= 0.200970 (Hartree/Particle)
Thermal correction to Energy= 0.214041
Thermal correction to Enthalpy= 0.214985
Thermal correction to Gibbs Free Energy= 0.160608
Sum of electronic and zero-point Energies= -840.390675
Sum of electronic and thermal Energies= -840.377605
Sum of electronic and thermal Enthalpies= -840.376660
Sum of electronic and thermal Free Energies= -840.431038

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	134.313	46.977	114.446



M062X /6-31++G**	**acetaldehydhausradpr**





xyz-matrix

24

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.1341600000	-0.1080810000	0.0442750000

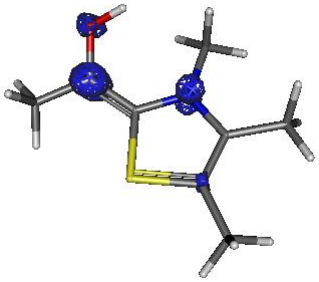
O	-2.8766410000	0.9687280000	0.3170310000
C	-2.9569920000	-1.3324710000	-0.1581940000
C	-0.7441470000	-0.1071040000	-0.0272550000
S	0.1586970000	-1.5913600000	-0.0284660000
C	1.6601250000	-0.7328640000	0.0197130000
C	1.4567390000	0.6181920000	0.0214640000
C	2.5154880000	1.6729950000	0.0626400000
H	2.6313290000	2.1687500000	-0.9066780000
H	3.4725300000	1.2220370000	0.3229660000
H	2.2895210000	2.4305480000	0.8179520000
C	2.9556220000	-1.4817660000	0.0717650000
H	3.7578400000	-0.8958070000	-0.3792550000
H	2.8837940000	-2.4222800000	-0.4787480000
H	3.2305010000	-1.7145390000	1.1050670000
N	0.1148380000	0.9662620000	-0.0286820000
C	-0.3198840000	2.3467340000	-0.2696510000
H	-0.5674570000	2.8534850000	0.6693480000
H	-1.1690270000	2.3460770000	-0.9542950000
H	0.4912150000	2.8945310000	-0.7450460000
H	-2.4142990000	-2.1246310000	-0.6741130000
H	-3.8370680000	-1.0647100000	-0.7489940000
H	-3.3119680000	-1.7068970000	0.8084770000
H	-2.3835420000	1.7077360000	0.6947530000

thermodynamic data

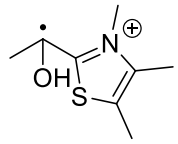
Zero-point correction= 0.201821 (Hartree/Particle)
Thermal correction to Energy= 0.213933
Thermal correction to Enthalpy= 0.214877
Thermal correction to Gibbs Free Energy= 0.163445
Sum of electronic and zero-point Energies= -840.173815

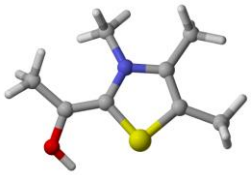
Sum of electronic and thermal Energies= -840.161703
Sum of electronic and thermal Enthalpies= -840.160759
Sum of electronic and thermal Free Energies= -840.212191

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	134.245	44.802	108.248



B3LYP/6-31G*	**Acetaldehydhausradpr2**





xyz-matrix

24

XYZ file generated by gabedit : coordinates in Angstrom

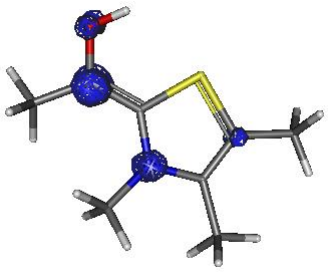
C	2.1321550000	-0.2474930000	-0.0004810000
O	2.7360770000	-1.4300070000	0.2090770000
C	3.1260530000	0.8158230000	-0.3485210000
C	0.7375500000	-0.1615650000	0.0275270000
S	-0.2611510000	-1.6019090000	-0.0194980000
C	-1.7246460000	-0.6480100000	-0.0340560000
C	-1.4311650000	0.6910760000	-0.0126190000
N	-0.0651930000	0.9582450000	0.0468940000
C	0.4496940000	2.3244470000	0.2340670000
C	-3.0511350000	-1.3413040000	-0.0766510000
H	3.9381100000	0.3379610000	-0.9057090000

H	3.5736210000	1.2555790000	0.5524400000
H	2.7046000000	1.6097550000	-0.9641360000
H	-0.3066910000	2.9220190000	0.7396540000
H	0.6880190000	2.7875440000	-0.7276880000
H	1.3378160000	2.2939340000	0.8628640000
H	-3.1338180000	-1.9862560000	-0.9587120000
H	-3.8700500000	-0.6203730000	-0.1102250000
H	-3.1946280000	-1.9688290000	0.8104690000
C	-2.4204970000	1.8170800000	-0.0365920000
H	-2.1791110000	2.5459040000	-0.8173580000
H	-2.4606320000	2.3450330000	0.9239630000
H	-3.4214120000	1.4358510000	-0.2399020000
H	2.1622850000	-2.0955610000	0.6294010000

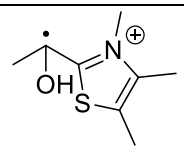
thermodynamic data

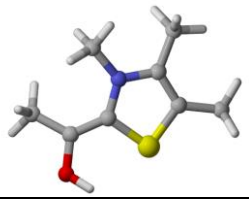
Zero-point correction= 0.201170 (Hartree/Particle)
Thermal correction to Energy= 0.214095
Thermal correction to Enthalpy= 0.215039
Thermal correction to Gibbs Free Energy= 0.161458
Sum of electronic and zero-point Energies= -840.390535
Sum of electronic and thermal Energies= -840.377610
Sum of electronic and thermal Enthalpies= -840.376665
Sum of electronic and thermal Free Energies= -840.430246

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	134.347	46.913	112.770



M062X /6-31++G**	**Acetaldehydhausradpr2**





xyz-matrix

24

XYZ file generated by gabedit : coordinates in Angstrom

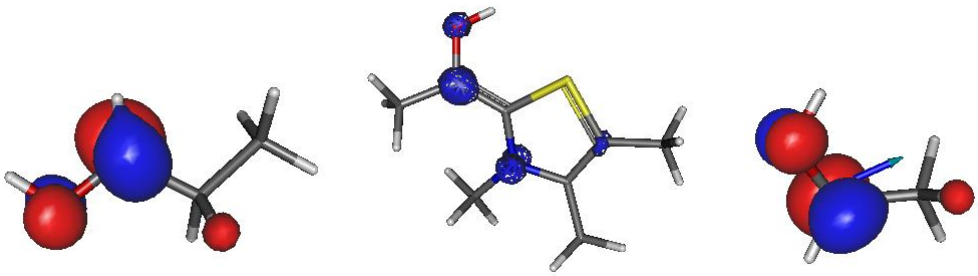
C	2.1227640000	-0.2500790000	0.0058720000
O	2.7318360000	-1.4186020000	-0.2061050000
C	3.0894500000	0.8218400000	0.3831470000
C	0.7299040000	-0.1719250000	-0.0356830000
S	-0.2636540000	-1.5983110000	0.0034650000
C	-1.7136240000	-0.6461030000	0.0304760000
C	-1.4193590000	0.6872160000	0.0170940000
N	-0.0572990000	0.9475400000	-0.0515120000
C	0.4550740000	2.3044380000	-0.2755650000
C	-3.0448870000	-1.3254570000	0.0894790000
H	3.5470450000	1.2720620000	-0.5050280000
H	3.8914730000	0.3464300000	0.9534230000
H	2.6370260000	1.5992080000	0.9957020000
H	0.6647850000	2.8031450000	0.6736320000
H	-0.2935280000	2.8727090000	-0.8242500000
H	1.3573740000	2.2518400000	-0.8812900000
H	-3.1178110000	-2.1028240000	-0.6754120000
H	-3.8485120000	-0.6103360000	-0.0868910000
H	-3.2042980000	-1.7913960000	1.0662310000
C	-2.3982360000	1.8175640000	0.0582330000

H	-2.4970340000	2.3008200000	-0.9190400000
H	-2.0966030000	2.5706900000	0.7908380000
H	-3.3803710000	1.4483550000	0.3496710000
H	2.1788000000	-2.0966610000	-0.6219170000

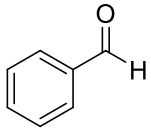
thermodynamic data

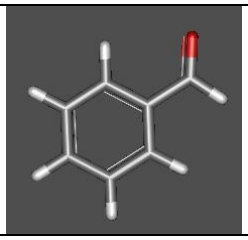
Zero-point correction=	0.202466 (Hartree/Particle)
Thermal correction to Energy=	0.215103
Thermal correction to Enthalpy=	0.216047
Thermal correction to Gibbs Free Energy=	0.163565
Sum of electronic and zero-point Energies=	-840.173530
Sum of electronic and thermal Energies=	-840.160893
Sum of electronic and thermal Enthalpies=	-840.159949
Sum of electronic and thermal Free Energies=	-840.212431

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	134.979	46.527	110.458



B3LYP/6-31G*	**Benzaldehyd**





xyz-matrix

14

XYZ file generated by gabedit : coordinates in Angstrom

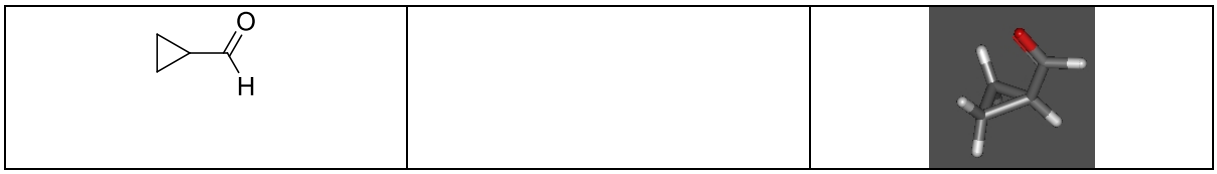
C	2.2172070000	-0.2508060000	-0.0000020000
C	1.3264450000	-1.3311570000	0.0000000000
C	-0.0453880000	-1.1010730000	0.0000030000
C	-0.5344530000	0.2143550000	0.0000040000
C	0.3611680000	1.2919900000	0.0000010000
C	1.7360410000	1.0606340000	-0.0000020000
H	3.2887010000	-0.4332280000	-0.0000040000
H	1.7077550000	-2.3487080000	0.0000000000
H	-0.7593100000	-1.9193330000	0.0000050000
H	-0.0251610000	2.3094770000	0.0000010000
H	2.4303830000	1.8963350000	-0.0000040000
C	-1.9921680000	0.4685000000	0.0000080000
O	-2.8477270000	-0.3956170000	-0.0000070000
H	-2.2736650000	1.5457360000	-0.0000100000

Thermodynamic data

Zero-point correction= 0.110217 (Hartree/Particle)
Thermal correction to Energy= 0.116506
Thermal correction to Enthalpy= 0.117450
Thermal correction to Gibbs Free Energy= 0.079695
Sum of electronic and zero-point Energies= -345.463224
Sum of electronic and thermal Energies= -345.456936
Sum of electronic and thermal Enthalpies= -345.455992
Sum of electronic and thermal Free Energies= -345.493747

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.108	23.815	79.462

B3LYP/6-31G*	**Aldehyd2**



xyz-matrix

11

XYZ file generated by gabedit : coordinates in Angstrom

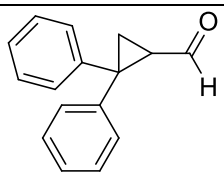
C	1.1848660000	-0.2826110000	0.7434950000
C	0.3051920000	0.7214930000	0.0000110000
C	1.1848730000	-0.2825830000	-0.7435010000
H	2.0449090000	0.1168250000	1.2729450000
H	0.6527480000	-1.0834720000	1.2482830000
H	0.6140920000	1.7632220000	0.0000320000
C	-1.1579140000	0.4778590000	0.0000000000
H	2.0449200000	0.1168730000	-1.2729290000
H	0.6527590000	-1.0834260000	-1.2483240000
O	-1.6646430000	-0.6280940000	-0.0000080000
H	-1.7943810000	1.3897830000	0.0000270000

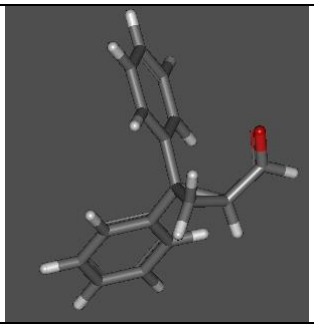
Thermodynamic data

Zero-point correction= 0.091439 (Hartree/Particle)
Thermal correction to Energy= 0.096482
Thermal correction to Enthalpy= 0.097427
Thermal correction to Gibbs Free Energy= 0.063495
Sum of electronic and zero-point Energies= -231.126708
Sum of electronic and thermal Energies= -231.121665
Sum of electronic and thermal Enthalpies= -231.120721
Sum of electronic and thermal Free Energies= -231.154653

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	60.544	17.196	71.416

B3LYP/6-31G*	**Aldehyd3**





xyz-matrix

31

XYZ file generated by gabedit : coordinates in Angstrom

C	0.0542950000	0.7039480000	0.3533520000
C	-0.1838800000	2.1823810000	-0.0594730000
C	-0.1441750000	1.7614000000	1.3951260000
C	-1.4825160000	2.6024720000	-0.6452170000
H	0.6857290000	2.6919010000	-0.4657090000
H	-1.1030940000	1.8015370000	1.9036820000
H	0.7141500000	2.0760660000	1.9814610000
C	-1.0227410000	-0.3304760000	0.1119200000
C	-1.2041680000	-0.8698600000	-1.1696910000
C	-2.1564000000	-1.8604900000	-1.3995740000
C	-2.9407620000	-2.3373570000	-0.3464520000
C	-2.7636740000	-1.8140020000	0.9336790000
C	-1.8109560000	-0.8186380000	1.1595550000
H	-0.5914400000	-0.5108720000	-1.9928490000
H	-2.2866140000	-2.2610460000	-2.4015380000
H	-3.6839500000	-3.1099640000	-0.5244000000
H	-3.3681330000	-2.1773140000	1.7606500000
H	-1.6815520000	-0.4172540000	2.1605960000
C	1.4605640000	0.1811530000	0.1464810000

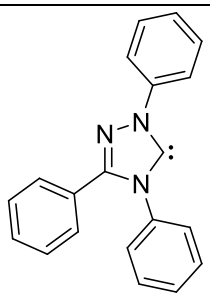
C	2.0574070000	-0.5975320000	1.1486970000
C	3.3360700000	-1.1251600000	0.9765870000
C	4.0408160000	-0.8853640000	-0.2055460000
C	3.4559370000	-0.1158350000	-1.2109800000
C	2.1750180000	0.4124510000	-1.0350180000
H	1.5097900000	-0.7909110000	2.0676640000
H	3.7834360000	-1.7231890000	1.7662310000
H	5.0383870000	-1.2946830000	-0.3402110000
H	3.9954760000	0.0766250000	-2.1346930000
H	1.7285370000	1.0128130000	-1.8236390000
O	-2.5705360000	2.3650550000	-0.1599810000
H	-1.4014420000	3.1713020000	-1.5980730000

Thermodynamic data

Zero-point correction= 0.253262 (Hartree/Particle)
Thermal correction to Energy= 0.267393
Thermal correction to Enthalpy= 0.268337
Thermal correction to Gibbs Free Energy= 0.210529
Sum of electronic and zero-point Energies= -693.063460
Sum of electronic and thermal Energies= -693.049330
Sum of electronic and thermal Enthalpies= -693.048386
Sum of electronic and thermal Free Energies= -693.106194

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.792	55.341	121.667

B3LYP/6-31G*	**Berkesselkat**



xyz-matrix

38

XYZ file generated by gabedit : coordinates in Angstrom

C	0.2640160000	-0.6488180000	-0.0233030000
N	-0.9815680000	-1.0417370000	-0.0188500000
N	-1.7010100000	0.1401130000	-0.0039680000
C	-0.9628210000	1.2772860000	0.0003210000
N	0.3100370000	0.7501960000	-0.0050000000
C	1.3927530000	-1.5921430000	-0.0893010000
C	2.5339610000	-1.3322310000	-0.8647220000
C	3.5593390000	-2.2734670000	-0.9406740000
C	3.4598600000	-3.4817880000	-0.2483840000
C	2.3234000000	-3.7499190000	0.5179090000
C	1.2952900000	-2.8134340000	0.5974810000
H	2.6143430000	-0.4025490000	-1.4179160000
H	4.4353100000	-2.0631420000	-1.5480090000
H	4.2622280000	-4.2120660000	-0.3084060000
H	2.2374520000	-4.6896170000	1.0565720000
H	0.4072920000	-3.0158070000	1.1874120000
C	1.4659420000	1.5915290000	0.0854610000

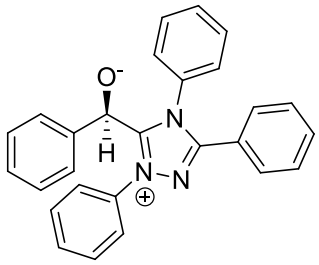
C	1.5707480000	2.6875420000	-0.7744820000
C	2.6748460000	3.5336710000	-0.6797410000
C	3.6735710000	3.2863060000	0.2645770000
C	3.5579220000	2.1931070000	1.1249350000
C	2.4522040000	1.3463780000	1.0443300000
H	0.7780590000	2.8708770000	-1.4915490000
H	2.7536320000	4.3873900000	-1.3470190000
H	4.5341800000	3.9456850000	0.3340270000
H	4.3241930000	2.0011240000	1.8707310000
H	2.3501840000	0.5064990000	1.7234130000
C	-3.1264520000	0.0837500000	-0.0016470000
C	-3.8579090000	1.2761750000	0.0249490000
C	-5.2495950000	1.2240570000	0.0270990000
C	-5.9162650000	-0.0036190000	0.0038380000
C	-5.1752020000	-1.1854140000	-0.0222620000
C	-3.7804840000	-1.1507750000	-0.0253990000
H	-3.3229680000	2.2183720000	0.0441790000
H	-5.8153390000	2.1516730000	0.0481380000
H	-7.0021720000	-0.0375740000	0.0060960000
H	-5.6817370000	-2.1466960000	-0.0412570000
H	-3.1975990000	-2.0633260000	-0.0475880000

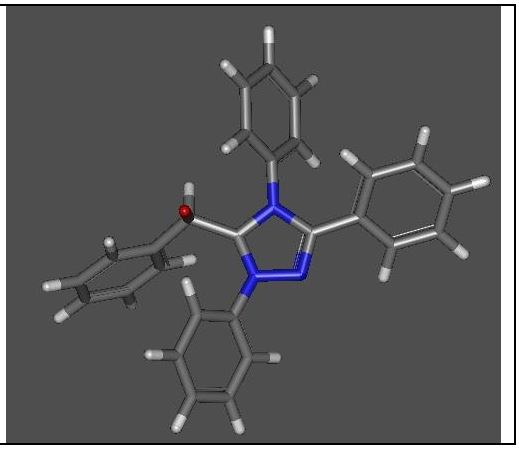
Thermodynamic data

Zero-point correction= 0.301919 (Hartree/Particle)
Thermal correction to Energy= 0.319275
Thermal correction to Enthalpy= 0.320219
Thermal correction to Gibbs Free Energy= 0.254483
Sum of electronic and zero-point Energies= -935.065482
Sum of electronic and thermal Energies= -935.048127
Sum of electronic and thermal Enthalpies= -935.047182
Sum of electronic and thermal Free Energies= -935.112919

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.348	69.723	138.354

B3LYP/6-31G*	**Job1de**





xyz-matrix

52

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.1951760000	-1.4389890000	-0.4445750000
O	-1.1624630000	-1.3738370000	-1.7888780000
H	-0.6625240000	-2.3197950000	-0.0071660000
C	-2.5692820000	-1.4558930000	0.2449330000
C	-2.7217090000	-1.2502470000	1.6203240000
C	-3.9769310000	-1.3628290000	2.2193820000
C	-5.0916970000	-1.7003620000	1.4474750000
C	-4.9407180000	-1.9215900000	0.0769520000
C	-3.6852530000	-1.7972410000	-0.5206100000
H	-1.8547580000	-0.9988550000	2.2309470000
H	-4.0855080000	-1.1904210000	3.2876330000
H	-6.0699080000	-1.7917160000	1.9129520000
H	-5.8038800000	-2.1901250000	-0.5278500000
H	-3.5365470000	-1.9587860000	-1.5840830000

C	-0.3061380000	-0.2515080000	-0.0749010000
N	1.0587640000	-0.3347500000	0.0109990000
C	1.5585200000	0.9654050000	0.0612380000
N	0.5775700000	1.8279220000	0.0284390000
N	-0.5702210000	1.0700170000	-0.0559350000
C	-1.8097830000	1.7538620000	-0.2859910000
C	1.8181670000	-1.5591910000	-0.0199830000
C	2.9709640000	1.3749890000	0.1254910000
C	2.7003960000	-1.8488500000	1.0223590000
C	1.6670760000	-2.4171520000	-1.1140620000
C	3.4648400000	-3.0134670000	0.9582550000
C	2.4322350000	-3.5830620000	-1.1553430000
C	3.3349130000	-3.8781590000	-0.1307550000
H	4.1558030000	-3.2462750000	1.7633020000
H	3.9300130000	-4.7861070000	-0.1751840000
H	2.7886560000	-1.1720600000	1.8662970000
H	0.9124920000	-2.1794320000	-1.8651390000
H	2.3167280000	-4.2646420000	-1.9932210000
C	3.9689240000	0.7363470000	-0.6275050000
C	3.3077080000	2.4855460000	0.9161710000
C	5.2826990000	1.1988140000	-0.5770140000
C	5.6144550000	2.2965710000	0.2192950000
C	4.6231230000	2.9406800000	0.9627400000
H	3.7182020000	-0.1065620000	-1.2620160000
H	6.0473250000	0.7019660000	-1.1672920000
H	2.5305450000	2.9834220000	1.4868220000
H	6.6407840000	2.6510740000	0.2572800000
H	4.8738450000	3.7979910000	1.5810170000

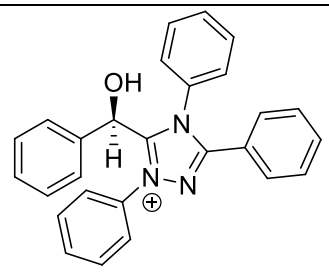
C	-2.1250600000	2.8556330000	0.5107170000
C	-2.6253010000	1.3486110000	-1.3428550000
C	-3.2977010000	3.5609060000	0.2492170000
C	-3.7996360000	2.0624970000	-1.5835380000
C	-4.1370560000	3.1638440000	-0.7951510000
H	-1.4563110000	3.1533630000	1.3113420000
H	-2.3259860000	0.4838130000	-1.9337530000
H	-3.5560910000	4.4190800000	0.8631180000
H	-4.4492400000	1.7562790000	-2.3985430000
H	-5.0521930000	3.7151630000	-0.9935450000

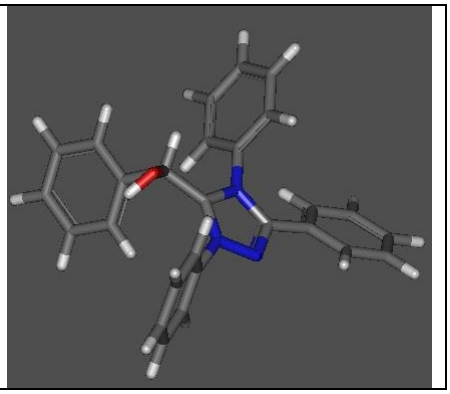
Thermodynamic data

Zero-point correction= 0.415427 (Hartree/Particle)
Thermal correction to Energy= 0.439636
Thermal correction to Enthalpy= 0.440580
Thermal correction to Gibbs Free Energy= 0.359947
Sum of electronic and zero-point Energies= -1280.517254
Sum of electronic and thermal Energies= -1280.493046
Sum of electronic and thermal Enthalpies= -1280.492101
Sum of electronic and thermal Free Energies= -1280.572734

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	275.875	96.930	169.705

B3LYP/6-31G*	**Job1pr**





xyz-matrix

53

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4003540000	-1.0567630000	-1.0374290000
H	-0.7440660000	-1.6876600000	-1.6465920000
O	-2.3890180000	-0.5639700000	-1.9227890000
H	-3.2175260000	-0.4539370000	-1.4282270000
C	-1.9684000000	-1.9095050000	0.0879690000
C	-2.4423020000	-1.3494950000	1.2825110000
C	-3.0322750000	-2.1608930000	2.2532580000
C	-3.1554260000	-3.5341780000	2.0374680000
C	-2.6883930000	-4.0975650000	0.8472540000
C	-2.0961370000	-3.2900720000	-0.1220900000
H	-2.3629450000	-0.2807270000	1.4620970000
H	-3.3959170000	-1.7187910000	3.1760740000
H	-3.6147340000	-4.1638880000	2.7935840000
H	-2.7851980000	-5.1651930000	0.6741090000
H	-1.7375060000	-3.7295810000	-1.0493490000
C	-0.5008760000	0.0689260000	-0.5414660000
N	-0.7857030000	1.3431960000	-0.2593530000
N	0.3257320000	2.0268630000	0.1610860000
C	1.3141590000	1.1623140000	0.1192590000
N	0.8323050000	-0.0724990000	-0.3180090000
C	1.5980040000	-1.2696220000	-0.6044060000
C	2.3974530000	-1.2960920000	-1.7483600000
C	3.1409200000	-2.4440130000	-2.0225200000
C	3.0783910000	-3.5429200000	-1.1623570000
C	2.2711070000	-3.5010830000	-0.0232260000

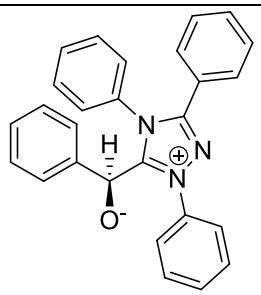
C	1.5226600000	-2.3589450000	0.2653130000
H	2.4395190000	-0.4339830000	-2.4067020000
H	3.7673720000	-2.4774320000	-2.9082610000
H	3.6601930000	-4.4333050000	-1.3801470000
H	2.2235480000	-4.3550160000	0.6452160000
H	0.8949540000	-2.3115400000	1.1491540000
C	2.6987930000	1.5100870000	0.4559470000
C	3.5915250000	0.5946710000	1.0378860000
C	4.8817490000	1.0013410000	1.3699520000
C	5.2914280000	2.3139590000	1.1271410000
C	4.4036840000	3.2294570000	0.5565960000
C	3.1119500000	2.8345150000	0.2232620000
H	3.2819120000	-0.4219440000	1.2502740000
H	5.5657460000	0.2918970000	1.8254690000
H	6.2996640000	2.6239600000	1.3853170000
H	4.7183960000	4.2512750000	0.3683800000
H	2.4181620000	3.5405510000	-0.2207590000
C	-2.0411580000	2.0647840000	-0.2867700000
C	-2.5362450000	2.5517830000	0.9239670000
C	-3.7121890000	3.3013500000	0.9175690000
C	-4.3677940000	3.5649530000	-0.2869580000
C	-3.8452290000	3.0878920000	-1.4913320000
C	-2.6682470000	2.3387300000	-1.5027020000
H	-2.0001620000	2.3606010000	1.8481420000
H	-4.1092780000	3.6835780000	1.8526380000
H	-5.2814570000	4.1514400000	-0.2886060000
H	-4.3456300000	3.3079900000	-2.4291440000
H	-2.2500380000	1.9688600000	-2.4308440000

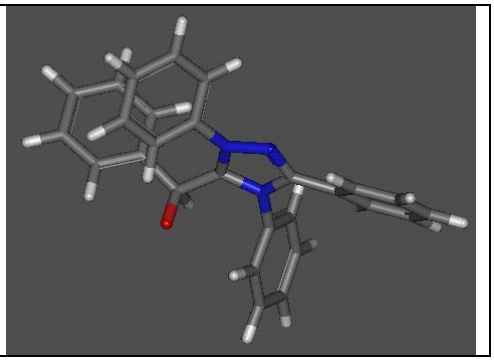
Thermodynamic data

Zero-point correction= 0.428903 (Hartree/Particle)
Thermal correction to Energy= 0.453906
Thermal correction to Enthalpy= 0.454850
Thermal correction to Gibbs Free Energy= 0.370667
Sum of electronic and zero-point Energies= -1280.947750
Sum of electronic and thermal Energies= -1280.922746
Sum of electronic and thermal Enthalpies= -1280.921802
Sum of electronic and thermal Free Energies= -1281.005985

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	284.830	98.869	177.178

B3LYP/6-31G*	**Job1deko2**





xyz-matrix

52

XYZ file generated by gabedit : coordinates in Angstrom

C	1.1741150000	-1.3697150000	-0.4961320000
H	0.6567510000	-2.2914070000	-0.1293190000
O	1.0909740000	-1.1695160000	-1.8217630000
C	2.5710440000	-1.4393610000	0.1425050000
C	3.6609920000	-1.7037610000	-0.6881980000
C	4.9369530000	-1.8730130000	-0.1479550000
C	5.1350120000	-1.7736310000	1.2308570000
C	4.0469210000	-1.5121490000	2.0676240000

C	2.7712440000	-1.3544880000	1.5244330000
H	3.4759040000	-1.7704440000	-1.7562470000
H	5.7794750000	-2.0810280000	-0.8036130000
H	6.1291930000	-1.8997180000	1.6523540000
H	4.1924520000	-1.4332400000	3.1424940000
H	1.9256040000	-1.1611720000	2.1841710000
C	0.2894300000	-0.2270930000	0.0099340000
N	0.5182100000	1.0984770000	0.0735810000
N	-0.6478450000	1.8180850000	0.1969020000
C	-1.6100610000	0.9317250000	0.2126410000
N	-1.0704820000	-0.3535600000	0.1330130000
C	1.7383000000	1.8256860000	-0.1272300000
C	2.0365940000	2.8848070000	0.7315100000
C	3.1899750000	3.6319320000	0.5015830000
C	4.0267590000	3.3178580000	-0.5727840000
C	3.7057480000	2.2585560000	-1.4232190000
C	2.5505480000	1.5042940000	-1.2146810000
H	1.3698080000	3.1172560000	1.5551580000
H	3.4356800000	4.4573920000	1.1636940000
H	4.9269150000	3.9014100000	-0.7462060000
H	4.3529710000	2.0177260000	-2.2617860000
H	2.2602670000	0.6712660000	-1.8540310000
C	-3.0272230000	1.3333360000	0.2456750000
C	-4.0556980000	0.5433740000	0.7811530000
C	-5.3689260000	1.0131380000	0.7922070000
C	-5.6744930000	2.2726240000	0.2775210000
C	-4.6548640000	3.0679510000	-0.2511520000
C	-3.3436230000	2.6041520000	-0.2703310000

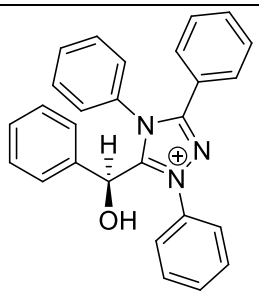
H	-3.8415200000	-0.4326730000	1.1956990000
H	-6.1535640000	0.3892770000	1.2109510000
H	-6.6995320000	2.6327150000	0.2870930000
H	-4.8820550000	4.0495870000	-0.6572390000
H	-2.5497150000	3.2143450000	-0.6866690000
C	-1.7571990000	-1.6080290000	-0.0674160000
C	-2.2433530000	-2.3244080000	1.0278080000
C	-2.9047200000	-3.5329570000	0.8102680000
C	-3.0595160000	-4.0196320000	-0.4902400000
C	-2.5400110000	-3.3073540000	-1.5728750000
C	-1.8803120000	-2.0944800000	-1.3700310000
H	-2.0965640000	-1.9414060000	2.0337680000
H	-3.2884290000	-4.0967480000	1.6555940000
H	-3.5721240000	-4.9629240000	-0.6568600000
H	-2.6363900000	-3.7001820000	-2.5807360000
H	-1.3939070000	-1.5610900000	-2.1794750000

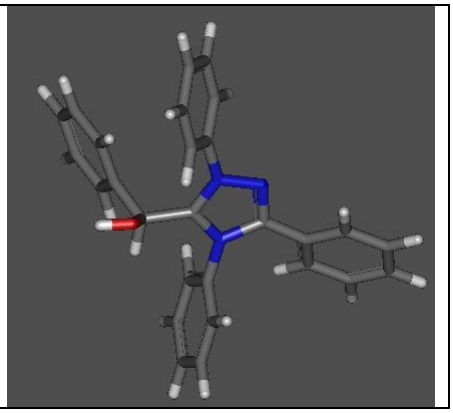
Thermodynamic data

Zero-point correction= 0.415098 (Hartree/Particle)
Thermal correction to Energy= 0.439495
Thermal correction to Enthalpy= 0.440440
Thermal correction to Gibbs Free Energy= 0.358418
Sum of electronic and zero-point Energies= -1280.513499
Sum of electronic and thermal Energies= -1280.489102
Sum of electronic and thermal Enthalpies= -1280.488157
Sum of electronic and thermal Free Energies= -1280.570179

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	275.788	97.201	172.628

B3LYP/6-31G*	**Job1prko2**





xyz-matrix

53

XYZ file generated by gabedit : coordinates in Angstrom

C	1.2152370000	-1.2892770000	-0.9454400000
H	0.5167390000	-2.1246600000	-1.0845500000
O	1.7754860000	-0.9010490000	-2.1900800000
H	2.4029780000	-1.5947730000	-2.4553850000
C	2.2417470000	-1.7083720000	0.1042660000
C	1.8999910000	-2.6941440000	1.0398700000
C	2.8237480000	-3.1079810000	1.9986090000
C	4.1027730000	-2.5478860000	2.0216600000
C	4.4537400000	-1.5784220000	1.0807870000
C	3.5287860000	-1.1554440000	0.1251560000
H	0.9161520000	-3.1563710000	1.0066200000
H	2.5511040000	-3.8768340000	2.7154740000
H	4.8263780000	-2.8747470000	2.7625210000
H	5.4519700000	-1.1506610000	1.0863540000
H	3.8111700000	-0.4076320000	-0.6078010000
C	0.3487240000	-0.1260300000	-0.4998690000
N	0.6866720000	1.1399860000	-0.2472380000

N	-0.3885360000	1.8752190000	0.1682190000
C	-1.4144100000	1.0530310000	0.1540730000
N	-0.9878560000	-0.2102290000	-0.2587560000
C	1.9667130000	1.8071640000	-0.3261970000
C	2.5027600000	2.3276330000	0.8519030000
C	3.7096530000	3.0215630000	0.7888010000
C	4.3558270000	3.1938900000	-0.4379420000
C	3.7937630000	2.6794120000	-1.6085080000
C	2.5842640000	1.9849630000	-1.5637520000
H	1.9824810000	2.1918570000	1.7940850000
H	4.1415680000	3.4293310000	1.6972800000
H	5.2941670000	3.7384070000	-0.4829920000
H	4.2884920000	2.8285850000	-2.5632390000
H	2.1339090000	1.5835380000	-2.4630860000
C	-2.7800050000	1.4813690000	0.4779940000
C	-3.7343180000	0.6324090000	1.0626270000
C	-5.0001870000	1.1227240000	1.3751870000
C	-5.3260550000	2.4543480000	1.1113150000
C	-4.3776980000	3.3044870000	0.5372220000
C	-3.1102840000	2.8254620000	0.2224820000
H	-3.4934780000	-0.3982010000	1.2926520000
H	-5.7308850000	0.4628390000	1.8327200000
H	-6.3155220000	2.8295980000	1.3550360000
H	-4.6261730000	4.3410230000	0.3312140000
H	-2.3709140000	3.4810130000	-0.2250710000
C	-1.8090160000	-1.3778910000	-0.5123000000
C	-1.9179810000	-2.3682430000	0.4666230000
C	-2.7146730000	-3.4847280000	0.2104550000

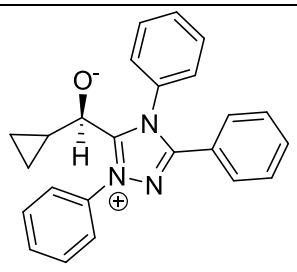
C	-3.3899910000	-3.5991320000	-1.0075740000
C	-3.2713080000	-2.5992920000	-1.9751690000
C	-2.4760410000	-1.4780710000	-1.7330240000
H	-1.3978360000	-2.2582080000	1.4135680000
H	-2.8094560000	-4.2608850000	0.9634270000
H	-4.0102440000	-4.4686990000	-1.2017620000
H	-3.7964260000	-2.6886590000	-2.9208780000
H	-2.3765720000	-0.6935550000	-2.4766600000

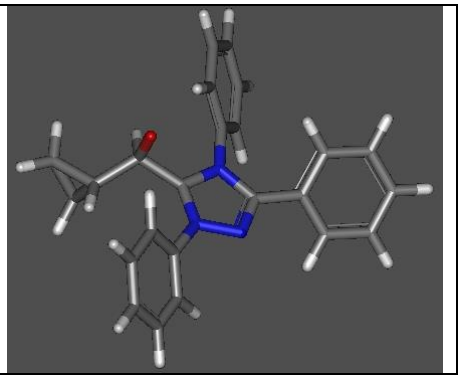
Thermodynamic data

Zero-point correction= 0.429112 (Hartree/Particle)
Thermal correction to Energy= 0.453992
Thermal correction to Enthalpy= 0.454936
Thermal correction to Gibbs Free Energy= 0.371248
Sum of electronic and zero-point Energies= -1280.947970
Sum of electronic and thermal Energies= -1280.923091
Sum of electronic and thermal Enthalpies= -1280.922147
Sum of electronic and thermal Free Energies= -1281.005834

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	284.884	98.713	176.136

B3LYP/6-31G*	**Job2de**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4177440000	1.8011280000	0.2316500000
H	-0.7131290000	2.5752690000	-0.1653720000
O	-1.4737550000	1.7138130000	1.5746620000
C	-2.7139860000	2.0478600000	-0.5447410000
C	-2.6438740000	2.4895720000	-1.9897760000
C	-3.0496060000	3.4689110000	-0.9171610000
H	-3.5555990000	1.4218160000	-0.2682450000
H	-3.3996990000	2.1270000000	-2.6815390000
H	-1.6582060000	2.6096370000	-2.4361190000
H	-4.0888180000	3.7826930000	-0.8664310000
H	-2.3379810000	4.2431130000	-0.6388710000
C	-0.7204250000	0.4726090000	-0.0726560000
N	-1.2033720000	-0.7884010000	-0.0921680000
N	-0.1971810000	-1.7325730000	-0.0903200000
C	0.9153430000	-1.0493250000	-0.0743340000
N	0.6423360000	0.3183130000	-0.0774590000
C	-2.5476260000	-1.2514630000	0.0923520000
C	-3.0142070000	-2.2918790000	-0.7125810000
C	-4.2973880000	-2.7902650000	-0.4948640000
C	-5.0977540000	-2.2508340000	0.5154920000
C	-4.6106210000	-1.2142470000	1.3145100000
C	-3.3246720000	-0.7083490000	1.1184270000
H	-2.3748500000	-2.7040960000	-1.4860600000
H	-4.6717170000	-3.5988180000	-1.1163680000
H	-6.0982310000	-2.6414120000	0.6808090000
H	-5.2293330000	-0.7991620000	2.1052840000
H	-2.9090940000	0.1084440000	1.7100410000
C	2.2387260000	-1.6932000000	-0.0444330000

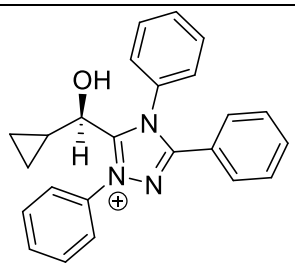
C	3.2901510000	-1.2066640000	0.7484310000
C	4.5071430000	-1.8851830000	0.7850130000
C	4.6887690000	-3.0503910000	0.0378110000
C	3.6423910000	-3.5435450000	-0.7447540000
C	2.4234330000	-2.8713670000	-0.7861740000
H	3.1539250000	-0.3126930000	1.3467400000
H	5.3129060000	-1.5039290000	1.4058260000
H	5.6402400000	-3.5740940000	0.0685120000
H	3.7752620000	-4.4521120000	-1.3252970000
H	1.6038490000	-3.2504450000	-1.3878780000
C	1.5942030000	1.3967090000	-0.0092490000
C	1.5287410000	2.2810660000	1.0722990000
C	2.4731390000	3.3046230000	1.1538180000
C	3.4668280000	3.4343470000	0.1802680000
C	3.5103190000	2.5475810000	-0.8977790000
C	2.5676200000	1.5246960000	-1.0015680000
H	0.7049770000	2.1797170000	1.7803790000
H	2.4273840000	4.0053920000	1.9826060000
H	4.2014560000	4.2313580000	0.2556510000
H	4.2736040000	2.6529930000	-1.6633740000
H	2.5871880000	0.8331130000	-1.8379680000

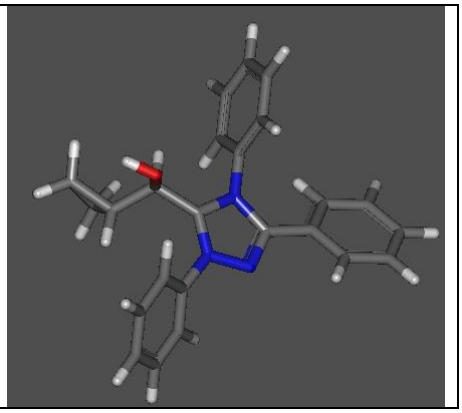
Thermodynamic data

Zero-point correction= 0.397101 (Hartree/Particle)
Thermal correction to Energy= 0.419837
Thermal correction to Enthalpy= 0.420781
Thermal correction to Gibbs Free Energy= 0.343714
Sum of electronic and zero-point Energies= -1166.179251
Sum of electronic and thermal Energies= -1166.156515
Sum of electronic and thermal Enthalpies= -1166.155571
Sum of electronic and thermal Free Energies= -1166.232637

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	263.451	90.242	162.200

B3LYP/6-31G*	**Job2pr**





xyz-matrix

50

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3671810000	1.7892800000	0.3277270000
H	-0.5819680000	2.5420290000	0.1734570000
O	-1.8204340000	1.8290510000	1.6783960000
H	-2.3759340000	2.6221790000	1.7685620000
C	-2.4611560000	2.0379030000	-0.6891390000
C	-2.1162340000	2.6317700000	-2.0363780000
C	-2.8169350000	3.4774650000	-1.0099260000
H	-3.2854090000	1.3323460000	-0.6582180000
H	-2.6769740000	2.2827240000	-2.8976370000
H	-1.0748630000	2.8614800000	-2.2486340000
H	-3.8660080000	3.7145470000	-1.1562780000
H	-2.2435230000	4.2702630000	-0.5345440000
C	-0.6799860000	0.4509310000	0.1664740000
N	-1.2065870000	-0.7739630000	0.0921040000

N	-0.2399180000	-1.7262250000	-0.0691370000
C	0.9065130000	-1.0807110000	-0.0738600000
N	0.6665010000	0.2850880000	0.0706170000
C	-2.5828110000	-1.2112690000	0.1323940000
C	-3.0173710000	-2.0738650000	-0.8761500000
C	-4.3281740000	-2.5439130000	-0.8354400000
C	-5.1816500000	-2.1579150000	0.2016450000
C	-4.7239770000	-1.3038240000	1.2066320000
C	-3.4127870000	-0.8262850000	1.1860750000
H	-2.3381320000	-2.3724790000	-1.6671040000
H	-4.6807600000	-3.2132790000	-1.6137750000
H	-6.2013520000	-2.5296870000	0.2297710000
H	-5.3822110000	-1.0164160000	2.0206510000
H	-3.0404400000	-0.1686700000	1.9623440000
C	2.2024930000	-1.7615920000	-0.1657780000
C	3.3325060000	-1.1819490000	-0.7661590000
C	4.5206000000	-1.9043650000	-0.8492230000
C	4.5945550000	-3.2019690000	-0.3393890000
C	3.4711170000	-3.7851320000	0.2519700000
C	2.2793050000	-3.0731920000	0.3387790000
H	3.2879830000	-0.1840410000	-1.1849760000
H	5.3885990000	-1.4533000000	-1.3201800000
H	5.5246720000	-3.7585760000	-0.4050770000
H	3.5239720000	-4.7940300000	0.6492880000
H	1.4046220000	-3.5200180000	0.7992320000
C	1.6422100000	1.3478120000	0.2149970000
C	2.2198030000	1.5648250000	1.4654180000
C	3.1589430000	2.5880930000	1.6031200000

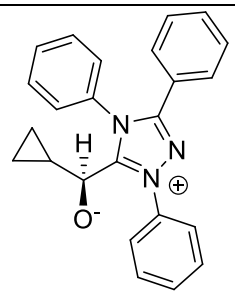
C	3.5028950000	3.3791550000	0.5049880000
C	2.9102250000	3.1531200000	-0.7401590000
C	1.9733190000	2.1306930000	-0.8934100000
H	1.9406110000	0.9451690000	2.3116500000
H	3.6181280000	2.7661530000	2.5703450000
H	4.2334880000	4.1740710000	0.6188160000
H	3.1779680000	3.7684830000	-1.5933790000
H	1.5137040000	1.9339490000	-1.8578180000

Thermodynamic data

Zero-point correction= 0.410790 (Hartree/Particle)
Thermal correction to Energy= 0.434185
Thermal correction to Enthalpy= 0.435129
Thermal correction to Gibbs Free Energy= 0.355427
Sum of electronic and zero-point Energies= -1166.616485
Sum of electronic and thermal Energies= -1166.593090
Sum of electronic and thermal Enthalpies= -1166.592146
Sum of electronic and thermal Free Energies= -1166.671847

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.455	91.967	167.746

B3LYP/6-31G*	**Job2deko2**



xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4177980000	1.8010720000	-0.2315600000
H	-0.7131000000	2.5751520000	0.1654500000
O	-1.4738290000	1.7139660000	-1.5746480000
C	-2.7140100000	2.0478830000	0.5448600000
C	-3.0490890000	3.4689800000	0.9176400000
C	-2.6436410000	2.4892490000	1.9900100000
H	-3.5557580000	1.4220740000	0.2683060000
H	-4.0881840000	3.7831600000	0.8671090000
H	-2.3371830000	4.2429570000	0.6394600000
H	-3.3996760000	2.1269210000	2.6816750000
H	-1.6579220000	2.6087250000	2.4363760000
C	-0.7205330000	0.4725370000	0.0725370000
N	-1.2035510000	-0.7884390000	0.0921630000
N	-0.1972980000	-1.7326490000	0.0903140000
C	0.9152470000	-1.0494100000	0.0743310000
N	0.6422090000	0.3182430000	0.0773290000
C	-2.5477420000	-1.2514590000	-0.0923940000
C	-3.0144240000	-2.2918900000	0.7124770000
C	-4.2976160000	-2.7902080000	0.4946880000
C	-5.0979450000	-2.2506640000	-0.5156420000
C	-4.6107520000	-1.2140460000	-1.3145610000
C	-3.3247690000	-0.7082240000	-1.1184360000
H	-2.3751140000	-2.7041390000	1.4859800000
H	-4.6720600000	-3.5987420000	1.1161470000
H	-6.0984430000	-2.6412010000	-0.6809390000
H	-5.2294100000	-0.7988540000	-2.1053190000
H	-2.9091390000	0.1086120000	-1.7100380000
C	1.5941590000	1.3965210000	0.0090810000

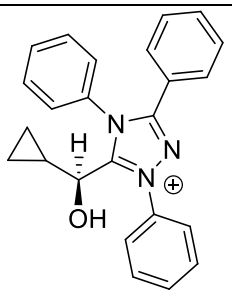
C	2.5676290000	1.5243310000	1.0013930000
C	3.5104010000	2.5471480000	0.8976870000
C	3.4669470000	3.4340560000	-0.1802480000
C	2.4731950000	3.3045320000	-1.1537560000
C	1.5286790000	2.2810730000	-1.0723010000
H	2.5872450000	0.8326420000	1.8377010000
H	4.2737080000	2.6524110000	1.6632830000
H	4.2016590000	4.2309930000	-0.2555800000
H	2.4275800000	4.0052920000	-1.9825610000
H	0.7048840000	2.1797470000	-1.7804160000
C	2.2387310000	-1.6932400000	0.0444790000
C	3.2897340000	-1.2069640000	-0.7491180000
C	4.5068500000	-1.8852510000	-0.7857390000
C	4.6889820000	-3.0499230000	-0.0378110000
C	3.6430260000	-3.5428340000	0.7454450000
C	2.4239160000	-2.8708890000	0.7868940000
H	3.1530390000	-0.3134000000	-1.3479040000
H	5.3123110000	-1.5043020000	-1.4071210000
H	5.6405570000	-3.5734490000	-0.0685000000
H	3.7764120000	-4.4509650000	1.3265450000
H	1.6046380000	-3.2497420000	1.3891460000

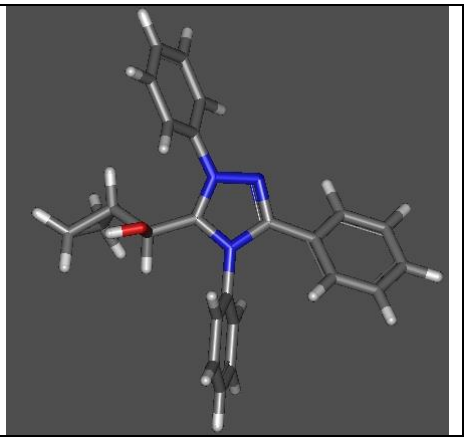
Thermodynamic data

Zero-point correction= 0.397099 (Hartree/Particle)
Thermal correction to Energy= 0.419835
Thermal correction to Enthalpy= 0.420779
Thermal correction to Gibbs Free Energy= 0.343713
Sum of electronic and zero-point Energies= -1166.179252
Sum of electronic and thermal Energies= -1166.156517
Sum of electronic and thermal Enthalpies= -1166.155572
Sum of electronic and thermal Free Energies= -1166.232639

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	263.450	90.242	162.200

B3LYP/6-31G*	**Job2prko2**





xyz-matrix

50

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3652400000	1.8062870000	-0.1800370000
H	-0.5870710000	2.5199480000	0.1257740000
O	-1.7279910000	2.0359310000	-1.5411310000
H	-2.2592630000	2.8505940000	-1.5617530000
C	-2.5165140000	1.9383070000	0.7918460000
C	-2.8329400000	3.3229390000	1.3268380000
C	-2.2337670000	2.2875250000	2.2362650000
H	-3.3648010000	1.2905710000	0.5975380000
H	-3.8790770000	3.5842510000	1.4514680000
H	-2.2002810000	4.1535190000	1.0217270000
H	-2.8623520000	1.8313500000	2.9943750000
H	-1.1987570000	2.4228210000	2.5408340000
C	-0.6831340000	0.4557870000	-0.1661870000

N	-1.2069940000	-0.7725970000	-0.1424180000
N	-0.2357430000	-1.7320260000	-0.0705220000
C	0.9085520000	-1.0837160000	-0.0646600000
N	0.6653560000	0.2866360000	-0.1334500000
C	-2.5812760000	-1.2010040000	-0.2281360000
C	-3.0298110000	-2.1505800000	0.6911710000
C	-4.3433870000	-2.6051160000	0.5957980000
C	-5.1857480000	-2.1169180000	-0.4066030000
C	-4.7143710000	-1.1749330000	-1.3232980000
C	-3.4001670000	-0.7123360000	-1.2474490000
H	-2.3601380000	-2.5261580000	1.4570330000
H	-4.7072010000	-3.3420060000	1.3048760000
H	-6.2074590000	-2.4771600000	-0.4775430000
H	-5.3638570000	-0.8073930000	-2.1116670000
H	-3.0165860000	0.0119050000	-1.9574490000
C	1.6366220000	1.3598980000	-0.1339280000
C	2.4253960000	1.5640070000	0.9994050000
C	3.3663340000	2.5932930000	0.9850470000
C	3.5058640000	3.4030080000	-0.1451320000
C	2.7027660000	3.1898260000	-1.2678800000
C	1.7600170000	2.1607500000	-1.2716210000
H	2.3100800000	0.9262360000	1.8700410000
H	3.9883200000	2.7619760000	1.8584590000
H	4.2407950000	4.2020730000	-0.1498660000
H	2.8099230000	3.8203660000	-2.1449360000
H	1.1243650000	1.9850320000	-2.1340740000
C	2.2115880000	-1.7537120000	0.0085430000
C	3.3408380000	-1.2796530000	-0.6798890000

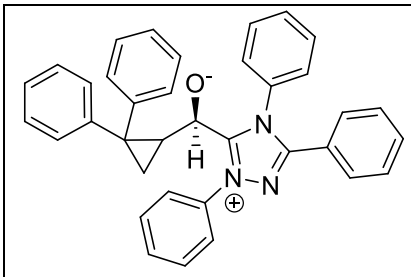
C	4.5391570000	-1.9864090000	-0.6123700000
C	4.6226280000	-3.1621240000	0.1365910000
C	3.4990430000	-3.6412820000	0.8144400000
C	2.2957490000	-2.9452820000	0.7499870000
H	3.2838890000	-0.3803270000	-1.2826770000
H	5.4069800000	-1.6212510000	-1.1528730000
H	5.5605520000	-3.7070470000	0.1874860000
H	3.5597220000	-4.5574510000	1.3936630000
H	1.4186160000	-3.3147500000	1.2708980000

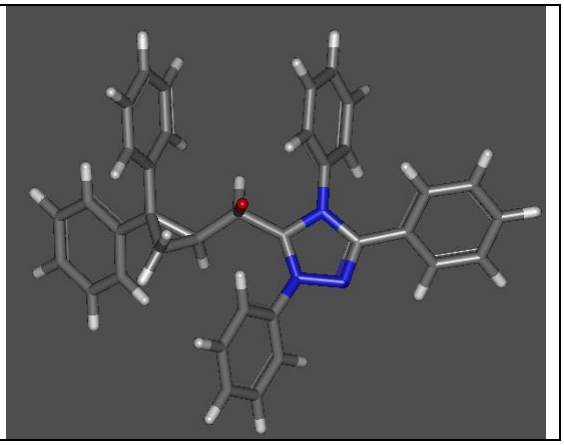
Thermodynamic data

Zero-point correction= 0.410870 (Hartree/Particle)
Thermal correction to Energy= 0.434188
Thermal correction to Enthalpy= 0.435132
Thermal correction to Gibbs Free Energy= 0.356025
Sum of electronic and zero-point Energies= -1166.617833
Sum of electronic and thermal Energies= -1166.594515
Sum of electronic and thermal Enthalpies= -1166.593571
Sum of electronic and thermal Free Energies= -1166.672678

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.457	91.904	166.495

B3LYP/6-31G*	**Job3de**





xyz-matrix

69

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.4361490000	0.1036700000	0.5969670000
H	-0.4615190000	1.0829710000	0.0683300000
O	-0.2293620000	0.1923350000	1.9276010000
C	-1.6925280000	-0.6618540000	0.1032680000
C	-3.0695310000	0.0336300000	0.1478850000
C	-2.7024990000	-1.0752830000	1.1208950000
H	-1.5380640000	-1.2986010000	-0.7659530000
H	-3.2210280000	-2.0252220000	1.0249110000
H	-2.4442050000	-0.7780720000	2.1339100000
C	0.8850700000	-0.5178180000	0.1557160000
N	1.3230340000	-1.7922910000	0.2037320000
N	2.6828680000	-1.8849800000	-0.0051230000
C	3.0856880000	-0.6556390000	-0.1889050000
N	2.0064190000	0.2232250000	-0.1127050000
C	0.6276530000	-2.9745300000	0.6214870000
C	-0.1311270000	-2.9375750000	1.7918260000
C	-0.7514970000	-4.1131650000	2.2166350000
C	-0.6023080000	-5.2976310000	1.4923330000
C	0.1724180000	-5.3146720000	0.3293310000
C	0.7949220000	-4.1491880000	-0.1137910000
H	-0.2284750000	-1.9893370000	2.3192450000
H	-1.3475650000	-4.1012310000	3.1248200000
H	-1.0856810000	-6.2088220000	1.8341160000
H	0.2932690000	-6.2354620000	-0.2342150000
H	1.4102160000	-4.1446590000	-1.0074160000

C	4.4985930000	-0.3129930000	-0.4192350000
C	5.1014610000	0.8076660000	0.1737220000
C	6.4580680000	1.0565290000	-0.0267540000
C	7.2247080000	0.1958480000	-0.8145310000
C	6.6312110000	-0.9253620000	-1.3985890000
C	5.2763680000	-1.1812100000	-1.2023260000
H	4.5184740000	1.4727370000	0.8010690000
H	6.9173070000	1.9228760000	0.4406510000
H	8.2813610000	0.3958280000	-0.9693970000
H	7.2231010000	-1.6012840000	-2.0092520000
H	4.8088530000	-2.0529830000	-1.6483150000
C	2.0432640000	1.6600240000	-0.2250770000
C	1.5818880000	2.4310940000	0.8463070000
C	1.6507840000	3.8207380000	0.7434370000
C	2.1801600000	4.4241370000	-0.3998410000
C	2.6269030000	3.6371970000	-1.4637790000
C	2.5542060000	2.2467160000	-1.3843890000
H	1.1224530000	1.9248840000	1.6965300000
H	1.2818380000	4.4317730000	1.5620540000
H	2.2352080000	5.5072220000	-0.4673320000
H	3.0265350000	4.1028270000	-2.3600400000
H	2.8915540000	1.6248590000	-2.2076210000
C	-3.1237820000	1.4532340000	0.6558710000
C	-3.6301170000	1.7633690000	1.9235420000
C	-3.6942760000	3.0845820000	2.3691980000
C	-3.2511520000	4.1241050000	1.5505820000
C	-2.7460240000	3.8319070000	0.2819570000
C	-2.6857920000	2.5097540000	-0.1590460000

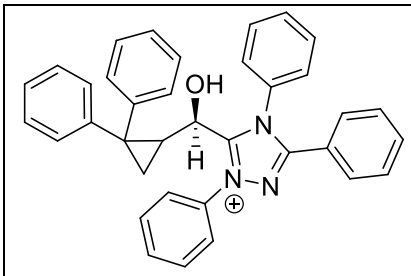
H	-3.9754600000	0.9599810000	2.5677560000
H	-4.0907500000	3.3005110000	3.3581510000
H	-3.2996240000	5.1533140000	1.8973170000
H	-2.3982970000	4.6330510000	-0.3656450000
H	-2.3049040000	2.2895160000	-1.1533130000
C	-4.0607670000	-0.3231890000	-0.9409730000
C	-5.0550390000	0.5801300000	-1.3509690000
C	-5.9815910000	0.2432030000	-2.3394690000
C	-5.9457400000	-1.0103990000	-2.9475300000
C	-4.9714540000	-1.9258180000	-2.5462780000
C	-4.0476020000	-1.5879650000	-1.5589070000
H	-5.1097260000	1.5598710000	-0.8900950000
H	-6.7366700000	0.9697280000	-2.6299840000
H	-6.6662650000	-1.2730450000	-3.7175750000
H	-4.9286210000	-2.9123370000	-3.0017410000
H	-3.3110130000	-2.3306930000	-1.2665050000

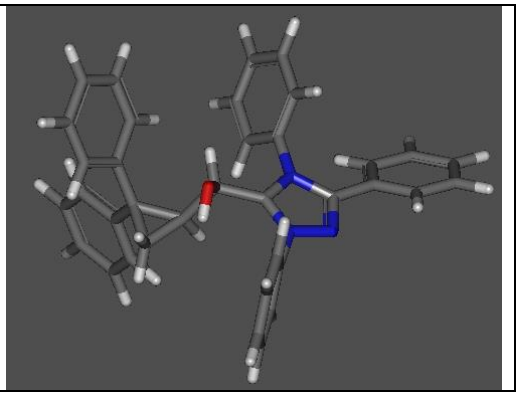
Thermodynamic data

Zero-point correction= 0.559193 (Hartree/Particle)
Thermal correction to Energy= 0.591098
Thermal correction to Enthalpy= 0.592042
Thermal correction to Gibbs Free Energy= 0.493011
Sum of electronic and zero-point Energies= -1628.116893
Sum of electronic and thermal Energies= -1628.084988
Sum of electronic and thermal Enthalpies= -1628.084043
Sum of electronic and thermal Free Energies= -1628.183074

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	370.919	128.151	208.428

B3LYP/6-31G*	**Job3pr**





xyz-matrix

70

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.4769160000	-0.7196440000	0.8550410000
H	-0.6523260000	0.2370100000	1.3560130000
O	-0.6865420000	-1.6948870000	1.8510720000
H	-0.8210040000	-2.5536630000	1.4174800000
C	-1.3818070000	-0.8289840000	-0.3843870000
C	-2.8525310000	-0.3777610000	-0.3691510000
C	-2.4886980000	-1.8481640000	-0.4669600000
H	-0.8637020000	-0.6204270000	-1.3173450000
H	-2.6492740000	-2.3602060000	-1.4109140000
H	-2.6902140000	-2.4552550000	0.4107940000
C	0.9832970000	-0.7064380000	0.4244330000
N	1.7617350000	-1.7427980000	0.1109760000
N	3.0285350000	-1.3460890000	-0.2282010000
C	3.0285850000	-0.0368000000	-0.1156920000
N	1.7613480000	0.3969530000	0.2881880000
C	1.4295420000	-3.1487980000	0.0501460000
C	1.3969790000	-3.8994100000	1.2269300000
C	1.1193210000	-5.2643870000	1.1410820000

C	0.8949110000	-5.8593570000	-0.1029480000
C	0.9471190000	-5.0945150000	-1.2705400000
C	1.2190010000	-3.7281560000	-1.2008640000
H	1.5824480000	-3.4227780000	2.1835060000
H	1.0894220000	-5.8621620000	2.0466270000
H	0.6851400000	-6.9229230000	-0.1627810000
H	0.7816290000	-5.5599960000	-2.2370480000
H	1.2786640000	-3.1225150000	-2.0994400000
C	4.2168740000	0.7888840000	-0.3576370000
C	4.1444910000	2.0867800000	-0.8904010000
C	5.3153110000	2.8000330000	-1.1371200000
C	6.5596100000	2.2313950000	-0.8575410000
C	6.6358160000	0.9379870000	-0.3351140000
C	5.4727320000	0.2158100000	-0.0873360000
H	3.1872880000	2.5338390000	-1.1319890000
H	5.2544170000	3.8001050000	-1.5552640000
H	7.4683880000	2.7939590000	-1.0497280000
H	7.6015580000	0.4919150000	-0.1184880000
H	5.5250750000	-0.7893510000	0.3175250000
C	1.3431740000	1.7500890000	0.5939630000
C	1.7986650000	2.3474220000	1.7697390000
C	1.4047750000	3.6545850000	2.0560010000
C	0.5667830000	4.3447600000	1.1768630000
C	0.1151490000	3.7310250000	0.0058770000
C	0.5031100000	2.4241080000	-0.2946890000
H	2.4491290000	1.8004540000	2.4448440000
H	1.7525040000	4.1306910000	2.9673240000
H	0.2651970000	5.3625870000	1.4044160000

H	-0.5356960000	4.2666130000	-0.6781340000
H	0.1638490000	1.9411780000	-1.2061870000
C	-3.4159410000	0.1063720000	0.9459780000
C	-4.3647320000	-0.6442850000	1.6509800000
C	-4.8953670000	-0.1771950000	2.8546040000
C	-4.4848630000	1.0517740000	3.3724220000
C	-3.5478550000	1.8159340000	2.6745040000
C	-3.0217010000	1.3480070000	1.4698920000
H	-4.7004910000	-1.5970180000	1.2507580000
H	-5.6328470000	-0.7730280000	3.3848340000
H	-4.8965470000	1.4145710000	4.3098050000
H	-3.2297480000	2.7786960000	3.0651520000
H	-2.3125790000	1.9615610000	0.9189510000
C	-3.3685170000	0.3022210000	-1.6252330000
C	-4.3716560000	1.2803870000	-1.5546130000
C	-4.8584230000	1.8981530000	-2.7083380000
C	-4.3568390000	1.5533550000	-3.9620350000
C	-3.3649610000	0.5755170000	-4.0509450000
C	-2.8804690000	-0.0416180000	-2.8986940000
H	-4.7851680000	1.5599000000	-0.5925080000
H	-5.6385030000	2.6493120000	-2.6203460000
H	-4.7377330000	2.0325570000	-4.8591400000
H	-2.9698210000	0.2847290000	-5.0205100000
H	-2.1218760000	-0.8122410000	-3.0128220000

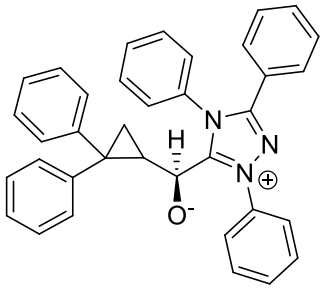
Thermodynamic data

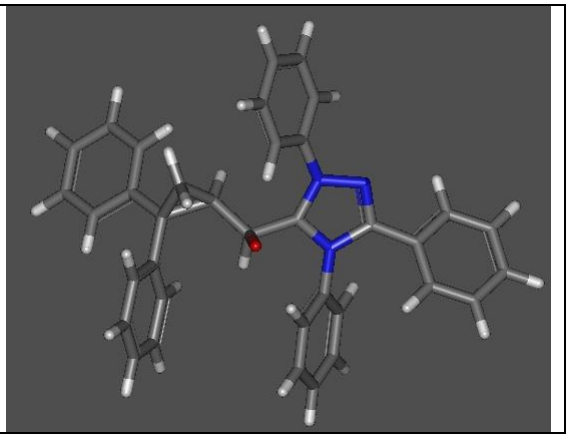
Zero-point correction= 0.572755 (Hartree/Particle)
Thermal correction to Energy= 0.605306
Thermal correction to Enthalpy= 0.606250

Thermal correction to Gibbs Free Energy= 0.503293
Sum of electronic and zero-point Energies= -1628.551361
Sum of electronic and thermal Energies= -1628.518810
Sum of electronic and thermal Enthalpies= -1628.517866
Sum of electronic and thermal Free Energies= -1628.620823

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	379.835	129.808	216.691

B3LYP/6-31G*	**Job3deko2**





xyz-matrix

69

XYZ file generated by gabedit : coordinates in Angstrom

C	0.4360930000	-0.1039180000	-0.5968280000
H	0.4614240000	-1.0831550000	-0.0680610000
O	0.2292200000	-0.1927110000	-1.9274700000
C	1.6924650000	0.6616560000	-0.1033000000
C	2.7023630000	1.0750470000	-1.1210570000
C	3.0694620000	-0.0337050000	-0.1479090000
H	1.5380150000	1.2985000000	0.7658600000
H	3.2207960000	2.0250460000	-1.0252280000
H	2.4441050000	0.7775600000	-2.1340030000
C	-0.8850940000	0.5176760000	-0.1556850000
N	-1.3229200000	1.7921990000	-0.2037050000

N	-2.6827430000	1.8850320000	0.0052520000
C	-3.0856810000	0.6557200000	0.1890200000
N	-2.0064850000	-0.2232450000	0.1128030000
C	-0.6274950000	2.9744030000	-0.6215100000
C	-0.7949010000	4.1491140000	0.1136480000
C	-0.1723640000	5.3145760000	-0.3294850000
C	0.6025140000	5.2974630000	-1.4923790000
C	0.7518020000	4.1129530000	-2.2165900000
C	0.1313940000	2.9373850000	-1.7917790000
H	-1.4103000000	4.1446350000	1.0072000000
H	-0.2933060000	6.2354070000	0.2339730000
H	1.0859220000	6.2086390000	-1.8341550000
H	1.3479870000	4.1009680000	-3.1246970000
H	0.2287840000	1.9891320000	-2.3191640000
C	-4.4986230000	0.3131730000	0.4192970000
C	-5.2764480000	1.1814460000	1.2022650000
C	-6.6313270000	0.9256910000	1.3983660000
C	-7.2248210000	-0.1955140000	0.8142900000
C	-6.4581390000	-1.0562560000	0.0266240000
C	-5.1014930000	-0.8074750000	-0.1736940000
H	-4.8089340000	2.0532160000	1.6482730000
H	-7.2232520000	1.6016610000	2.0089420000
H	-8.2815000000	-0.3954180000	0.9690800000
H	-6.9173510000	-1.9226020000	-0.4408080000
H	-4.5184990000	-1.4725920000	-0.8009800000
C	-2.0433680000	-1.6600520000	0.2251120000
C	-1.5822530000	-2.4311230000	-0.8463810000
C	-1.6513040000	-3.8207590000	-0.7435680000

C	-2.1805590000	-4.4241440000	0.3997770000
C	-2.6269760000	-3.6372000000	1.4638450000
C	-2.5541700000	-2.2467240000	1.3844890000
H	-1.1229170000	-1.9249220000	-1.6966810000
H	-1.2826100000	-4.4318000000	-1.5622940000
H	-2.2357550000	-5.5072240000	0.4672260000
H	-3.0265040000	-4.1028220000	2.3601590000
H	-2.8913490000	-1.6248440000	2.2077800000
C	4.0607670000	0.3232920000	0.9408470000
C	5.0550030000	-0.5799980000	1.3510120000
C	5.9815510000	-0.2429100000	2.3394490000
C	5.9457480000	1.0108210000	2.9472560000
C	4.9715140000	1.9262050000	2.5458260000
C	4.0476520000	1.5881880000	1.5585180000
H	5.1096430000	-1.5598300000	0.8903300000
H	6.7366070000	-0.9693970000	2.6301200000
H	6.6662870000	1.2735920000	3.7172470000
H	4.9287160000	2.9128120000	3.0011010000
H	3.3110670000	2.3308690000	1.2659790000
C	3.1238340000	-1.4533530000	-0.6557180000
C	3.6303200000	-1.7635510000	-1.9233170000
C	3.6946390000	-3.0847970000	-2.3688260000
C	3.2515180000	-4.1242800000	-1.5501400000
C	2.7462200000	-3.8320030000	-0.2816110000
C	2.6858260000	-2.5098060000	0.1592540000
H	3.9756090000	-0.9601640000	-2.5675660000
H	4.0912090000	-3.3008180000	-3.3577200000
H	3.3000860000	-5.1535090000	-1.8968020000

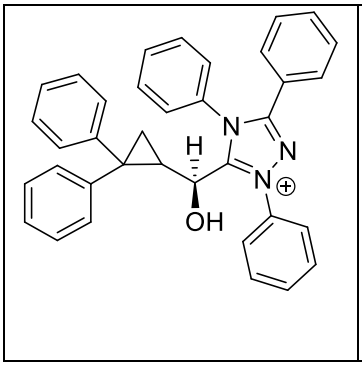
H	2.3984640000	-4.6330980000	0.3660370000
H	2.3047990000	-2.2895080000	1.1534550000

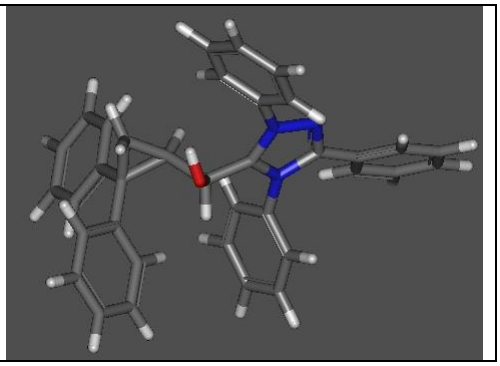
Thermodynamic data

Zero-point correction=	0.559193 (Hartree/Particle)
Thermal correction to Energy=	0.591098
Thermal correction to Enthalpy=	0.592042
Thermal correction to Gibbs Free Energy=	0.493013
Sum of electronic and zero-point Energies=	-1628.116892
Sum of electronic and thermal Energies=	-1628.084987
Sum of electronic and thermal Enthalpies=	-1628.084043
Sum of electronic and thermal Free Energies=	-1628.183073

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	370.920	128.151	208.425

B3LYP/6-31G*	**Job3prko2**





xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	0.4008390000	0.9868000000	-0.6673240000
H	0.6357770000	0.1678230000	-1.3553220000
O	0.4955930000	2.1514400000	-1.4513340000
H	0.5439750000	2.9229360000	-0.8623160000
C	1.3459620000	0.9154730000	0.5456250000
C	2.4279210000	1.9438070000	0.7574170000

C	2.8281010000	0.5230790000	0.4064750000
H	0.8703110000	0.5399050000	1.4480950000
H	2.6152730000	2.2980070000	1.7670670000
H	2.5703780000	2.6922320000	-0.0164070000
C	-1.0426650000	0.7542450000	-0.2378160000
N	-1.9754860000	1.6565230000	0.0756430000
N	-3.1949720000	1.0727280000	0.2983260000
C	-3.0050530000	-0.2163590000	0.1294110000
N	-1.6665250000	-0.4521290000	-0.1957290000
C	-1.8600740000	3.0860640000	0.2023820000
C	-0.9145920000	3.6312790000	1.0736580000
C	-0.8287330000	5.0202420000	1.1881430000
C	-1.6914550000	5.8392430000	0.4571460000
C	-2.6470420000	5.2736420000	-0.3910320000
C	-2.7380700000	3.8893260000	-0.5248540000
H	-0.2770970000	2.9855420000	1.6689720000
H	-0.1004440000	5.4576090000	1.8639060000
H	-1.6253960000	6.9183590000	0.5550540000
H	-3.3216650000	5.9104320000	-0.9544360000
H	-3.4718190000	3.4352000000	-1.1815900000
C	-4.0766810000	-1.2097930000	0.2575380000
C	-5.3835990000	-0.8064250000	-0.0703720000
C	-6.4435140000	-1.6965660000	0.0702480000
C	-6.2136750000	-2.9911860000	0.5424970000
C	-4.9194780000	-3.3921790000	0.8797820000
C	-3.8508140000	-2.5097580000	0.7399050000
H	-5.5565350000	0.2004900000	-0.4352440000
H	-7.4488150000	-1.3803730000	-0.1904630000
H	-7.0421740000	-3.6847490000	0.6511340000
H	-4.7403370000	-4.3932160000	1.2599250000

H	-2.8552140000	-2.8294540000	1.0246460000
C	-1.0530550000	-1.7146460000	-0.5550260000
C	-1.3644830000	-2.2858120000	-1.7899970000
C	-0.7811190000	-3.5051180000	-2.1340290000
C	0.0999210000	-4.1361280000	-1.2521260000
C	0.4038520000	-3.5503690000	-0.0207270000
C	-0.1742680000	-2.3312480000	0.3375320000
H	-2.0515310000	-1.7861350000	-2.4656380000
H	-1.0159790000	-3.9594340000	-3.0914050000
H	0.5498850000	-5.0859120000	-1.5245200000
H	1.0896050000	-4.0381590000	0.6647610000
H	0.0516250000	-1.8741470000	1.2956670000
C	3.4100580000	-0.3383330000	1.5137070000
C	4.4343920000	-1.2588580000	1.2467570000
C	4.9801700000	-2.0452000000	2.2634320000
C	4.5175070000	-1.9311640000	3.5731400000
C	3.5053330000	-1.0134730000	3.8579610000
C	2.9621060000	-0.2275480000	2.8424880000
H	4.8184120000	-1.3598970000	0.2383300000
H	5.7760800000	-2.7452770000	2.0248040000
H	4.9445380000	-2.5408740000	4.3639690000
H	3.1405650000	-0.9004250000	4.8752530000
H	2.1908290000	0.4903960000	3.1109310000
C	3.3568310000	0.2861230000	-0.9887980000
C	4.2589240000	1.1780040000	-1.5821740000
C	4.7639510000	0.9398190000	-2.8613630000
C	4.3740400000	-0.1978060000	-3.5690430000
C	3.4840440000	-1.1013110000	-2.9854530000
C	2.9837900000	-0.8629720000	-1.7047440000
H	4.5793640000	2.0609100000	-1.0359870000

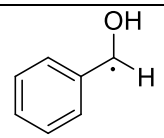
H	5.4652550000	1.6424100000	-3.3024180000
H	4.7653720000	-0.3824320000	-4.5652940000
H	3.1828890000	-1.9953350000	-3.5246450000
H	2.3147810000	-1.5871800000	-1.2460140000

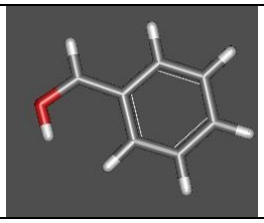
Thermodynamic data

Zero-point correction= 0.573104 (Hartree/Particle)
Thermal correction to Energy= 0.605461
Thermal correction to Enthalpy= 0.606406
Thermal correction to Gibbs Free Energy= 0.505707
Sum of electronic and zero-point Energies= -1628.551873
Sum of electronic and thermal Energies= -1628.519516
Sum of electronic and thermal Enthalpies= -1628.518572
Sum of electronic and thermal Free Energies= -1628.619271

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	379.933	129.681	211.938

B3LYP/6-31G*	**Benzaldehydradikal**





xyz-matrix

15

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4938410000	1.2452920000	0.0074270000
C	-0.0898070000	1.3029310000	0.2295400000
C	0.7042180000	0.1284260000	0.1729180000
C	0.0723800000	-1.1160270000	-0.1109950000

C	-1.3315080000	-1.1810670000	-0.3342040000
C	-2.1166170000	0.0008080000	-0.2751130000
H	-2.0786930000	2.1455590000	0.0544440000
H	0.3879520000	2.2409560000	0.4437710000
H	0.6610670000	-2.0129420000	-0.1569210000
H	-1.7938910000	-2.1273950000	-0.5473540000
H	-3.1772120000	-0.0463650000	-0.4434450000
C	2.0982210000	0.2509740000	0.4033060000
O	2.8109940000	-0.7519380000	0.3602380000
H	2.8114860000	-1.3055750000	-0.4206060000
H	2.5352470000	1.2263630000	0.6169870000

Thermodynamic data

Zero-point correction= 0.119793 (Hartree/Particle)
Thermal correction to Energy= 0.126838
Thermal correction to Enthalpy= 0.127782
Thermal correction to Gibbs Free Energy= 0.087808
Sum of electronic and zero-point Energies= -346.011317
Sum of electronic and thermal Energies= -346.004273
Sum of electronic and thermal Enthalpies= -346.003329
Sum of electronic and thermal Free Energies= -346.043302

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.592	26.982	84.131

B3LYP/6-31G*	**Aldehyd2**

xyz-matrix

12

XYZ file generated by gabedit : coordinates in Angstrom

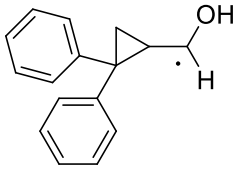
C	-0.3000640000	-0.1895800000	0.4920100000
C	-1.6126040000	-0.5351580000	-0.1699270000
C	-1.1594100000	0.9001700000	-0.1412840000
H	-0.3174100000	-0.1978760000	1.5881970000
C	0.9686920000	-0.5807690000	-0.1520930000
H	-2.4427480000	-0.8279380000	0.4665810000
H	-1.5667770000	-1.0571030000	-1.1215230000
H	-1.6748860000	1.5920580000	0.5191890000
H	-0.8165550000	1.3368030000	-1.0757230000
H	1.2754480000	-1.6198740000	-0.2303730000
O	2.0555100000	0.2561750000	-0.0512090000
H	1.7191720000	1.1565570000	0.0910810000

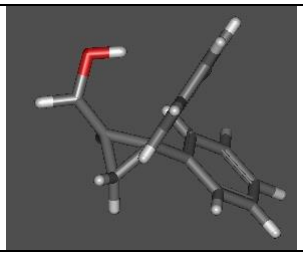
Thermodynamic data

```
Zero-point correction=                           0.101423
(Hartree/Particle)
 Thermal correction to Energy=                    0.107066
 Thermal correction to Enthalpy=                  0.108010
 Thermal correction to Gibbs Free Energy=         0.072138
 Sum of electronic and zero-point Energies=           -231.658544
 Sum of electronic and thermal Energies=              -231.652902
 Sum of electronic and thermal Enthalpies=            -231.651958
 Sum of electronic and thermal Free Energies=         -231.687830

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  67.185             19.885            75.499
```

B3LYP/6-31G*	**Aldehyd3**





xyz-matrix

32

XYZ file generated by gabedit : coordinates in Angstrom

C	0.0294610000	1.5573050000	1.7478770000
C	-0.0805820000	0.6236830000	0.5602070000
C	0.1857900000	2.1246660000	0.3576770000
H	-0.8848950000	1.7750160000	2.2922600000
H	0.9227290000	1.5197900000	2.3634500000
H	-0.6813610000	2.6802150000	-0.0147850000
C	1.5131020000	2.6150240000	-0.0774740000
C	1.0304180000	-0.3584930000	0.2509660000
C	1.0956920000	-0.9383840000	-1.0292590000
C	2.1142150000	-1.8297210000	-1.3667820000
C	3.0876410000	-2.1715650000	-0.4259030000
C	3.0256680000	-1.6172600000	0.8521440000
C	2.0073500000	-0.7216170000	1.1862110000
H	0.3226730000	-0.7069300000	-1.7585880000
H	2.1419250000	-2.2622910000	-2.3635510000
H	3.8812190000	-2.8668930000	-0.6852140000
H	3.7710620000	-1.8821440000	1.5975750000
H	1.9739080000	-0.3085010000	2.1892090000
C	-1.4651330000	0.1134940000	0.2233960000
C	-2.1678000000	0.5548540000	-0.9048230000
C	-3.4329990000	0.0442180000	-1.2066480000
C	-4.0145980000	-0.9188070000	-0.3827240000
C	-3.3220580000	-1.3702710000	0.7439490000
C	-2.0599020000	-0.8595500000	1.0410500000
H	-1.7236550000	1.3069130000	-1.5518200000
H	-3.9619110000	0.4016400000	-2.0864340000
H	-4.9997220000	-1.3148410000	-0.6143600000
H	-3.7672070000	-2.1204380000	1.3925290000
H	-1.5231620000	-1.2153030000	1.9171300000
O	1.9575440000	2.3614000000	-1.3507690000

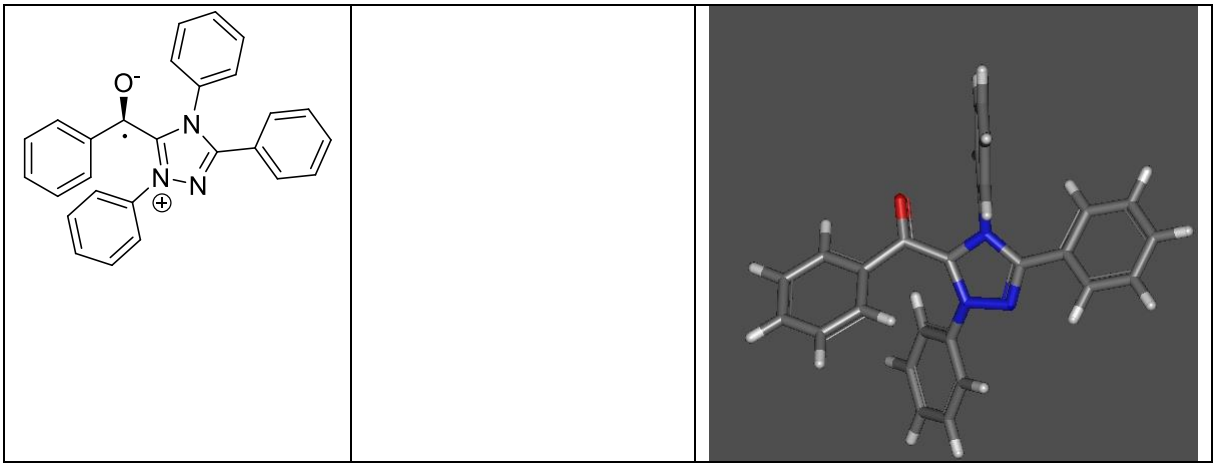
H	1.7020540000	1.4512390000	-1.5820440000
H	1.8883990000	3.5658670000	0.2916160000

Thermodynamic data

Zero-point correction= 0.263563 (Hartree/Particle)
Thermal correction to Energy= 0.278147
Thermal correction to Enthalpy= 0.279091
Thermal correction to Gibbs Free Energy= 0.220188
Sum of electronic and zero-point Energies= -693.598448
Sum of electronic and thermal Energies= -693.583864
Sum of electronic and thermal Enthalpies= -693.582920
Sum of electronic and thermal Free Energies= -693.641823

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	174.540	57.837	123.972

B3LYP/6-31G*	**Job1radde**



xyz-matrix

51

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2128200000	-1.4408480000	0.3960280000
O	-0.7796080000	-2.4530350000	1.0070360000
C	-2.5729160000	-1.4768340000	-0.2241300000
C	-3.4986450000	-2.3922720000	0.3039010000

C	-4.7617250000	-2.5351100000	-0.2640010000
C	-5.1192630000	-1.7769880000	-1.3823720000
C	-4.1997780000	-0.8793010000	-1.9289140000
C	-2.9377930000	-0.7301070000	-1.3559730000
H	-3.1963570000	-2.9916240000	1.1565490000
H	-5.4686170000	-3.2425300000	0.1624710000
H	-6.1037800000	-1.8901950000	-1.8288320000
H	-4.4627960000	-0.2976840000	-2.8087700000
H	-2.2285670000	-0.0409150000	-1.8045280000
C	-0.3665100000	-0.2862020000	0.2746840000
N	1.0395570000	-0.3270380000	0.2890870000
C	1.4831870000	0.9591160000	0.0037470000
N	0.4922240000	1.7982550000	-0.1185930000
N	-0.6591400000	1.0551180000	0.0725250000
C	-1.8488130000	1.7760690000	0.3638350000
C	1.8467320000	-1.5131180000	0.1754730000
C	2.8838870000	1.3991750000	-0.1120240000
C	2.0709150000	-2.3224840000	1.2918960000
C	2.4381780000	-1.8144180000	-1.0524920000
C	2.9051170000	-3.4314520000	1.1743290000
C	3.2736590000	-2.9276210000	-1.1613180000
C	3.5098700000	-3.7349850000	-0.0492520000
H	3.0774260000	-4.0648840000	2.0396990000
H	4.1592560000	-4.6018720000	-0.1343170000
H	1.5747150000	-2.0909280000	2.2261670000
H	2.2466850000	-1.1805240000	-1.9130020000
H	3.7345710000	-3.1613140000	-2.1168120000
C	3.9210580000	0.8199110000	0.6357820000
C	3.1723410000	2.4805700000	-0.9613970000
C	5.2201300000	1.3137040000	0.5287820000

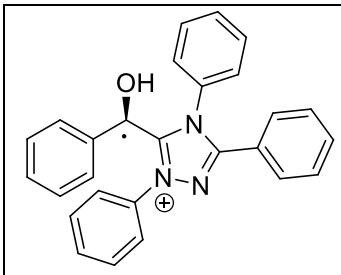
C	5.5014760000	2.3843870000	-0.3212330000
C	4.4723040000	2.9679710000	-1.0637850000
H	3.7151470000	-0.0072370000	1.3053210000
H	6.0137400000	0.8597840000	1.1156160000
H	2.3672570000	2.9301580000	-1.5329670000
H	6.5165930000	2.7629670000	-0.4038580000
H	4.6825990000	3.8023300000	-1.7271280000
C	-2.7392160000	1.3384690000	1.3508540000
C	-2.0970000000	2.9653000000	-0.3338150000
C	-3.8835800000	2.0856510000	1.6217960000
C	-3.2410780000	3.7052200000	-0.0464580000
C	-4.1427930000	3.2682640000	0.9268320000
H	-2.5352500000	0.4287780000	1.9032750000
H	-1.3874960000	3.3008150000	-1.0815990000
H	-4.5714400000	1.7407490000	2.3886770000
H	-3.4294560000	4.6264930000	-0.5909390000
H	-5.0373990000	3.8451710000	1.1429010000

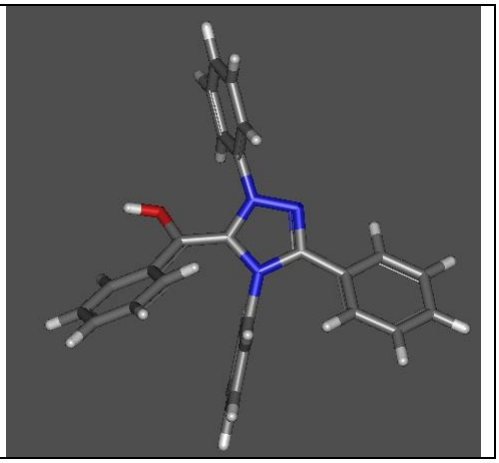
Thermodynamic data

Zero-point correction= 0.403004 (Hartree/Particle)
Thermal correction to Energy= 0.427437
Thermal correction to Enthalpy= 0.428381
Thermal correction to Gibbs Free Energy= 0.345460
Sum of electronic and zero-point Energies= -1279.943044
Sum of electronic and thermal Energies= -1279.918611
Sum of electronic and thermal Enthalpies= -1279.917667
Sum of electronic and thermal Free Energies= -1280.000588

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	268.220	97.162	174.522

B3LYP/6-31G*	**Job1radpr**





xyz-matrix

52

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.6070220000	-1.0061160000	-0.3999370000
O	-2.6472230000	-0.7277010000	-1.2258640000
H	-3.3553210000	-1.3815460000	-1.0836730000
C	-1.4744620000	-2.3361060000	0.1632250000
C	-0.9979120000	-2.5377110000	1.4768330000
C	-0.9766570000	-3.8135160000	2.0279990000
C	-1.4300670000	-4.9099400000	1.2867150000
C	-1.9089660000	-4.7240000000	-0.0134220000
C	-1.9361810000	-3.4509990000	-0.5728210000
H	-0.6908230000	-1.6847800000	2.0750500000
H	-0.6252320000	-3.9543120000	3.0458160000
H	-1.4149640000	-5.9039990000	1.7230910000
H	-2.2531500000	-5.5742050000	-0.5943560000
H	-2.2752440000	-3.3196340000	-1.5971750000
C	-0.7518420000	0.1082800000	-0.1655970000
N	-1.1148190000	1.4160240000	-0.0963940000
N	-0.0360180000	2.2228760000	0.1202180000
C	1.0128300000	1.4305020000	0.1534620000
N	0.6206850000	0.1013220000	-0.0127710000

C	1.4806230000	-0.9933980000	-0.4270270000
C	1.7237840000	-1.1563590000	-1.7921410000
C	2.5581320000	-2.1910380000	-2.2149820000
C	3.1405620000	-3.0482190000	-1.2791580000
C	2.8888350000	-2.8747710000	0.0832640000
C	2.0532130000	-1.8452160000	0.5166740000
H	1.2740070000	-0.4779720000	-2.5109880000
H	2.7560800000	-2.3212000000	-3.2743600000
H	3.7924240000	-3.8503660000	-1.6114390000
H	3.3409310000	-3.5406600000	0.8116980000
H	1.8482450000	-1.7072220000	1.5729130000
C	2.3782080000	1.9481700000	0.2886810000
C	3.3948560000	1.2601890000	0.9706050000
C	4.6599580000	1.8300250000	1.0919340000
C	4.9232040000	3.0850070000	0.5396140000
C	3.9126380000	3.7786840000	-0.1307030000
C	2.6455770000	3.2183530000	-0.2554780000
H	3.2004510000	0.2961460000	1.4234910000
H	5.4390570000	1.2949760000	1.6262480000
H	5.9121380000	3.5234260000	0.6351300000
H	4.1121590000	4.7562030000	-0.5588270000
H	1.8573160000	3.7521280000	-0.7755020000
C	-2.4316160000	2.0086800000	-0.0470640000
C	-2.9252220000	2.4143470000	1.1929890000
C	-4.1714970000	3.0376800000	1.2504720000
C	-4.8996620000	3.2557950000	0.0790290000
C	-4.3843700000	2.8544720000	-1.1557430000
C	-3.1405330000	2.2285120000	-1.2274760000
H	-2.3392820000	2.2525630000	2.0921960000
H	-4.5681550000	3.3568630000	2.2091840000

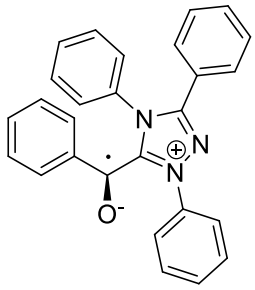
H	-5.8675660000	3.7455090000	0.1274460000
H	-4.9467510000	3.0341710000	-2.0667420000
H	-2.7259370000	1.9161110000	-2.1793280000

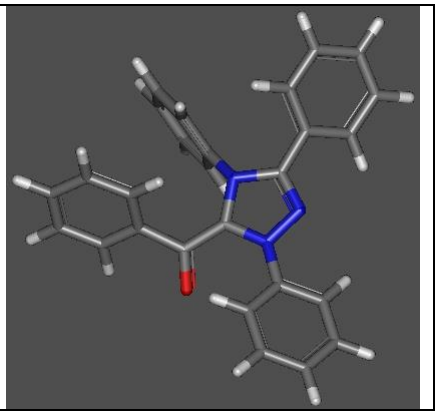
Thermodynamic data

Zero-point correction= 0.415939 (Hartree/Particle)
Thermal correction to Energy= 0.440731
Thermal correction to Enthalpy= 0.441675
Thermal correction to Gibbs Free Energy= 0.357235
Sum of electronic and zero-point Energies= -1280.331430
Sum of electronic and thermal Energies= -1280.306638
Sum of electronic and thermal Enthalpies= -1280.305694
Sum of electronic and thermal Free Energies= -1280.390134

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	276.563	98.385	177.719

B3LYP/6-31G*	**Job1raddeko2**





xyz-matrix

51

XYZ file generated by gabedit : coordinates in Angstrom

C	1.4227450000	-1.3904850000	-0.3875900000
O	2.4532550000	-1.4112130000	-1.1049080000
C	0.8539710000	-2.6664400000	0.1421350000
C	1.0360480000	-3.8358750000	-0.6136360000
C	0.6005440000	-5.0669730000	-0.1313010000

C	-0.0046860000	-5.1562800000	1.1260990000
C	-0.1655760000	-4.0040780000	1.8980700000
C	0.2604900000	-2.7689690000	1.4097590000
H	1.5326100000	-3.7547800000	-1.5753100000
H	0.7385280000	-5.9621290000	-0.7325440000
H	-0.3368140000	-6.1189690000	1.5060010000
H	-0.6107860000	-4.0693280000	2.8879390000
H	0.1588690000	-1.8808000000	2.0283610000
C	0.8373490000	-0.1239860000	-0.0267550000
N	1.4749020000	1.1050420000	-0.0487250000
N	0.5743100000	2.1380690000	0.0950860000
C	-0.5998960000	1.5881180000	0.2028960000
N	-0.5257400000	0.1896560000	0.1709340000
C	2.8581850000	1.4282220000	-0.0252140000
C	3.2551190000	2.6764440000	-0.5233250000
C	4.5976680000	3.0424160000	-0.4797560000
C	5.5512760000	2.1739230000	0.0553460000
C	5.1457860000	0.9352100000	0.5547760000
C	3.8055750000	0.5557690000	0.5236280000
H	2.5093710000	3.3471130000	-0.9331950000
H	4.8976370000	4.0106670000	-0.8713150000
H	6.5989540000	2.4598010000	0.0837570000
H	5.8767510000	0.2523680000	0.9788700000
H	3.5054120000	-0.4054140000	0.9171440000
C	-1.8244460000	2.3893050000	0.3478930000
C	-2.8894380000	1.9924920000	1.1702280000
C	-4.0118700000	2.8073310000	1.3077590000
C	-4.0844580000	4.0265390000	0.6322660000
C	-3.0230070000	4.4326750000	-0.1800250000
C	-1.9007780000	3.6215110000	-0.3231670000

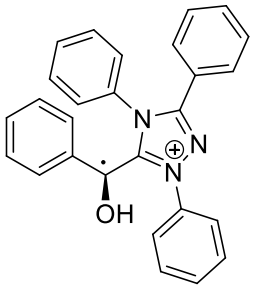
H	-2.8326310000	1.0596220000	1.7182360000
H	-4.8279920000	2.4907830000	1.9512760000
H	-4.9619100000	4.6581490000	0.7402410000
H	-3.0710520000	5.3813510000	-0.7073090000
H	-1.0733730000	3.9292010000	-0.9538900000
C	-1.5846000000	-0.6242020000	-0.3879350000
C	-2.4802980000	-1.2953730000	0.4432050000
C	-3.5107190000	-2.0498880000	-0.1190670000
C	-3.6382950000	-2.1399270000	-1.5054380000
C	-2.7318930000	-1.4744480000	-2.3337490000
C	-1.7030770000	-0.7155930000	-1.7775650000
H	-2.3607780000	-1.2384990000	1.5196830000
H	-4.2073040000	-2.5737200000	0.5290400000
H	-4.4396370000	-2.7306160000	-1.9402720000
H	-2.8260030000	-1.5421180000	-3.4137550000
H	-0.9904930000	-0.1969670000	-2.4120030000

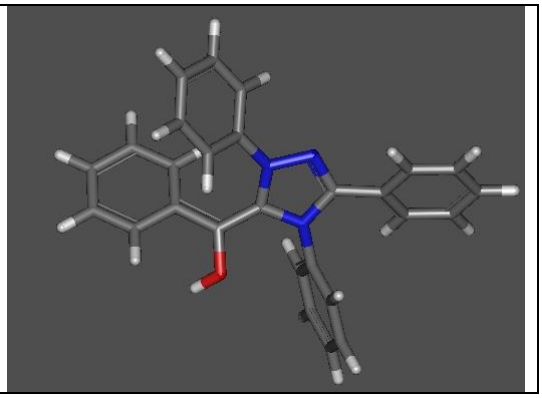
Thermodynamic data

Zero-point correction= 0.402991 (Hartree/Particle)
Thermal correction to Energy= 0.427398
Thermal correction to Enthalpy= 0.428342
Thermal correction to Gibbs Free Energy= 0.345472
Sum of electronic and zero-point Energies= -1279.938960
Sum of electronic and thermal Energies= -1279.914552
Sum of electronic and thermal Enthalpies= -1279.913608
Sum of electronic and thermal Free Energies= -1279.996478

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	268.196	97.135	174.414

B3LYP/6-31G*	**Job1radprko2**





xyz-matrix

52

XYZ file generated by gabedit : coordinates in Angstrom

C	1.2195260000	-1.3066800000	-0.4044320000
O	0.7146250000	-2.3059770000	-1.1718590000
H	1.2005350000	-3.1302760000	-0.9908000000
C	2.5569600000	-1.4111030000	0.1408870000
C	3.5138820000	-2.2186710000	-0.5170840000
C	4.7822210000	-2.3934000000	0.0254080000
C	5.1243870000	-1.7681110000	1.2278900000
C	4.1877700000	-0.9647360000	1.8878440000
C	2.9164310000	-0.7879350000	1.3573030000
H	3.2766170000	-2.6702580000	-1.4770680000
H	5.5098740000	-3.0073700000	-0.4964860000
H	6.1153960000	-1.9056610000	1.6493960000
H	4.4477840000	-0.4875600000	2.8277790000
H	2.1880530000	-0.1901660000	1.8961710000
C	0.3129490000	-0.2214460000	-0.2204730000
N	0.5905030000	1.1043020000	-0.1030940000
N	-0.5418790000	1.8369700000	0.1034310000
C	-1.5409130000	0.9806450000	0.0760450000

N	-1.0627000000	-0.3066640000	-0.1357270000
C	1.8286230000	1.8090360000	-0.2883060000
C	2.1642030000	2.8078910000	0.6274490000
C	3.3398990000	3.5306340000	0.4331730000
C	4.1624370000	3.2557670000	-0.6618830000
C	3.8049100000	2.2615600000	-1.5753520000
C	2.6293740000	1.5340070000	-1.3984150000
H	1.5080370000	3.0169470000	1.4654370000
H	3.6109090000	4.3101040000	1.1384170000
H	5.0764080000	3.8229540000	-0.8090070000
H	4.4328590000	2.0603150000	-2.4376410000
H	2.3316840000	0.7808420000	-2.1202560000
C	-2.9386300000	1.4063970000	0.2206700000
C	-3.9185270000	0.6210460000	0.8511630000
C	-5.2152960000	1.1107530000	0.9899820000
C	-5.5475230000	2.3772850000	0.5053630000
C	-4.5745660000	3.1648900000	-0.1148310000
C	-3.2755550000	2.6871920000	-0.2551150000
H	-3.6730630000	-0.3557170000	1.2500250000
H	-5.9660840000	0.5020050000	1.4844680000
H	-6.5613140000	2.7511750000	0.6139970000
H	-4.8279120000	4.1510170000	-0.4916870000
H	-2.5158660000	3.2944740000	-0.7355740000
C	-1.8430810000	-1.5241810000	-0.1922710000
C	-1.8223610000	-2.3974410000	0.8960070000
C	-2.5887500000	-3.5620070000	0.8413350000
C	-3.3646230000	-3.8381720000	-0.2872000000
C	-3.3750360000	-2.9523660000	-1.3668860000
C	-2.6087770000	-1.7874310000	-1.3266840000
H	-1.2246060000	-2.1650970000	1.7726790000

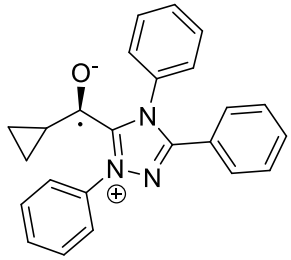
H	-2.5833640000	-4.2484050000	1.6825080000
H	-3.9627820000	-4.7435390000	-0.3240090000
H	-3.9773690000	-3.1671130000	-2.2440750000
H	-2.6038710000	-1.0936570000	-2.1611820000

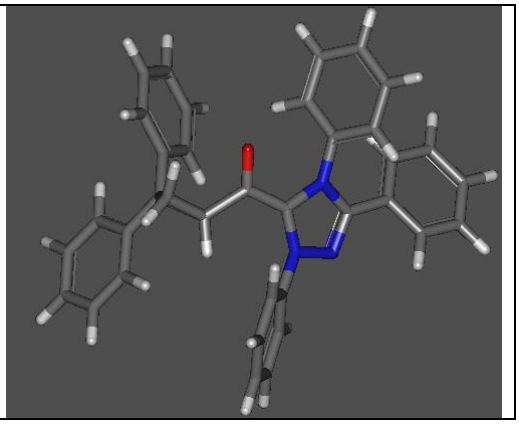
Thermodynamic data

Zero-point correction= 0.416089 (Hartree/Particle)
Thermal correction to Energy= 0.440808
Thermal correction to Enthalpy= 0.441753
Thermal correction to Gibbs Free Energy= 0.358420
Sum of electronic and zero-point Energies= -1280.336290
Sum of electronic and thermal Energies= -1280.311571
Sum of electronic and thermal Enthalpies= -1280.310627
Sum of electronic and thermal Free Energies= -1280.393960

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	276.611	98.417	175.389

B3LYP/6-31G*	**Job2radde**





xyz-matrix

68

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.4524580000	0.3291820000	1.2944250000
O	-0.1221640000	1.3948770000	1.8641090000
C	-1.9066230000	-0.0196760000	1.1307160000

C	-2.8591100000	0.9958700000	0.4281480000
C	-2.8940360000	0.7829090000	1.9262190000
H	-2.1455630000	-1.0514000000	0.9124280000
H	-3.7651490000	0.2877100000	2.3460430000
H	-2.4435820000	1.5538320000	2.5443040000
C	0.5535250000	-0.5215130000	0.7267420000
N	0.4637960000	-1.7979900000	0.1761430000
N	1.6069630000	-2.1190500000	-0.5366840000
C	2.4207760000	-1.1111860000	-0.3781110000
N	1.8662040000	-0.1146740000	0.4127330000
C	-0.3946780000	-2.8729750000	0.5213850000
C	-0.8952690000	-3.0087200000	1.8234310000
C	-1.7187130000	-4.0895170000	2.1352630000
C	-2.0324770000	-5.0453410000	1.1667940000
C	-1.5128080000	-4.9133700000	-0.1238390000
C	-0.6988810000	-3.8328790000	-0.4533920000
H	-0.6318460000	-2.2777190000	2.5811000000
H	-2.1021910000	-4.1901030000	3.1469730000
H	-2.6724370000	-5.8868640000	1.4158740000
H	-1.7481970000	-5.6530900000	-0.8840670000
H	-0.2886970000	-3.7233740000	-1.4508980000
C	3.7535230000	-1.0992200000	-1.0098710000
C	4.3534580000	0.0743350000	-1.4925600000
C	5.5916920000	0.0159930000	-2.1305110000
C	6.2443000000	-1.2065250000	-2.2956970000
C	5.6490370000	-2.3787190000	-1.8236560000
C	4.4126980000	-2.3277650000	-1.1855850000
H	3.8540990000	1.0293490000	-1.3779820000
H	6.0444070000	0.9309720000	-2.5022030000
H	7.2109500000	-1.2462830000	-2.7904390000

H	6.1500850000	-3.3346040000	-1.9490470000
H	3.9421830000	-3.2338160000	-0.8186660000
C	2.5763320000	1.0283570000	0.9244070000
C	3.6457460000	0.8163750000	1.7952160000
C	4.3901090000	1.9052160000	2.2526550000
C	4.0604420000	3.1972090000	1.8443670000
C	2.9825290000	3.4003380000	0.9777890000
C	2.2372090000	2.3195290000	0.5123040000
H	3.8906010000	-0.1934790000	2.1101160000
H	5.2229100000	1.7395880000	2.9303130000
H	4.6373470000	4.0452120000	2.2031270000
H	2.7139660000	4.4057680000	0.6665320000
H	1.3877020000	2.4725110000	-0.1433260000
C	-2.2641050000	2.2679560000	-0.1196700000
C	-2.5455030000	3.5135820000	0.4511720000
C	-2.0213830000	4.6874010000	-0.0938050000
C	-1.2091470000	4.6335990000	-1.2269210000
C	-0.9263270000	3.3965130000	-1.8126320000
C	-1.4504110000	2.2264270000	-1.2623630000
H	-3.1775130000	3.5627980000	1.3334820000
H	-2.2490660000	5.6444250000	0.3686430000
H	-0.8026710000	5.5469700000	-1.6536660000
H	-0.3013200000	3.3432780000	-2.7009260000
H	-1.2334750000	1.2659440000	-1.7234330000
C	-3.9983960000	0.3987080000	-0.3734260000
C	-4.5399440000	1.0730470000	-1.4799310000
C	-5.6065280000	0.5387710000	-2.2050880000
C	-6.1653230000	-0.6860880000	-1.8450250000
C	-5.6444420000	-1.3678130000	-0.7440830000
C	-4.5813010000	-0.8326050000	-0.0194730000

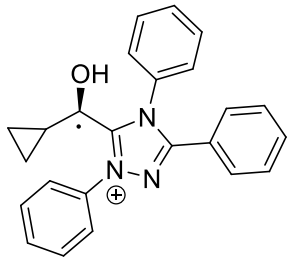
H	-4.1272150000	2.0299020000	-1.7780730000
H	-5.9999900000	1.0898900000	-3.0556730000
H	-6.9945120000	-1.1032470000	-2.4101370000
H	-6.0665000000	-2.3236100000	-0.4436520000
H	-4.2068440000	-1.3920150000	0.8326750000

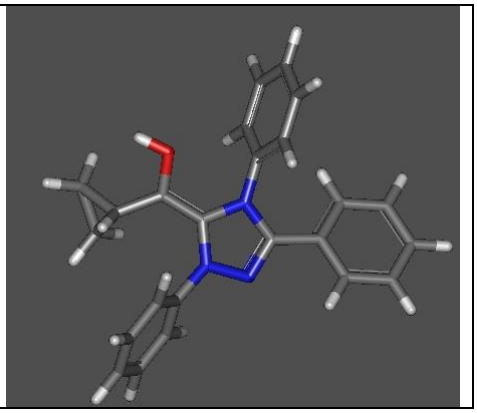
Thermodynamic data

Zero-point correction= 0.546764 (Hartree/Particle)
Thermal correction to Energy= 0.578877
Thermal correction to Enthalpy= 0.579821
Thermal correction to Gibbs Free Energy= 0.478469
Sum of electronic and zero-point Energies= -1627.545403
Sum of electronic and thermal Energies= -1627.513290
Sum of electronic and thermal Enthalpies= -1627.512346
Sum of electronic and thermal Free Energies= -1627.613698

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	363.251	128.363	213.314

B3LYP/6-31G*	**Job2radpr**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3452500000	1.8098440000	0.1953080000
O	-0.5999320000	2.8540930000	0.6169900000

H	-1.1363030000	3.6636370000	0.5389180000
C	-2.7669640000	2.0476610000	-0.1462770000
C	-3.3229480000	1.7149370000	-1.5120520000
C	-3.0937160000	3.1540610000	-1.1468350000
H	-3.4669360000	1.9512510000	0.6830540000
H	-4.3397610000	1.3386120000	-1.5528880000
H	-2.6506460000	1.2735960000	-2.2420300000
H	-3.9506140000	3.7836910000	-0.9290910000
H	-2.2728040000	3.6679810000	-1.6411550000
C	-0.6729210000	0.5709540000	0.1212620000
N	-1.2329840000	-0.6688410000	0.0070370000
N	-0.2852850000	-1.6364370000	-0.1468350000
C	0.8779140000	-1.0215140000	-0.0947930000
N	0.6941610000	0.3445810000	0.0843610000
C	-2.5992000000	-1.0813100000	0.1643490000
C	-3.1746080000	-1.8771480000	-0.8277930000
C	-4.4828130000	-2.3266680000	-0.6557200000
C	-5.1986670000	-1.9862740000	0.4949880000
C	-4.6024990000	-1.2043490000	1.4874340000
C	-3.2922600000	-0.7532260000	1.3318200000
H	-2.6010990000	-2.1410800000	-1.7099870000
H	-4.9413510000	-2.9449210000	-1.4211320000
H	-6.2165970000	-2.3408940000	0.6243870000
H	-5.1492410000	-0.9608000000	2.3932000000
H	-2.8063370000	-0.1780800000	2.1142570000
C	2.1455380000	-1.7573150000	-0.1804470000
C	3.3157940000	-1.2186680000	-0.7420180000
C	4.4671060000	-1.9982590000	-0.8267800000
C	4.4671490000	-3.3124890000	-0.3559140000
C	3.3044530000	-3.8553200000	0.1966280000

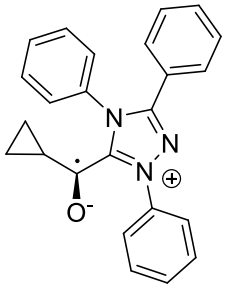
C	2.1483620000	-3.0870100000	0.2827230000
H	3.3302630000	-0.2077330000	-1.1294310000
H	5.3651980000	-1.5774700000	-1.2685450000
H	5.3694580000	-3.9131320000	-0.4223640000
H	3.2985690000	-4.8772300000	0.5631340000
H	1.2431020000	-3.5040740000	0.7105340000
C	1.7370140000	1.3421790000	0.2077250000
C	2.4142740000	1.4645440000	1.4194750000
C	3.4359840000	2.4086530000	1.5293910000
C	3.7657940000	3.2162290000	0.4394060000
C	3.0763210000	3.0829380000	-0.7687940000
C	2.0558000000	2.1406390000	-0.8915570000
H	2.1489900000	0.8301680000	2.2593670000
H	3.9722140000	2.5110840000	2.4676630000
H	4.5619550000	3.9489100000	0.5297250000
H	3.3348380000	3.7088000000	-1.6174460000
H	1.5173710000	2.0212880000	-1.8272050000

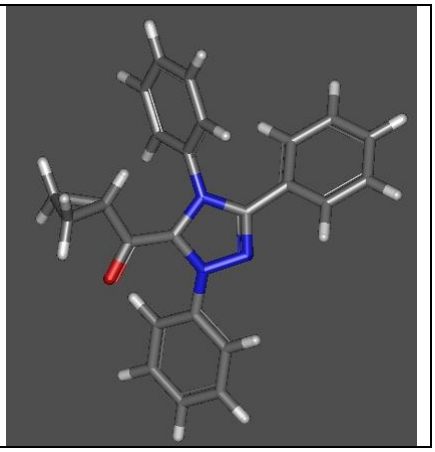
Thermodynamic data

Zero-point correction= 0.397797 (Hartree/Particle)
Thermal correction to Energy= 0.420988
Thermal correction to Enthalpy= 0.421932
Thermal correction to Gibbs Free Energy= 0.342305
Sum of electronic and zero-point Energies= -1165.996090
Sum of electronic and thermal Energies= -1165.972898
Sum of electronic and thermal Enthalpies= -1165.971954
Sum of electronic and thermal Free Energies= -1166.051581

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.174	91.542	167.589

B3LYP/6-31G*	**Job2raddeko2**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4706840000	1.7726780000	0.4789140000
O	-2.7188900000	1.8493440000	0.4916020000
C	-0.6609270000	2.9778200000	0.8630290000
C	-1.3483270000	3.9936430000	1.7558480000
C	-1.1134840000	4.3259910000	0.3159760000
H	0.4036730000	2.8549560000	1.0126520000
H	-0.7396310000	4.4825280000	2.5116340000
H	-2.3641700000	3.7512500000	2.0498660000
H	-0.3449510000	5.0488850000	0.0557750000
H	-1.9767660000	4.3051210000	-0.3427600000
C	-0.8280610000	0.5422390000	0.0953900000
N	-1.4486650000	-0.7074860000	0.0523410000
N	-0.5240540000	-1.7247890000	0.1188240000
C	0.6506360000	-1.1622480000	0.1156960000
N	0.5499820000	0.2266200000	0.0704960000
C	-2.8022910000	-1.0727710000	-0.1643360000
C	-3.2842270000	-2.2350740000	0.4523400000

C	-4.5901040000	-2.6547810000	0.2103640000
C	-5.4209270000	-1.9247460000	-0.6415620000
C	-4.9299350000	-0.7708100000	-1.2575370000
C	-3.6249870000	-0.3422370000	-1.0311850000
H	-2.6307510000	-2.7984100000	1.1083970000
H	-4.9585640000	-3.5546970000	0.6954440000
H	-6.4404950000	-2.2517710000	-0.8256330000
H	-5.5657330000	-0.1983110000	-1.9273710000
H	-3.2502530000	0.5546660000	-1.5052990000
C	1.6118720000	1.1366030000	-0.2158170000
C	2.6969880000	1.2431020000	0.6615370000
C	3.7384070000	2.1225940000	0.3654450000
C	3.6957770000	2.9032600000	-0.7913590000
C	2.6051490000	2.7986760000	-1.6594030000
C	1.5647210000	1.9152880000	-1.3787470000
H	2.7165290000	0.6437680000	1.5658440000
H	4.5801450000	2.2027540000	1.0474450000
H	4.5054610000	3.5921030000	-1.0142510000
H	2.5655620000	3.4025690000	-2.5615700000
H	0.7117490000	1.8275640000	-2.0444020000
C	1.8866190000	-1.9677940000	0.1280990000
C	2.9755340000	-1.7005650000	-0.7169580000
C	4.0931820000	-2.5338900000	-0.7034670000
C	4.1393310000	-3.6400380000	0.1467140000
C	3.0547820000	-3.9173970000	0.9814360000
C	1.9351280000	-3.0889070000	0.9728040000
H	2.9451250000	-0.8565610000	-1.3967590000
H	4.9271020000	-2.3201910000	-1.3662600000
H	5.0137210000	-4.2850240000	0.1553470000
H	3.0804600000	-4.7791480000	1.6426010000

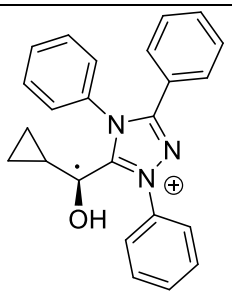
H 1.0870500000 -3.3010380000 1.6155210000

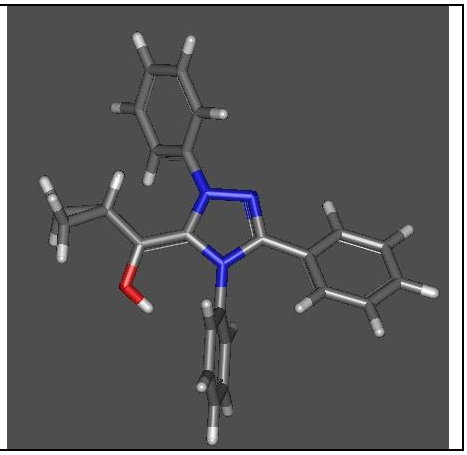
Thermodynamic data

Zero-point correction= 0.384784 (Hartree/Particle)
Thermal correction to Energy= 0.407712
Thermal correction to Enthalpy= 0.408656
Thermal correction to Gibbs Free Energy= 0.329123
Sum of electronic and zero-point Energies= -1165.607693
Sum of electronic and thermal Energies= -1165.584766
Sum of electronic and thermal Enthalpies= -1165.583822
Sum of electronic and thermal Free Energies= -1165.663355

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	255.843	90.342	167.392

B3LYP/6-31G*	**Job2radprko2**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C -1.4162670000 1.6859090000 -0.0708250000

O -0.8408490000 2.8513630000 0.2907940000

H 0.0727150000 2.7341680000 0.6089720000

C -2.8068440000 1.8159500000 -0.5051270000

C -3.2934840000 3.1529030000 -1.0710210000

C	-3.7763950000	2.7202990000	0.2691650000
H	-3.2358890000	0.9286440000	-0.9509160000
H	-3.9669460000	3.0850060000	-1.9199170000
H	-2.5734230000	3.9624540000	-1.1166270000
H	-4.7918070000	2.3513470000	0.3762360000
H	-3.3750960000	3.2301900000	1.1395360000
C	-0.6939620000	0.4731320000	-0.0524370000
N	-1.1802550000	-0.8068860000	-0.1244820000
N	-0.1717460000	-1.7264570000	-0.1951610000
C	0.9517840000	-1.0503790000	-0.1301060000
N	0.6899320000	0.3120890000	-0.0266440000
C	-2.5227070000	-1.2972880000	0.0125600000
C	-3.2836320000	-0.9396770000	1.1287280000
C	-4.5675090000	-1.4652920000	1.2649220000
C	-5.0728170000	-2.3455560000	0.3049040000
C	-4.2927120000	-2.7068620000	-0.7963040000
C	-3.0089860000	-2.1850360000	-0.9494250000
H	-2.8745040000	-0.2729420000	1.8810720000
H	-5.1660700000	-1.1981900000	2.1303650000
H	-6.0713400000	-2.7560660000	0.4193660000
H	-4.6815950000	-3.3967790000	-1.5386450000
H	-2.3867740000	-2.4623530000	-1.7936400000
C	1.6600930000	1.3742740000	0.1042980000
C	2.2789690000	1.5828230000	1.3418310000
C	3.2284510000	2.5998350000	1.4629830000
C	3.5490920000	3.3952240000	0.3609530000
C	2.9215400000	3.1811380000	-0.8699440000
C	1.9744510000	2.1666950000	-1.0070330000
H	2.0269500000	0.9511260000	2.1881310000
H	3.7160800000	2.7660270000	2.4183280000

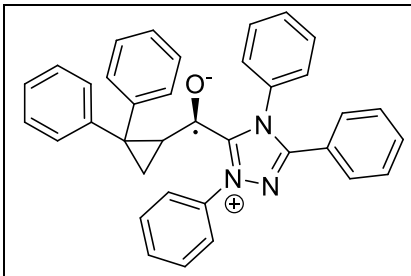
H	4.2874120000	4.1848280000	0.4606210000
H	3.1701380000	3.8014910000	-1.7252600000
H	1.4828750000	1.9866270000	-1.9583680000
C	2.2641400000	-1.7080290000	-0.1270110000
C	3.4108130000	-1.1349990000	-0.7024730000
C	4.6144320000	-1.8363690000	-0.6977320000
C	4.6882610000	-3.1071800000	-0.1242100000
C	3.5488850000	-3.6850900000	0.4412300000
C	2.3415380000	-2.9941020000	0.4394270000
H	3.3667640000	-0.1606680000	-1.1741730000
H	5.4945920000	-1.3911580000	-1.1514940000
H	5.6301170000	-3.6477140000	-0.1220800000
H	3.6009240000	-4.6741590000	0.8858170000
H	1.4533510000	-3.4379270000	0.8762160000

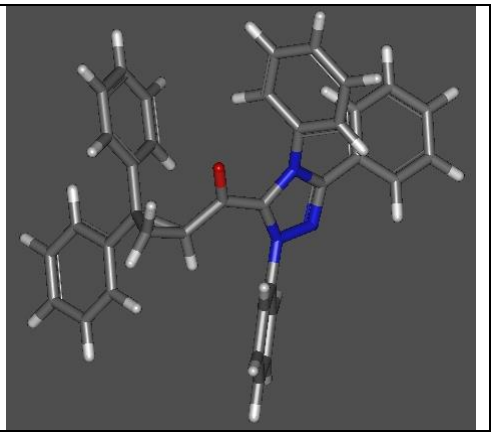
Thermodynamic data

Zero-point correction= 0.397815 (Hartree/Particle)
Thermal correction to Energy= 0.421027
Thermal correction to Enthalpy= 0.421971
Thermal correction to Gibbs Free Energy= 0.342119
Sum of electronic and zero-point Energies= -1165.999003
Sum of electronic and thermal Energies= -1165.975792
Sum of electronic and thermal Enthalpies= -1165.974847
Sum of electronic and thermal Free Energies= -1166.054700

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.198	91.705	168.063

B3LYP/6-31G*	**Job3radde**





xyz-matrix

68

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.4524330000	0.3291410000	1.2942940000
O	-0.1222260000	1.3948520000	1.8640260000
C	-1.9065520000	-0.0198260000	1.1305690000
C	-2.8592150000	0.9956950000	0.4281280000
C	-2.8939690000	0.7826450000	1.9261830000
H	-2.1454250000	-1.0515400000	0.9121710000
H	-3.7649860000	0.2874300000	2.3461800000
H	-2.4433920000	1.5535880000	2.5441550000
C	0.5536260000	-0.5214540000	0.7265890000
N	0.4640350000	-1.7980000000	0.1761380000
N	1.6073040000	-2.1190910000	-0.5365070000
C	2.4210500000	-1.1111760000	-0.3779460000
N	1.8663300000	-0.1146020000	0.4127110000
C	-0.3944570000	-2.8729780000	0.5213210000
C	-0.8951160000	-3.0087490000	1.8233310000
C	-1.7185360000	-4.0895840000	2.1351130000
C	-2.0322030000	-5.0454120000	1.1666240000
C	-1.5124660000	-4.9134110000	-0.1239860000

C	-0.6985600000	-3.8328950000	-0.4534810000
H	-0.6318000000	-2.2777260000	2.5810170000
H	-2.1020810000	-4.1901720000	3.1467970000
H	-2.6721490000	-5.8869630000	1.4156440000
H	-1.7477960000	-5.6531490000	-0.8842170000
H	-0.2883110000	-3.7233650000	-1.4509570000
C	3.7538350000	-1.0991570000	-1.0096070000
C	4.3536040000	0.0743840000	-1.4925360000
C	5.5918480000	0.0160830000	-2.1304630000
C	6.2446310000	-1.2063820000	-2.2953770000
C	5.6495320000	-2.3785600000	-1.8230960000
C	4.4131730000	-2.3276450000	-1.1850580000
H	3.8541030000	1.0293500000	-1.3781720000
H	6.0444420000	0.9310420000	-2.5023510000
H	7.2112920000	-1.2461130000	-2.7901000000
H	6.1507220000	-3.3343970000	-1.9482830000
H	3.9427760000	-3.2336900000	-0.8179690000
C	2.5763120000	1.0285630000	0.9242420000
C	3.6458330000	0.8168330000	1.7949810000
C	4.3900640000	1.9058270000	2.2522730000
C	4.0601350000	3.1977400000	1.8439460000
C	2.9820960000	3.4006210000	0.9774660000
C	2.2369250000	2.3196610000	0.5121130000
H	3.8908960000	-0.1929460000	2.1099610000
H	5.2229530000	1.7403750000	2.9298660000
H	4.6369230000	4.0458660000	2.2026030000
H	2.7133160000	4.4059870000	0.6661790000
H	1.3873320000	2.4724730000	-0.1434420000
C	-2.2644070000	2.2679010000	-0.1196280000
C	-2.5461310000	3.5134660000	0.4512060000

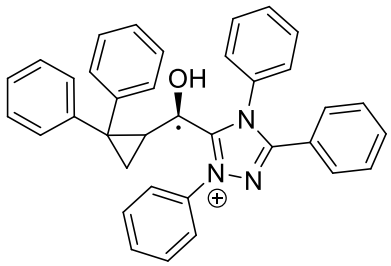
C	-2.0222270000	4.6874000000	-0.0937040000
C	-1.2099030000	4.6337920000	-1.2267780000
C	-0.9267820000	3.3967850000	-1.8124910000
C	-1.4506400000	2.2265690000	-1.2622630000
H	-3.1782210000	3.5625220000	1.3334690000
H	-2.2501370000	5.6443780000	0.3687240000
H	-0.8036090000	5.5472650000	-1.6534780000
H	-0.3017130000	3.3436950000	-2.7007500000
H	-1.2334550000	1.2661500000	-1.7233470000
C	-3.9984640000	0.3984350000	-0.3734050000
C	-4.5399410000	1.0725530000	-1.4800750000
C	-5.6064720000	0.5381250000	-2.2051970000
C	-6.1653040000	-0.6866540000	-1.8449210000
C	-5.6445130000	-1.3681530000	-0.7437940000
C	-4.5814290000	-0.8327920000	-0.0192220000
H	-4.1271980000	2.0293510000	-1.7783820000
H	-5.9998830000	1.0890690000	-3.0559190000
H	-6.9944590000	-1.1039170000	-2.4100080000
H	-6.0666180000	-2.3238710000	-0.4431800000
H	-4.2070520000	-1.3920070000	0.8330880000

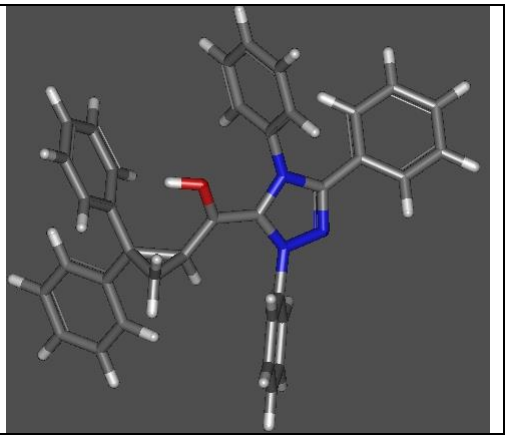
Thermodynamic data

Zero-point correction= 0.546764 (Hartree/Particle)
Thermal correction to Energy= 0.578877
Thermal correction to Enthalpy= 0.579822
Thermal correction to Gibbs Free Energy= 0.478467
Sum of electronic and zero-point Energies= -1627.545403
Sum of electronic and thermal Energies= -1627.513289
Sum of electronic and thermal Enthalpies= -1627.512345
Sum of electronic and thermal Free Energies= -1627.613700

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	363.251	128.363	213.318

B3LYP/6-31G*	**Job3radpr**





xyz-matrix

69

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.3863790000	0.1665720000	0.8155420000
O	-0.2320790000	1.3839340000	1.3706630000
H	-1.0557660000	1.9062740000	1.2619570000
C	-1.7105200000	-0.4392440000	0.6572740000
C	-3.0270490000	0.3876120000	0.3990100000
C	-2.7784950000	-0.2755560000	1.7249940000
H	-1.6987580000	-1.3823050000	0.1283550000
H	-3.3678040000	-1.1486820000	1.9880680000
H	-2.5137260000	0.3567070000	2.5687680000
C	0.8206820000	-0.4744330000	0.4476340000
N	1.0454430000	-1.8076740000	0.2420850000
N	2.3215600000	-2.0446230000	-0.1847530000
C	2.9191130000	-0.8745070000	-0.2136770000
N	2.0416270000	0.1292610000	0.1809750000
C	0.2190450000	-2.9426200000	0.5418540000
C	-0.2983610000	-3.1061840000	1.8295990000
C	-1.0665810000	-4.2356230000	2.1091970000

C	-1.2974410000	-5.1925320000	1.1173180000
C	-0.7563580000	-5.0242120000	-0.1595930000
C	0.0075850000	-3.8959850000	-0.4560020000
H	-0.0924860000	-2.3695660000	2.5996920000
H	-1.4686390000	-4.3758540000	3.1079310000
H	-1.8896460000	-6.0741290000	1.3430580000
H	-0.9268240000	-5.7716920000	-0.9281250000
H	0.4415200000	-3.7536500000	-1.4399420000
C	4.3350580000	-0.7374040000	-0.5830590000
C	4.8527310000	0.3824320000	-1.2552950000
C	6.1993940000	0.4178090000	-1.6107650000
C	7.0398120000	-0.6534180000	-1.3030230000
C	6.5284260000	-1.7728540000	-0.6420940000
C	5.1846390000	-1.8193750000	-0.2854120000
H	4.2121780000	1.2146130000	-1.5192780000
H	6.5902480000	1.2839850000	-2.1360170000
H	8.0892240000	-0.6177760000	-1.5803820000
H	7.1771370000	-2.6096590000	-0.4018050000
H	4.7824630000	-2.6864480000	0.2274310000
C	2.3416200000	1.5423520000	0.2588930000
C	3.0870730000	2.0181410000	1.3357520000
C	3.4035010000	3.3758950000	1.3918390000
C	2.9726710000	4.2395300000	0.3830740000
C	2.2228960000	3.7485810000	-0.6889330000
C	1.9042850000	2.3926860000	-0.7573540000
H	3.4147300000	1.3367480000	2.1144380000
H	3.9861970000	3.7563400000	2.2250350000
H	3.2227310000	5.2950850000	0.4304720000
H	1.8908670000	4.4193000000	-1.4755790000
H	1.3295440000	1.9956850000	-1.5889510000

C	-2.9328440000	1.8933480000	0.3265650000
C	-3.5112680000	2.6997180000	1.3209110000
C	-3.4728370000	4.0927490000	1.2221130000
C	-2.8608030000	4.7007880000	0.1255580000
C	-2.2842680000	3.9114730000	-0.8734490000
C	-2.3203040000	2.5211970000	-0.7747680000
H	-4.0078070000	2.2328430000	2.1669200000
H	-3.9291550000	4.6994280000	1.9987100000
H	-2.8340480000	5.7836430000	0.0476570000
H	-1.8118150000	4.3794570000	-1.7323440000
H	-1.8823880000	1.9088890000	-1.5591780000
C	-4.0217920000	-0.2688930000	-0.5410300000
C	-4.8262910000	0.5039390000	-1.3917910000
C	-5.7619400000	-0.0945910000	-2.2376280000
C	-5.9154840000	-1.4791660000	-2.2548140000
C	-5.1260160000	-2.2614610000	-1.4102310000
C	-4.1944000000	-1.6647250000	-0.5636120000
H	-4.7361130000	1.5839420000	-1.3920930000
H	-6.3731640000	0.5312470000	-2.8816340000
H	-6.6430240000	-1.9444960000	-2.9131380000
H	-5.2369520000	-3.3421500000	-1.4051690000
H	-3.6071120000	-2.3102220000	0.0840930000

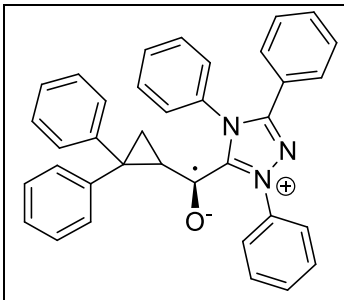
Thermodynamic data

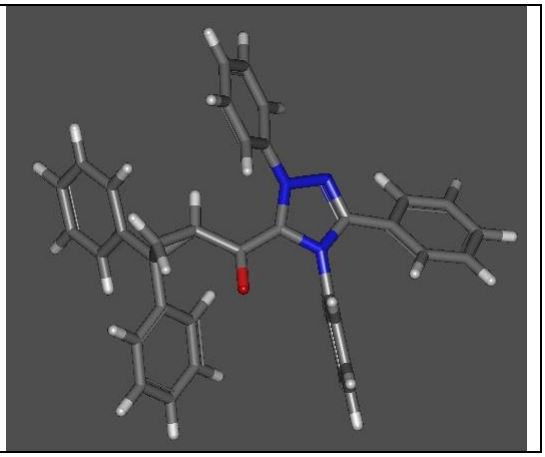
Zero-point correction= 0.559818 (Hartree/Particle)
Thermal correction to Energy= 0.592159
Thermal correction to Enthalpy= 0.593104
Thermal correction to Gibbs Free Energy= 0.491097
Sum of electronic and zero-point Energies= -1627.942974
Sum of electronic and thermal Energies= -1627.910633
Sum of electronic and thermal Enthalpies= -1627.909688
Sum of electronic and thermal Free Energies= -1628.011695

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	371.586	129.517	214.691

B3LYP/6-31G*	**Job3raddeko2**





xyz-matrix

68

XYZ file generated by gabedit : coordinates in Angstrom

C	0.4645270000	-0.1816000000	-1.2255250000
O	0.2908470000	-1.2536450000	-1.8488080000
C	1.8496000000	0.3117840000	-0.9242940000
C	2.9754780000	-0.1625270000	-1.8013310000
C	2.9351340000	-0.6608980000	-0.3745360000
H	1.9275180000	1.3065080000	-0.5050530000
H	3.7598880000	0.5333520000	-2.0859890000
H	2.6756140000	-0.8736340000	-2.5659110000
C	-0.6596140000	0.5710800000	-0.7460400000
N	-0.7369790000	1.8768850000	-0.2703240000
N	-1.9560180000	2.1158070000	0.3427950000
C	-2.6435130000	1.0154430000	0.2116770000
N	-1.9385250000	0.0396950000	-0.4835910000
C	0.0212550000	3.0152500000	-0.6474990000
C	0.1126810000	4.0894870000	0.2484780000

C	0.8303430000	5.2269410000	-0.1113800000
C	1.4637410000	5.3051850000	-1.3545450000
C	1.3617610000	4.2343950000	-2.2451000000
C	0.6384800000	3.0930560000	-1.9033750000
H	-0.3851390000	4.0229430000	1.2090710000
H	0.8989000000	6.0553740000	0.5883210000
H	2.0271770000	6.1926840000	-1.6276510000
H	1.8352650000	4.2888590000	-3.2215900000
H	0.5441150000	2.2706500000	-2.6042900000
C	-4.0235600000	0.9091770000	0.7169390000
C	-5.0145910000	0.1698140000	0.0521940000
C	-6.3192820000	0.1509910000	0.5422730000
C	-6.6513480000	0.8639140000	1.6954920000
C	-5.6704590000	1.6056600000	2.3576720000
C	-4.3653080000	1.6299100000	1.8733060000
H	-4.7712120000	-0.3827160000	-0.8481440000
H	-7.0786390000	-0.4216610000	0.0172140000
H	-7.6690230000	0.8426390000	2.0756670000
H	-5.9209600000	2.1644150000	3.2551580000
H	-3.5985580000	2.2062220000	2.3802820000
C	-2.3182870000	-1.3426150000	-0.5722500000
C	-2.5329440000	-2.0678990000	0.6016730000
C	-2.9643090000	-3.3932160000	0.5247750000
C	-3.1727210000	-3.9902930000	-0.7179850000
C	-2.9451760000	-3.2602950000	-1.8885640000
C	-2.5177190000	-1.9370600000	-1.8210910000
H	-2.3677990000	-1.5953740000	1.5650970000
H	-3.1341670000	-3.9557620000	1.4385440000
H	-3.5066430000	-5.0224560000	-0.7769730000
H	-3.0951760000	-3.7249860000	-2.8587960000

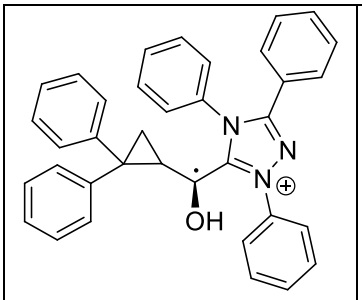
H	-2.3185350000	-1.3678050000	-2.7211010000
C	3.9174680000	-0.0452890000	0.6027020000
C	4.4302040000	-0.7850610000	1.6803460000
C	5.3419820000	-0.2242020000	2.5766030000
C	5.7695100000	1.0931470000	2.4219460000
C	5.2727830000	1.8431240000	1.3547140000
C	4.3636500000	1.2820980000	0.4598810000
H	4.1166130000	-1.8129590000	1.8208430000
H	5.7184730000	-0.8275510000	3.3989890000
H	6.4792290000	1.5298130000	3.1195380000
H	5.5936150000	2.8722830000	1.2137340000
H	4.0004830000	1.8983910000	-0.3575490000
C	2.5890160000	-2.1080730000	-0.1318050000
C	3.2638680000	-3.1233400000	-0.8198830000
C	2.9985590000	-4.4675990000	-0.5552870000
C	2.0520200000	-4.8177980000	0.4083480000
C	1.3751780000	-3.8142830000	1.1046270000
C	1.6456090000	-2.4727160000	0.8380930000
H	4.0022080000	-2.8547750000	-1.5710160000
H	3.5311560000	-5.2408190000	-1.1033180000
H	1.8408880000	-5.8641390000	0.6136510000
H	0.6305160000	-4.0764050000	1.8518690000
H	1.1139790000	-1.6947970000	1.3802160000

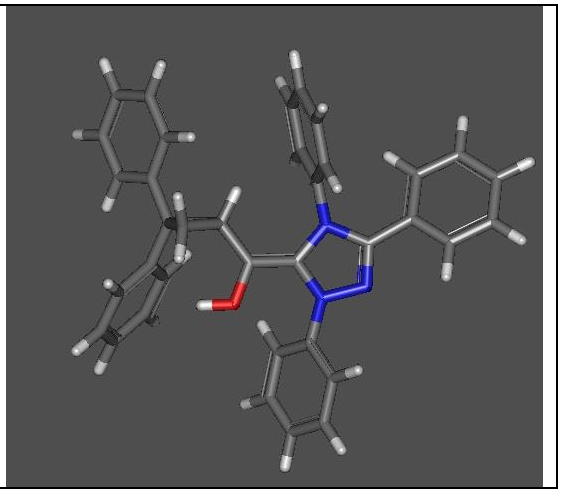
Thermodynamic data

Zero-point correction= 0.546713 (Hartree/Particle)
Thermal correction to Energy= 0.578830
Thermal correction to Enthalpy= 0.579774
Thermal correction to Gibbs Free Energy= 0.478483
Sum of electronic and zero-point Energies= -1627.545829
Sum of electronic and thermal Energies= -1627.513712
Sum of electronic and thermal Enthalpies= -1627.512768
Sum of electronic and thermal Free Energies= -1627.614058

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	363.221	128.397	213.184

B3LYP/6-31G*	**Job3radprko2**





xyz-matrix

69

XYZ file generated by gabedit : coordinates in Angstrom

C	0.4916320000	0.5965360000	0.7931030000
O	1.0109210000	1.7726110000	1.1996440000
H	1.9886400000	1.7554760000	1.1292520000
C	1.2690930000	-0.6338280000	0.9402040000
C	2.2852390000	-0.7616060000	2.0589530000
C	2.8300480000	-0.7003510000	0.6608960000
H	0.7571530000	-1.5380020000	0.6505730000
H	2.3285660000	-1.7069440000	2.5910120000
H	2.4085960000	0.1090300000	2.6974340000
C	-0.8334610000	0.7047520000	0.3068760000
N	-1.5156890000	1.8768670000	0.0904540000
N	-2.8353670000	1.6491960000	-0.1728580000
C	-2.9969640000	0.3473350000	-0.1538670000

N	-1.7887490000	-0.2890130000	0.1091570000
C	-1.0568970000	3.2350670000	-0.0245360000
C	-1.7342680000	4.2194450000	0.6949480000
C	-1.3489670000	5.5509530000	0.5467940000
C	-0.3028030000	5.8882170000	-0.3138240000
C	0.3585050000	4.8913570000	-1.0356150000
C	-0.0190480000	3.5574110000	-0.8998130000
H	-2.5492960000	3.9426870000	1.3547400000
H	-1.8684850000	6.3234260000	1.1052240000
H	-0.0070970000	6.9267060000	-0.4276950000
H	1.1633460000	5.1528930000	-1.7157910000
H	0.4792850000	2.7798490000	-1.4690950000
C	-4.3112510000	-0.2754770000	-0.3637770000
C	-4.4880620000	-1.4997880000	-1.0292660000
C	-5.7716280000	-2.0021950000	-1.2318160000
C	-6.8863270000	-1.2961890000	-0.7759820000
C	-6.7167610000	-0.0742220000	-0.1208080000
C	-5.4392050000	0.4375680000	0.0826610000
H	-3.6366890000	-2.0514780000	-1.4082740000
H	-5.8998570000	-2.9451830000	-1.7545810000
H	-7.8840670000	-1.6945400000	-0.9347370000
H	-7.5802220000	0.4808860000	0.2328480000
H	-5.3027940000	1.3878310000	0.5875940000
C	-1.6231080000	-1.7107260000	0.2988440000
C	-2.0059880000	-2.2848060000	1.5115810000
C	-1.8723940000	-3.6640130000	1.6808230000
C	-1.3607630000	-4.4522140000	0.6476610000
C	-0.9795740000	-3.8655060000	-0.5624710000
C	-1.1133920000	-2.4888810000	-0.7443660000
H	-2.4069010000	-1.6623290000	2.3053930000

H	-2.1719260000	-4.1203480000	2.6192050000
H	-1.2625590000	-5.5250150000	0.7835330000
H	-0.5814910000	-4.4767470000	-1.3662590000
H	-0.8264420000	-2.0201580000	-1.6811720000
C	3.3181870000	-1.9891330000	0.0305520000
C	4.3610490000	-1.9851350000	-0.9084380000
C	4.8292230000	-3.1746340000	-1.4696290000
C	4.2670930000	-4.3969490000	-1.1072920000
C	3.2320610000	-4.4182600000	-0.1706750000
C	2.7656430000	-3.2317120000	0.3909910000
H	4.8267840000	-1.0508170000	-1.1991910000
H	5.6420430000	-3.1389890000	-2.1893570000
H	4.6335210000	-5.3220850000	-1.5422210000
H	2.7892930000	-5.3631280000	0.1321530000
H	1.9647350000	-3.2922240000	1.1225070000
C	3.5151240000	0.5698180000	0.2182890000
C	4.4240630000	1.2320530000	1.0601230000
C	5.0872940000	2.3847400000	0.6285670000
C	4.8577450000	2.8868750000	-0.6520690000
C	3.9595500000	2.2348090000	-1.5026950000
C	3.2936480000	1.0889810000	-1.0712850000
H	4.6268550000	0.8330080000	2.0502410000
H	5.7894260000	2.8806560000	1.2922090000
H	5.3767960000	3.7794430000	-0.9885520000
H	3.7835400000	2.6165590000	-2.5044680000
H	2.6044990000	0.5775570000	-1.7388090000

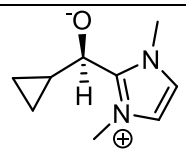
Thermodynamic data

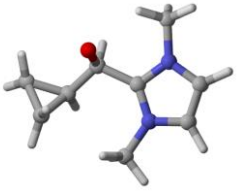
Zero-point correction= 0.559783 (Hartree/Particle)
Thermal correction to Energy= 0.592067
Thermal correction to Enthalpy= 0.593012
Thermal correction to Gibbs Free Energy= 0.491375

Sum of electronic and zero-point Energies= -1627.941290
Sum of electronic and thermal Energies= -1627.909005
Sum of electronic and thermal Enthalpies= -1627.908061
Sum of electronic and thermal Free Energies= -1628.009698

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	371.528	129.599	213.912

M062X/6-31++G**	**Job8de**





xyz-matrix

26

XYZ file generated by gabedit : coordinates in Angstrom

C	0.7299990000	-0.8483160000	-0.2160890000
H	0.5903360000	-1.5773840000	-1.0620040000
O	0.7948520000	-1.3976450000	0.9976010000
C	1.9441810000	-0.0070160000	-0.6265390000
C	3.2763910000	-0.5896410000	-0.2548990000
C	2.7653090000	0.6307070000	0.4572460000
H	1.8867470000	0.4928930000	-1.5945590000
H	4.0983500000	-0.4736110000	-0.9529930000
H	3.2383590000	-1.5167440000	0.3073640000
H	3.2440160000	1.5856210000	0.2589250000
H	2.4029310000	0.4609440000	1.4672530000
C	-0.5930430000	-0.0489300000	-0.2323920000
N	-0.8718840000	1.2574820000	-0.0641210000

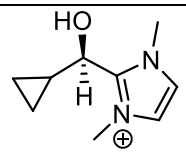
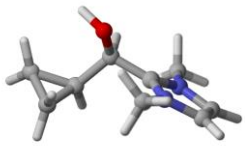
C	-2.2335840000	1.4228130000	0.1261850000
N	-1.7677980000	-0.7012080000	-0.1595890000
C	-2.7929910000	0.1889140000	0.0661570000
C	0.0887240000	2.3553470000	0.0080170000
C	-1.8719190000	-2.1599140000	-0.1519680000
H	-1.8207830000	-2.5477850000	-1.1711290000
H	-2.8282100000	-2.4283580000	0.2970290000
H	-1.0364970000	-2.5291300000	0.4530660000
H	-2.6729040000	2.3946600000	0.2829990000
H	-3.8181350000	-0.1299400000	0.1646230000
H	0.7190410000	2.2379570000	0.8895610000
H	-0.4777970000	3.2844540000	0.0730300000
H	0.7150870000	2.3698810000	-0.8823150000

thermodynamic data

Zero-point correction= 0.224665 (Hartree/Particle)
Thermal correction to Energy= 0.236282
Thermal correction to Enthalpy= 0.237227
Thermal correction to Gibbs Free Energy= 0.187504
Sum of electronic and zero-point Energies= -535.590569
Sum of electronic and thermal Energies= -535.578952
Sum of electronic and thermal Enthalpies= -535.578008
Sum of electronic and thermal Free Energies= -535.627730

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.269	44.440	104.650

B3LYP/6-31G*	**Job8pr**

xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

C	0.7749020000	-0.5520470000	0.6307480000
H	0.6406630000	-1.5564250000	1.0585330000
O	1.2243040000	0.3416440000	1.6352910000
H	1.9987130000	-0.0481380000	2.0714000000
C	1.7119570000	-0.6692040000	-0.5730620000
C	3.2092550000	-0.7030670000	-0.3816330000
C	2.5617930000	0.4838210000	-1.0488410000
H	1.3227640000	-1.3340010000	-1.3433660000
H	3.7784050000	-1.4043560000	-0.9835440000
H	3.6185420000	-0.5488840000	0.6139290000
H	2.6892700000	0.6159890000	-2.1188750000
H	2.5400070000	1.4063890000	-0.4776030000
C	-0.6040470000	-0.0845090000	0.2147310000
N	-1.0302040000	1.1738630000	-0.0076840000
C	-2.3510500000	1.1375090000	-0.4156450000
N	-1.6368900000	-0.9142120000	-0.0490230000
C	-2.7307820000	-0.1667220000	-0.4448110000
C	-0.2594770000	2.4249350000	0.1140180000
C	-1.6358880000	-2.3787720000	0.0823700000
H	-0.8772160000	-2.8201080000	-0.5668070000
H	-2.6166470000	-2.7442640000	-0.2212730000
H	-1.4560390000	-2.6650710000	1.1210150000

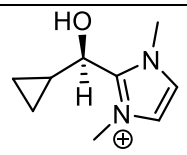
H	-2.8997270000	2.0385270000	-0.6418280000
H	-3.6735720000	-0.6244940000	-0.7002170000
H	-0.9368130000	3.2047000000	0.4651350000
H	0.1453960000	2.6993090000	-0.8625510000
H	0.5414870000	2.2784580000	0.8334230000

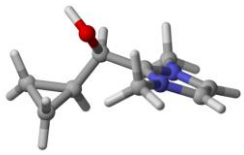
thermodynamic data

Zero-point correction= 0.237118 (Hartree/Particle)
Thermal correction to Energy= 0.249708
Thermal correction to Enthalpy= 0.250652
Thermal correction to Gibbs Free Energy= 0.198058
Sum of electronic and zero-point Energies= -536.221554
Sum of electronic and thermal Energies= -536.208964
Sum of electronic and thermal Enthalpies= -536.208020
Sum of electronic and thermal Free Energies= -536.260614

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.694	46.778	110.694

M062X/6-31++G**	**Job8pr**	





xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

C	0.7931760000	-0.4163730000	0.6831990000
H	0.7055880000	-1.3314900000	1.2856070000
O	1.2463400000	0.6561130000	1.4776650000

H	1.8222900000	0.3337530000	2.1803590000
C	1.6922170000	-0.6913560000	-0.5145650000
C	3.1805570000	-0.7339080000	-0.3314760000
C	2.5517380000	0.3975750000	-1.0949200000
H	1.2739410000	-1.4079760000	-1.2183530000
H	3.7333990000	-1.4897060000	-0.8762570000
H	3.5845600000	-0.4949220000	0.6473650000
H	2.6727690000	0.4288040000	-2.1711490000
H	2.5521480000	1.3591420000	-0.5939890000
C	-0.6031550000	-0.0687920000	0.2292120000
N	-1.0922160000	1.1430020000	-0.0581080000
C	-2.4008860000	1.0107470000	-0.4716770000
N	-1.5708060000	-0.9683090000	-0.0037680000
C	-2.7021680000	-0.3129880000	-0.4408950000
C	-0.3903160000	2.4318450000	0.0482340000
C	-1.4619600000	-2.4157920000	0.2023670000
H	-0.5979270000	-2.8075510000	-0.3353550000
H	-2.3649450000	-2.8791280000	-0.1913780000
H	-1.3789520000	-2.6362820000	1.2679570000
H	-2.9974810000	1.8649440000	-0.7503340000
H	-3.6097360000	-0.8406190000	-0.6879590000
H	-0.2322720000	2.6773050000	1.0966590000
H	-1.0151150000	3.1817140000	-0.4339540000
H	0.5669570000	2.3645060000	-0.4642820000

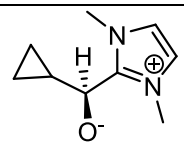
thermodynamic data

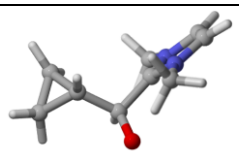
Zero-point correction= 0.238504 (Hartree/Particle)
Thermal correction to Energy= 0.251000
Thermal correction to Enthalpy= 0.251945

Thermal correction to Gibbs Free Energy= 0.199875
Sum of electronic and zero-point Energies= -536.021759
Sum of electronic and thermal Energies= -536.009263
Sum of electronic and thermal Enthalpies= -536.008319
Sum of electronic and thermal Free Energies= -536.060388

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	157.505	46.455	109.589

B3LYP/6-31G*	**Job8deko2**





xyz-matrix

26

XYZ file generated by gabedit : coordinates in Angstrom

C	0.9095610000	-0.3216430000	0.7392130000
H	1.1651890000	0.6223640000	1.3131790000
O	0.8547660000	-1.4194890000	1.4558550000
C	1.8933160000	-0.3214550000	-0.4576980000
C	3.3389560000	-0.0198320000	-0.1887480000
C	2.5080720000	0.9547250000	-0.9913350000
H	1.6970080000	-1.1095870000	-1.1843480000
H	4.0997360000	-0.6003970000	-0.7041700000
H	3.6056420000	0.2558370000	0.8293310000
H	2.6946390000	1.0456170000	-2.0589160000
H	2.2406170000	1.8951100000	-0.5116260000
C	-0.5272590000	0.0086940000	0.1594000000
N	-1.4040780000	-0.9314620000	-0.2581640000

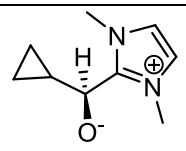
C	-2.6346050000	-0.3547250000	-0.5161970000
N	-1.2119270000	1.1808590000	0.1689090000
C	-2.5196020000	0.9710420000	-0.2504690000
C	-1.0915290000	-2.3624670000	-0.3582970000
C	-0.6598320000	2.4908450000	0.4984650000
H	0.0881900000	2.3796180000	1.2846840000
H	-1.4692320000	3.1325370000	0.8536980000
H	-0.1910870000	2.9460970000	-0.3786540000
H	-0.2464950000	-2.5138780000	0.3346700000
H	-0.8216180000	-2.6143000000	-1.3882310000
H	-1.9745680000	-2.9330830000	-0.0599590000
H	-3.4773360000	-0.9397100000	-0.8501360000
H	-3.2392520000	1.7728030000	-0.3075860000

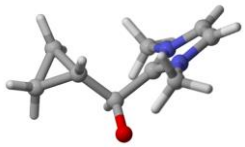
thermodynamic data

Zero-point correction= 0.221749 (Hartree/Particle)
Thermal correction to Energy= 0.233958
Thermal correction to Enthalpy= 0.234902
Thermal correction to Gibbs Free Energy= 0.182941
Sum of electronic and zero-point Energies= -535.784685
Sum of electronic and thermal Energies= -535.772476
Sum of electronic and thermal Enthalpies= -535.771532
Sum of electronic and thermal Free Energies= -535.823493

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	146.811	45.487	109.363

M062X/6-31++G**	**Job8deko2**





xyz-matrix

26

XYZ file generated by gabedit : coordinates in Angstrom

C	0.9040900000	-0.3630380000	0.7464250000
H	1.1995680000	0.5449720000	1.3439690000
O	0.8871810000	-1.4982200000	1.4181720000
C	1.8173970000	-0.3212180000	-0.4932000000
C	3.2680140000	-0.0521820000	-0.2655280000
C	2.4178520000	0.9778800000	-0.9655920000
H	1.5742450000	-1.0652290000	-1.2505990000
H	3.9967660000	-0.5995620000	-0.8527450000
H	3.5653950000	0.1485480000	0.7596220000
H	2.5650640000	1.1350850000	-2.0289680000
H	2.1813610000	1.8799570000	-0.4064310000
C	-0.5232200000	-0.0066220000	0.2287610000
N	-1.4100690000	-0.9106710000	-0.2176420000
C	-2.5970750000	-0.2883110000	-0.5395500000
N	-1.1480370000	1.1877440000	0.1960490000
C	-2.4368480000	1.0329910000	-0.2806490000
C	-1.1514800000	-2.3479620000	-0.3607140000
C	-0.5615960000	2.4731290000	0.5539760000
H	0.1693860000	2.3267790000	1.3480730000
H	-1.3580440000	3.1285450000	0.9083720000

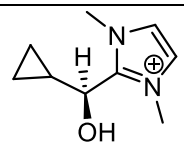
H	-0.0723050000	2.9199680000	-0.3136050000
H	-0.3075670000	-2.5697510000	0.3056980000
H	-0.9115730000	-2.5678600000	-1.4035130000
H	-2.0525160000	-2.8870080000	-0.0640580000
H	-3.4466990000	-0.8408010000	-0.9081500000
H	-3.1165850000	1.8645980000	-0.3754730000

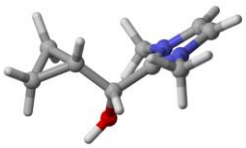
thermodynamic data

Zero-point correction= 0.223251 (Hartree/Particle)
Thermal correction to Energy= 0.235364
Thermal correction to Enthalpy= 0.236308
Thermal correction to Gibbs Free Energy= 0.184443
Sum of electronic and zero-point Energies= -535.589435
Sum of electronic and thermal Energies= -535.577322
Sum of electronic and thermal Enthalpies= -535.576378
Sum of electronic and thermal Free Energies= -535.628242

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.693	45.069	109.158

B3LYP/6-31G*	**Job8prko2**





xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

C	0.8740510000	-0.0720600000	0.6778190000
H	1.1108670000	0.8880060000	1.1606460000
O	0.9178470000	-1.1252120000	1.6322130000

H	1.8545900000	-1.3179200000	1.8081880000
C	1.8423660000	-0.2762060000	-0.4731690000
C	3.3019420000	0.0808150000	-0.2647850000
C	2.4541080000	0.9044180000	-1.1936570000
H	1.6452950000	-1.1632240000	-1.0714430000
H	4.0477470000	-0.5837400000	-0.6892720000
H	3.5940050000	0.5307600000	0.6815310000
H	2.6117060000	0.8139740000	-2.2636490000
H	2.1895570000	1.9081590000	-0.8701270000
C	-0.5630550000	0.0111300000	0.2154470000
N	-1.3376040000	-1.0023380000	-0.2198740000
C	-2.5756860000	-0.5038740000	-0.5781840000
N	-1.2967440000	1.1416550000	0.1414280000
C	-2.5507010000	0.8366520000	-0.3549800000
C	-0.9646070000	-2.4230620000	-0.3351130000
C	-0.8689200000	2.4925420000	0.5341500000
H	-0.0768660000	2.8472980000	-0.1277380000
H	-0.5255230000	2.4922920000	1.5705410000
H	-1.7294150000	3.1557750000	0.4479710000
H	-0.1636020000	-2.6300100000	0.3705610000
H	-0.6491790000	-2.6383080000	-1.3591620000
H	-1.8392790000	-3.0261720000	-0.0872210000
H	-3.3607110000	-1.1440080000	-0.9497590000
H	-3.3085260000	1.5914720000	-0.4948180000

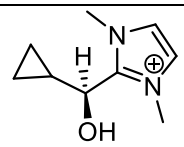
thermodynamic data

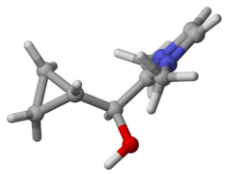
Zero-point correction= 0.237197 (Hartree/Particle)
Thermal correction to Energy= 0.249734
Thermal correction to Enthalpy= 0.250679

Thermal correction to Gibbs Free Energy= 0.198338
Sum of electronic and zero-point Energies= -536.224794
Sum of electronic and thermal Energies= -536.212256
Sum of electronic and thermal Enthalpies= -536.211312
Sum of electronic and thermal Free Energies= -536.263653

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.711	46.697	110.160

M062X/6-31++G**	**Job8prko2**





xyz-matrix

27

XYZ file generated by gabedit : coordinates in Angstrom

C	0.8770740000	-0.0261990000	0.6879580000
H	1.1065700000	0.9682100000	1.0996620000
O	0.9224750000	-1.0063730000	1.7028310000
H	1.8445370000	-1.1476120000	1.9577170000
C	1.8340050000	-0.2968740000	-0.4489320000
C	3.2637110000	0.1510940000	-0.2868490000
C	2.3640290000	0.8547230000	-1.2590050000
H	1.6724660000	-1.2377500000	-0.9687440000
H	4.0398530000	-0.4954580000	-0.6780860000
H	3.5311860000	0.6842060000	0.6211370000
H	2.5210970000	0.6946450000	-2.3186990000
H	2.0405500000	1.8578010000	-0.9979340000

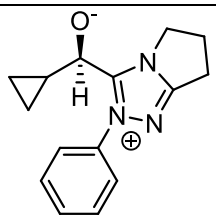
C	-0.5534820000	0.0149130000	0.2162700000
N	-1.2853520000	-1.0231560000	-0.2090900000
C	-2.5319900000	-0.5734020000	-0.5835140000
N	-1.3148560000	1.1154430000	0.1236780000
C	-2.5513250000	0.7689290000	-0.3769580000
C	-0.8566790000	-2.4252580000	-0.3051850000
C	-0.9258430000	2.4765570000	0.5081760000
H	-0.1485280000	2.8484150000	-0.1597610000
H	-0.5828270000	2.4867370000	1.5430600000
H	-1.8063980000	3.1108360000	0.4209990000
H	-0.0820530000	-2.6058390000	0.4361890000
H	-0.4912360000	-2.6253710000	-1.3138310000
H	-1.7196530000	-3.0553380000	-0.0924180000
H	-3.2909080000	-1.2443450000	-0.9545190000
H	-3.3300010000	1.4989450000	-0.5313020000

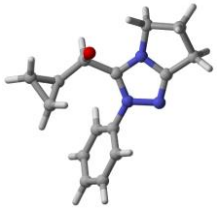
thermodynamic data

Zero-point correction= 0.238842 (Hartree/Particle)
Thermal correction to Energy= 0.251204
Thermal correction to Enthalpy= 0.252148
Thermal correction to Gibbs Free Energy= 0.200134
Sum of electronic and zero-point Energies= -536.023870
Sum of electronic and thermal Energies= -536.011508
Sum of electronic and thermal Enthalpies= -536.010564
Sum of electronic and thermal Free Energies= -536.062578

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	157.633	46.164	109.472

B3LYP/6-31G*	**Job11de**





xyz-matrix

36

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.5539000000	1.8626050000	0.4029260000
H	-0.9957530000	2.2430890000	1.3646410000
O	-1.2105100000	2.1635570000	-0.7101380000
C	0.9299900000	2.2442780000	0.4218340000
C	1.2799160000	3.5537950000	-0.2403140000
C	1.6841640000	2.2521800000	-0.8833060000
H	1.4820540000	1.9905800000	1.3261680000
H	2.0487260000	4.1716510000	0.2169890000
H	0.4562340000	4.0890200000	-0.7023040000
H	2.7320010000	1.9639910000	-0.8805900000
H	1.1114700000	1.9522530000	-1.7557380000
C	-0.8038800000	0.2978010000	0.4700000000
N	-0.0902860000	-0.7977940000	0.1122950000
N	-0.8972500000	-1.8989000000	-0.2196120000
N	-2.0823930000	-0.1570740000	0.4537490000
C	-2.0963470000	-1.4436980000	-0.0002310000
C	1.3264370000	-0.9894240000	0.0908320000
C	2.0773060000	-0.7641860000	1.2448460000
C	1.9267050000	-1.4643790000	-1.0758880000

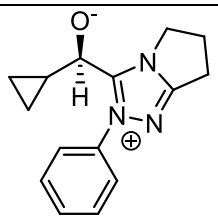
C	3.4537000000	-0.9857230000	1.2179820000
C	3.3011840000	-1.6953020000	-1.0889640000
C	4.0671770000	-1.4510770000	0.0532170000
H	1.5845490000	-0.4259560000	2.1506180000
H	1.3168750000	-1.6462080000	-1.9540910000
H	4.0433310000	-0.8060770000	2.1123450000
H	3.7744130000	-2.0610040000	-1.9956360000
H	5.1387590000	-1.6287080000	0.0373120000
C	-3.3923560000	0.4956750000	0.4517980000
C	-3.5042490000	-1.9154830000	-0.1897750000
C	-4.2695470000	-0.5573450000	-0.2841270000
H	-3.2666860000	1.4433000000	-0.0809360000
H	-3.7220120000	0.6775580000	1.4798400000
H	-3.8306000000	-2.5088070000	0.6734630000
H	-3.6183950000	-2.5357040000	-1.0816130000
H	-4.3630990000	-0.2701390000	-1.3358410000
H	-5.2760760000	-0.6192210000	0.1364690000

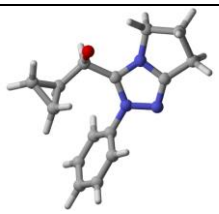
thermodynamic data

Zero-point correction= 0.299452 (Hartree/Particle)
Thermal correction to Energy= 0.315536
Thermal correction to Enthalpy= 0.316481
Thermal correction to Gibbs Free Energy= 0.255006
Sum of electronic and zero-point Energies= -820.898876
Sum of electronic and thermal Energies= -820.882792
Sum of electronic and thermal Enthalpies= -820.881847
Sum of electronic and thermal Free Energies= -820.943322

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	198.002	62.945	129.383

M062X/6-31++G**	**Job11de**





xyz-matrix

36

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.5034030000	1.8448890000	0.4572930000
H	-0.8762990000	2.1831490000	1.4602890000
O	-1.1849930000	2.2971450000	-0.5896930000
C	1.0024300000	2.1076440000	0.4369160000
C	1.4446480000	3.3563940000	-0.2663180000
C	1.7209510000	2.0102700000	-0.8768160000
H	1.5557770000	1.8266150000	1.3306590000
H	2.2761850000	3.9118930000	0.1539700000
H	0.6490240000	3.9330010000	-0.7255220000
H	2.7381220000	1.6288860000	-0.8738320000
H	1.1075740000	1.7430810000	-1.7327380000
C	-0.8147250000	0.3060130000	0.4511520000
N	-0.1254890000	-0.8147970000	0.1707700000
N	-0.9377360000	-1.8942580000	-0.1252410000
N	-2.0949040000	-0.0966760000	0.3852620000
C	-2.1329340000	-1.4044400000	0.0162480000
C	1.2928590000	-1.0035510000	0.1185970000
C	2.0541440000	-0.8254330000	1.2667880000
C	1.8676100000	-1.3924140000	-1.0860860000

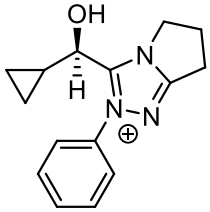
C	3.4333920000	-1.0017880000	1.1948480000
C	3.2448250000	-1.5823730000	-1.1443050000
C	4.0281200000	-1.3784770000	-0.0086520000
H	1.5694770000	-0.5418850000	2.1958890000
H	1.2375480000	-1.5276400000	-1.9589590000
H	4.0410180000	-0.8524810000	2.0814050000
H	3.7071920000	-1.8782210000	-2.0802310000
H	5.1031310000	-1.5179980000	-0.0602340000
C	-3.3953760000	0.5719780000	0.3756130000
C	-3.5483250000	-1.8474480000	-0.1739090000
C	-4.2611470000	-0.4783330000	-0.3640040000
H	-3.2652260000	1.5238880000	-0.1468420000
H	-3.7232300000	0.7414760000	1.4053140000
H	-3.8997050000	-2.3693430000	0.7223680000
H	-3.6621900000	-2.5164620000	-1.0272360000
H	-4.2813320000	-0.2302100000	-1.4282550000
H	-5.2886400000	-0.4923570000	0.0017610000

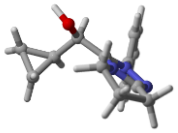
thermodynamic data

Zero-point correction= 0.301392 (Hartree/Particle)
Thermal correction to Energy= 0.317250
Thermal correction to Enthalpy= 0.318194
Thermal correction to Gibbs Free Energy= 0.257197
Sum of electronic and zero-point Energies= -820.605410
Sum of electronic and thermal Energies= -820.589552
Sum of electronic and thermal Enthalpies= -820.588608
Sum of electronic and thermal Free Energies= -820.649605

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	199.077	62.314	128.379

B3LYP/6-31G*	**Job11pr**





xyz-matrix

37

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.3493310000	1.4821760000	0.7691690000
H	0.5014820000	1.5175900000	1.4626400000
O	-1.5458680000	1.8861530000	1.4139680000
H	-1.3780880000	2.7219970000	1.8763920000
C	-0.0045230000	2.2978640000	-0.4778720000
C	-0.3583570000	3.7631310000	-0.5612700000
C	-1.0754170000	2.7634630000	-1.4326540000
H	0.9519420000	2.0119600000	-0.9105020000
H	0.3715660000	4.4292120000	-1.0103630000
H	-0.9307600000	4.2147880000	0.2443450000
H	-0.8576780000	2.7420850000	-2.4959710000
H	-2.1110700000	2.5562560000	-1.1783700000
C	-0.5838730000	0.0357500000	0.3993060000
N	0.3372680000	-0.8817670000	0.0607980000
N	-0.2363080000	-2.0785120000	-0.3206610000
N	-1.7674920000	-0.5784160000	0.2412710000
C	-1.5162350000	-1.8575300000	-0.1927900000
C	1.7723140000	-0.7393500000	0.0490950000
C	2.4484380000	-0.5248970000	1.2511360000

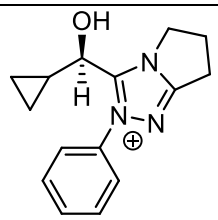
C	2.4470460000	-0.8555560000	-1.1667210000
C	3.8374830000	-0.3974010000	1.2255520000
C	3.8360510000	-0.7345720000	-1.1745020000
C	4.5284950000	-0.5002770000	0.0163500000
H	1.9042900000	-0.4865630000	2.1901580000
H	1.8945560000	-1.0453570000	-2.0810990000
H	4.3778670000	-0.2343880000	2.1526130000
H	4.3761400000	-0.8253190000	-2.1115830000
H	5.6100380000	-0.4075280000	0.0029540000
C	-3.2092190000	-0.3097010000	0.4510100000
C	-2.7836360000	-2.6334200000	-0.3520110000
C	-3.8570160000	-1.5047050000	-0.2985820000
H	-3.4756720000	0.6650230000	0.0465640000
H	-3.4061450000	-0.3093540000	1.5255780000
H	-2.8892380000	-3.3449330000	0.4755100000
H	-2.8085070000	-3.2054070000	-1.2822970000
H	-4.1176110000	-1.1979660000	-1.3155330000
H	-4.7737570000	-1.8303110000	0.1960670000

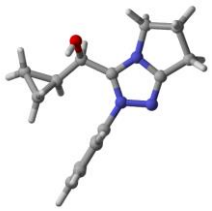
thermodynamic data

Zero-point correction= 0.313747 (Hartree/Particle)
Thermal correction to Energy= 0.330282
Thermal correction to Enthalpy= 0.331226
Thermal correction to Gibbs Free Energy= 0.268126
Sum of electronic and zero-point Energies= -821.337562
Sum of electronic and thermal Energies= -821.321027
Sum of electronic and thermal Enthalpies= -821.320083
Sum of electronic and thermal Free Energies= -821.383183

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	207.255	64.412	132.805

M062X/6-31++G**	**Job11pr**





xyz-matrix

37

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.3980440000	1.7846880000	0.3719510000
H	-0.9330080000	2.1925470000	1.2395040000
O	-0.9427130000	2.4610140000	-0.7392350000
H	-0.3911460000	2.3154160000	-1.5203340000
C	1.0842580000	1.9877130000	0.5810960000
C	1.6990050000	3.3068870000	0.2125230000
C	2.0430790000	2.0717310000	-0.5714900000
H	1.4588450000	1.5173670000	1.4852680000
H	2.4457970000	3.7149130000	0.8828290000
H	1.0576660000	4.0405220000	-0.2641190000
H	3.0170460000	1.6136930000	-0.4349080000
H	1.6684340000	1.9945250000	-1.5900230000
C	-0.8452270000	0.3339370000	0.2657840000
N	-0.1867370000	-0.8239220000	0.1355630000
N	-1.0342680000	-1.8888880000	-0.0073160000
N	-2.1392600000	-0.0016040000	0.2055490000
C	-2.2206210000	-1.3530830000	0.0410720000
C	1.2359590000	-1.0615300000	0.0620690000

C	1.9750480000	-1.1500870000	1.2346530000
C	1.8034650000	-1.2443260000	-1.1929320000
C	3.3438810000	-1.3894210000	1.1387560000
C	3.1708780000	-1.4928650000	-1.2750060000
C	3.9387230000	-1.5574580000	-0.1122070000
H	1.4893600000	-1.0361600000	2.1992200000
H	1.1836080000	-1.1998880000	-2.0831950000
H	3.9415250000	-1.4577070000	2.0413240000
H	3.6339620000	-1.6397910000	-2.2446880000
H	5.0039850000	-1.7515950000	-0.1797820000
C	-3.4491780000	0.6685770000	0.2586230000
C	-3.6467740000	-1.7931830000	-0.0221500000
C	-4.3701360000	-0.4458730000	-0.2974100000
H	-3.4263400000	1.5742350000	-0.3475900000
H	-3.6706730000	0.9231900000	1.2985900000
H	-3.9379990000	-2.2281070000	0.9392510000
H	-3.8167530000	-2.5394400000	-0.7983660000
H	-4.4868870000	-0.3085050000	-1.3749890000
H	-5.3597540000	-0.4066750000	0.1573220000

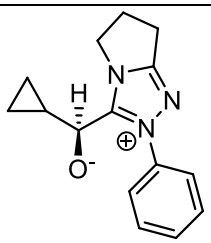
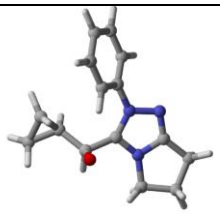
thermodynamic data

Zero-point correction= 0.316498 (Hartree/Particle)
Thermal correction to Energy= 0.332558
Thermal correction to Enthalpy= 0.333503
Thermal correction to Gibbs Free Energy= 0.272222
Sum of electronic and zero-point Energies= -821.031655
Sum of electronic and thermal Energies= -821.015595
Sum of electronic and thermal Enthalpies= -821.014651
Sum of electronic and thermal Free Energies= -821.075932

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	208.684	63.469	128.976

M062X/6-31++G**	**Job11deko2**

xyz-matrix

36

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.3113060000	1.7984040000	-0.0442980000
H	-1.1175970000	2.3919140000	-0.5562210000
O	-0.2717250000	1.9427550000	1.2805340000
C	0.9674130000	2.1161890000	-0.8374080000
C	2.2333930000	2.4144390000	-0.0932780000
C	1.4641370000	3.5320400000	-0.7338300000
H	1.0566180000	1.6426320000	-1.8149850000
H	3.1764000000	2.1021840000	-0.5303560000
H	2.1551750000	2.3508810000	0.9874390000
H	1.8663570000	4.0055980000	-1.6230800000
H	0.9100210000	4.1821000000	-0.0624040000
C	-0.8170070000	0.3564840000	-0.2528800000
N	-0.2301160000	-0.8515020000	-0.2115730000
N	-1.1371180000	-1.8898190000	-0.1342340000
N	-2.1280540000	0.0694440000	-0.2120310000
C	-2.2838680000	-1.2819390000	-0.1327990000

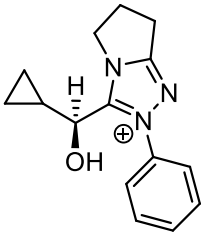
C	1.1629500000	-1.1336920000	-0.0402550000
C	1.8520840000	-0.4511340000	0.9559040000
C	1.7631260000	-2.1059130000	-0.8336130000
C	3.2018760000	-0.7439080000	1.1393270000
C	3.1094000000	-2.3925700000	-0.6289370000
C	3.8285120000	-1.7089820000	0.3531760000
H	1.3256340000	0.3053910000	1.5393330000
H	1.1794640000	-2.6257110000	-1.5863060000
H	3.5971380000	-3.1472250000	-1.2372420000
H	4.8793740000	-1.9337110000	0.5065110000
H	3.7612630000	-0.2146920000	1.9042360000
C	-3.3653400000	0.8296070000	-0.0652540000
C	-3.7339130000	-1.6298100000	-0.0264070000
C	-4.3296020000	-0.2728150000	0.4445620000
H	-3.6649790000	1.2424130000	-1.0322610000
H	-3.2036780000	1.6387380000	0.6499380000
H	-3.9159670000	-2.4431140000	0.6763720000
H	-4.1217110000	-1.9272310000	-1.0061950000
H	-5.3475550000	-0.1186090000	0.0848440000
H	-4.3462680000	-0.2488540000	1.5368990000

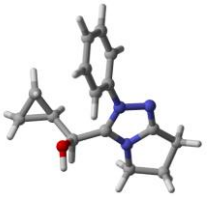
thermodynamic data

Zero-point correction= 0.301633 (Hartree/Particle)
Thermal correction to Energy= 0.317567
Thermal correction to Enthalpy= 0.318511
Thermal correction to Gibbs Free Energy= 0.257251
Sum of electronic and zero-point Energies= -820.604447
Sum of electronic and thermal Energies= -820.588513
Sum of electronic and thermal Enthalpies= -820.587568
Sum of electronic and thermal Free Energies= -820.648828

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	199.276	62.223	128.932

B3LYP/6-31G*	**Job11prko2**





xyz-matrix

37

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.3406870000	1.7946430000	0.3613400000
H	-1.2423350000	2.4186020000	0.4457360000
O	0.4437690000	1.8987080000	1.5371780000
H	-0.1052610000	2.2294670000	2.2643860000
C	0.4465140000	2.2613330000	-0.8557280000
C	1.9558400000	2.2311830000	-0.8937450000
C	1.2340580000	3.5471060000	-0.7756330000
H	-0.0743530000	2.0693940000	-1.7926880000
H	2.4246420000	1.9726210000	-1.8382410000
H	2.4793900000	1.8742920000	-0.0141770000
H	1.1995910000	4.2117840000	-1.6333640000
H	1.2810280000	4.0474330000	0.1868870000
C	-0.8593720000	0.3736040000	0.1797300000
N	-0.1940820000	-0.7877790000	0.0371660000
N	-1.0475850000	-1.8506740000	-0.1836640000

N	-2.1607460000	0.0390060000	0.0654030000
C	-2.2347430000	-1.3100030000	-0.1659010000
C	1.2251230000	-1.0557990000	0.0795550000
C	1.9540180000	-0.7865680000	1.2373330000
C	1.8073640000	-1.6518650000	-1.0400790000
C	3.3135100000	-1.0990130000	1.2558260000
C	3.1653840000	-1.9610470000	-1.0033590000
C	3.9180110000	-1.6823710000	0.1405360000
H	1.4728540000	-0.3355040000	2.0959330000
H	1.2065720000	-1.8715760000	-1.9162560000
H	3.6333360000	-2.4220710000	-1.8673870000
H	4.9753680000	-1.9275530000	0.1649070000
H	3.8954060000	-0.8958860000	2.1493230000
C	-3.4803390000	0.7041590000	0.0567150000
C	-3.6506910000	-1.7517870000	-0.3502530000
C	-4.4404870000	-0.5131800000	0.1722400000
H	-3.5971720000	1.2521460000	-0.8829530000
H	-3.5680830000	1.4022990000	0.8912590000
H	-3.8786330000	-2.6661870000	0.2019980000
H	-3.8456760000	-1.9489810000	-1.4110010000
H	-5.3618490000	-0.3427330000	-0.3870630000
H	-4.7090990000	-0.6634610000	1.2214580000

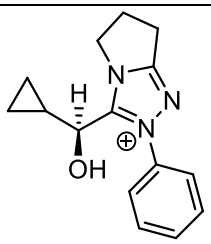
thermodynamic data

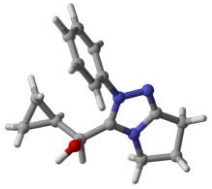
Zero-point correction= 0.313436 (Hartree/Particle)
Thermal correction to Energy= 0.330108
Thermal correction to Enthalpy= 0.331052
Thermal correction to Gibbs Free Energy= 0.267993
Sum of electronic and zero-point Energies= -821.331030
Sum of electronic and thermal Energies= -821.314358

Sum of electronic and thermal Enthalpies= -821.313414
Sum of electronic and thermal Free Energies= -821.376472

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	207.146	64.590	132.718

M062X/6-31++G**	**Job11prko2**





xyz-matrix

37

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.2778570000	1.7645160000	0.3592650000
H	-1.1418890000	2.4431940000	0.4270720000
O	0.4160780000	1.7262810000	1.5841220000
H	0.5958820000	2.6268180000	1.8824340000
C	0.5701870000	2.1785300000	-0.8325730000
C	2.0456850000	1.9040290000	-0.8799780000
C	1.5526050000	3.3087570000	-0.6884300000
H	0.0258000000	2.1392310000	-1.7738310000
H	2.4736690000	1.6299660000	-1.8373790000
H	2.4912170000	1.4183560000	-0.0178550000
H	1.6290840000	4.0109380000	-1.5098980000
H	1.6995400000	3.7533910000	0.2914840000
C	-0.8711360000	0.3905010000	0.1576470000

N	-0.2567230000	-0.7860120000	0.0042570000
N	-1.1366820000	-1.8036600000	-0.2276710000
N	-2.1762520000	0.1165120000	0.0362340000
C	-2.3013280000	-1.2231660000	-0.2066810000
C	1.1555770000	-1.0709120000	0.0698560000
C	1.8167800000	-0.9444520000	1.2850700000
C	1.7952460000	-1.4822300000	-1.0939740000
C	3.1831900000	-1.2135620000	1.3224790000
C	3.1596850000	-1.7496350000	-1.0392730000
C	3.8515700000	-1.6087290000	0.1644190000
H	1.2776890000	-0.6300510000	2.1715590000
H	1.2347110000	-1.5857480000	-2.0176940000
H	3.6817840000	-2.0679870000	-1.9350920000
H	4.9155700000	-1.8176830000	0.2008160000
H	3.7216300000	-1.1208690000	2.2594010000
C	-3.4666870000	0.8273160000	0.0542560000
C	-3.7343750000	-1.6012250000	-0.3886000000
C	-4.4551670000	-0.3564930000	0.1949700000
H	-3.5839730000	1.3699890000	-0.8873760000
H	-3.5078070000	1.5256810000	0.8906310000
H	-3.9883470000	-2.5249940000	0.1316880000
H	-3.9454420000	-1.7394590000	-1.4536800000
H	-5.3980010000	-0.1469960000	-0.3098080000
H	-4.6659910000	-0.5213770000	1.2541010000

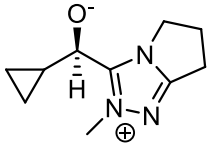
thermodynamic data

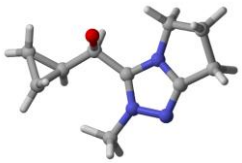
Zero-point correction=	0.315756 (Hartree/Particle)
Thermal correction to Energy=	0.332046

Thermal correction to Enthalpy= 0.332990
Thermal correction to Gibbs Free Energy= 0.271258
Sum of electronic and zero-point Energies= -821.034177
Sum of electronic and thermal Energies= -821.017887
Sum of electronic and thermal Enthalpies= -821.016943
Sum of electronic and thermal Free Energies= -821.078675

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	208.362	63.864	129.928

B3LYP/6-31G*	**Job14de**





xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

C	1.2141700000	-0.8568750000	-0.4111930000
H	1.0494340000	-1.4334110000	-1.3657030000
O	0.9883150000	-1.5141230000	0.7211360000
C	2.6091610000	-0.2251280000	-0.5523140000
C	3.7506900000	-1.0646800000	-0.0407460000
C	3.3423750000	0.1761070000	0.7091680000
H	2.7903860000	0.3499040000	-1.4625090000
H	4.6869560000	-1.0549130000	-0.5926850000
H	3.4745530000	-2.0128810000	0.4101600000
H	4.0042600000	1.0394010000	0.6885970000
H	2.7939630000	0.0169300000	1.6330830000
C	0.0359770000	0.1796130000	-0.4144060000

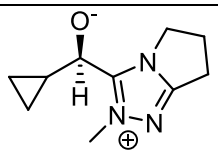
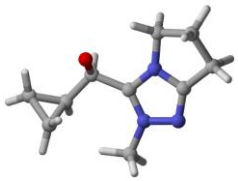
N	-0.1099390000	1.4818290000	-0.0940090000
N	-1.4297840000	1.8382400000	0.1839900000
N	-1.2389430000	-0.2843730000	-0.3929870000
C	-2.0730540000	0.7205810000	-0.0028680000
C	0.8928500000	2.5328140000	-0.0244660000
C	-1.8398790000	-1.6180600000	-0.3607510000
C	-3.1982950000	-1.3306000000	0.3410140000
C	-3.4648690000	0.2008020000	0.1808260000
H	-1.1528270000	-2.2590560000	0.1998350000
H	-1.9624790000	-1.9990910000	-1.3797760000
H	-3.1084950000	-1.5703980000	1.4048840000
H	-4.0087590000	-1.9366860000	-0.0707340000
H	-4.0773510000	0.4173360000	-0.7033780000
H	-3.9637350000	0.6422430000	1.0465310000
H	0.7628650000	3.2263280000	-0.8608380000
H	1.8787010000	2.0760070000	-0.0559970000
H	0.7619100000	3.0739440000	0.9149140000

thermodynamic data

Zero-point correction= 0.247224 (Hartree/Particle)
Thermal correction to Energy= 0.260295
Thermal correction to Enthalpy= 0.261239
Thermal correction to Gibbs Free Energy= 0.207276
Sum of electronic and zero-point Energies= -629.217925
Sum of electronic and thermal Energies= -629.204853
Sum of electronic and thermal Enthalpies= -629.203909
Sum of electronic and thermal Free Energies= -629.257872

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.338	49.362	113.575

M062X/6-31++G**	**Job14de**

xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

C	1.2220000000	-0.8424790000	-0.5131130000
H	1.0851200000	-1.2264220000	-1.5611270000
O	1.0113420000	-1.7317260000	0.4498340000
C	2.5934900000	-0.1583040000	-0.4961520000
C	3.7246620000	-0.9997380000	0.0121600000
C	3.2100280000	0.1423920000	0.8430590000
H	2.8155140000	0.5090680000	-1.3295820000
H	4.6948660000	-0.8914940000	-0.4604740000
H	3.4443960000	-1.9931270000	0.3449970000
H	3.8339070000	1.0256730000	0.9468290000
H	2.6099120000	-0.1317070000	1.7056130000
C	0.0483160000	0.1852060000	-0.3782900000
N	-0.0989630000	1.4909010000	-0.1122050000
N	-1.4021970000	1.8483550000	0.1477450000
N	-1.2076000000	-0.2898980000	-0.3027290000
C	-2.0467000000	0.7252240000	0.0238600000
C	0.9006630000	2.5463890000	-0.0484450000
C	-1.8362430000	-1.6109250000	-0.3256680000
C	-3.1801070000	-1.3057910000	0.3810320000
C	-3.4427150000	0.2151480000	0.1878860000

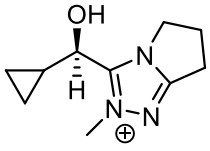
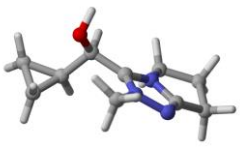
H	-1.1681700000	-2.3008320000	0.1953450000
H	-1.9671270000	-1.9281340000	-1.3645830000
H	-3.0729450000	-1.5173990000	1.4480420000
H	-3.9944540000	-1.9190930000	-0.0069040000
H	-4.0219630000	0.4174010000	-0.7191900000
H	-3.9567860000	0.6755980000	1.0319940000
H	0.7175470000	3.2598690000	-0.8535400000
H	1.8856780000	2.0994940000	-0.1393480000
H	0.8047280000	3.0466800000	0.9156140000

thermodynamic data

Zero-point correction= 0.248905 (Hartree/Particle)
Thermal correction to Energy= 0.261778
Thermal correction to Enthalpy= 0.262722
Thermal correction to Gibbs Free Energy= 0.208931
Sum of electronic and zero-point Energies= -628.989067
Sum of electronic and thermal Energies= -628.976195
Sum of electronic and thermal Enthalpies= -628.975251
Sum of electronic and thermal Free Energies= -629.029042

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.268	48.807	113.213

B3LYP/6-31G*	**Job14pr**

xyz-matrix

30

XYZ file generated by gabedit : coordinates in Angstrom

C	1.2805190000	-0.5433710000	0.6999420000
H	0.9630590000	-1.4369510000	1.2576910000
O	2.1052130000	0.2806510000	1.4995960000
H	1.8783930000	0.1639240000	2.4354390000
C	2.0396670000	-0.9906690000	-0.5448170000
C	3.4738750000	-1.4410640000	-0.4286160000
C	3.1475290000	-0.1538640000	-1.1419690000
H	1.4130960000	-1.5423890000	-1.2440250000
H	3.7774820000	-2.3048280000	-1.0118690000
H	3.9511430000	-1.3549370000	0.5424650000
H	3.2226660000	-0.1197050000	-2.2245760000
H	3.4304420000	0.7645470000	-0.6380000000
C	0.0024420000	0.1839750000	0.3054690000
N	-0.1893360000	1.4757500000	0.0044900000
N	-1.4876590000	1.7405470000	-0.3605640000
N	-1.2046370000	-0.3924640000	0.1322130000
C	-2.0802560000	0.5803100000	-0.2771040000
C	0.7686080000	2.5880880000	-0.0037380000
C	-1.8190110000	-1.7332540000	0.2198490000
C	-3.3331100000	-1.3828620000	0.1647690000
C	-3.4416230000	0.0143740000	-0.5201190000
H	-1.5247360000	-2.2337950000	1.1445360000
H	-1.4879870000	-2.3332950000	-0.6328620000
H	-3.7282840000	-1.3255940000	1.1826490000
H	-3.8958740000	-2.1503800000	-0.3690220000
H	-3.6246650000	-0.0664310000	-1.5981100000
H	-4.2343160000	0.6355980000	-0.0973020000
H	0.9948850000	2.8513700000	-1.0390450000

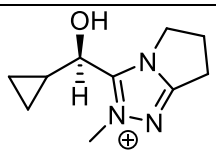
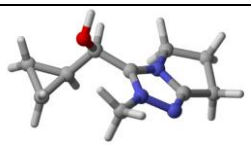
H	1.6657320000	2.2756230000	0.5247550000
H	0.2968480000	3.4352260000	0.4955410000

thermodynamic data

Zero-point correction=	0.261460 (Hartree/Particle)
Thermal correction to Energy=	0.274861
Thermal correction to Enthalpy=	0.275805
Thermal correction to Gibbs Free Energy=	0.221142
Sum of electronic and zero-point Energies=	-629.648643
Sum of electronic and thermal Energies=	-629.635243
Sum of electronic and thermal Enthalpies=	-629.634298
Sum of electronic and thermal Free Energies=	-629.688961

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	172.478	50.886	115.048

M062X/6-31++G**	**Job14pr**

xyz-matrix

30

XYZ file generated by gabedit : coordinates in Angstrom

C	1.2489740000	-0.6551440000	0.6501270000
H	0.9133050000	-1.6070050000	1.0849350000
O	2.0415740000	0.0681960000	1.5588370000
H	1.8764200000	-0.2150190000	2.4654280000
C	2.0328550000	-0.9351380000	-0.6203620000
C	3.4648460000	-1.3662990000	-0.5169060000
C	3.1322640000	-0.0021810000	-1.0522870000
H	1.4346110000	-1.3933760000	-1.4047240000

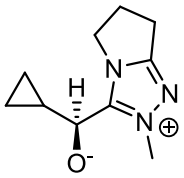
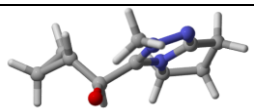
H	3.8104440000	-2.1262380000	-1.2074400000
H	3.9015820000	-1.4018000000	0.4751700000
H	3.2458460000	0.1813100000	-2.1143060000
H	3.3706900000	0.8342560000	-0.4053030000
C	-0.0030260000	0.1234410000	0.3042740000
N	-0.1364660000	1.4249060000	0.0534790000
N	-1.4098290000	1.7559950000	-0.2985140000
N	-1.2249120000	-0.3952970000	0.1118500000
C	-2.0543690000	0.6256810000	-0.2603400000
C	0.8806870000	2.4796740000	0.0717930000
C	-1.8936480000	-1.7072970000	0.1436680000
C	-3.3830420000	-1.2820190000	0.1345750000
C	-3.4349190000	0.1227750000	-0.5248220000
H	-1.6100440000	-2.2643540000	1.0373900000
H	-1.6061700000	-2.2720810000	-0.7469410000
H	-3.7422900000	-1.2151940000	1.1640440000
H	-3.9986480000	-2.0109960000	-0.3919350000
H	-3.6023360000	0.0657620000	-1.6049930000
H	-4.2015030000	0.7683620000	-0.0956580000
H	1.2103850000	2.6667130000	-0.9511370000
H	1.7087150000	2.1519700000	0.6955470000
H	0.4111330000	3.3719410000	0.4832000000

thermodynamic data

Zero-point correction= 0.263281 (Hartree/Particle)
Thermal correction to Energy= 0.276474
Thermal correction to Enthalpy= 0.277418
Thermal correction to Gibbs Free Energy= 0.223261
Sum of electronic and zero-point Energies= -629.416100
Sum of electronic and thermal Energies= -629.402908
Sum of electronic and thermal Enthalpies= -629.401964
Sum of electronic and thermal Free Energies= -629.456121

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	173.490	50.365	113.983

B3LYP/6-31G*	**Job14deko2**

xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.5460100000	0.1435320000	0.7168790000
H	-1.3381960000	-0.7836820000	1.3440230000
O	-1.9926910000	1.1877980000	1.3599420000
C	-2.3974850000	-0.3719400000	-0.4693550000
C	-3.5451080000	-1.2928230000	-0.1733300000
C	-2.3421040000	-1.8150990000	-0.9240040000
H	-2.5700010000	0.3803300000	-1.2384560000
H	-4.4767110000	-1.1580590000	-0.7166670000
H	-3.6752240000	-1.6055160000	0.8604940000
H	-2.4433580000	-2.0405300000	-1.9830480000
H	-1.6828110000	-2.4988940000	-0.3902040000
C	-0.0927190000	0.4269620000	0.1333880000
N	0.3888580000	1.6223600000	-0.2424540000
N	1.7482950000	1.6146140000	-0.5017350000
N	1.0025910000	-0.3702470000	0.1171920000
C	2.0843940000	0.3770730000	-0.2701450000
C	-0.3790100000	2.8622650000	-0.3156070000
C	1.3198270000	-1.7740390000	0.3798120000
C	2.8713170000	-1.7302750000	0.4724320000

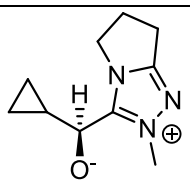
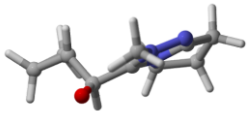
C	3.3211570000	-0.4638220000	-0.3203520000
H	-0.6233560000	3.0857630000	-1.3579930000
H	0.2333770000	3.6650860000	0.0989110000
H	-1.2788600000	2.6648690000	0.2891870000
H	0.9617630000	-2.3930240000	-0.4487940000
H	0.8351300000	-2.1089900000	1.2995460000
H	3.3243340000	-2.6463980000	0.0869980000
H	3.1671870000	-1.6269690000	1.5208780000
H	4.1878800000	0.0299210000	0.1259400000
H	3.5766160000	-0.7043840000	-1.3596770000

thermodynamic data

Zero-point correction= 0.246441 (Hartree/Particle)
Thermal correction to Energy= 0.259453
Thermal correction to Enthalpy= 0.260397
Thermal correction to Gibbs Free Energy= 0.206324
Sum of electronic and zero-point Energies= -629.214897
Sum of electronic and thermal Energies= -629.201886
Sum of electronic and thermal Enthalpies= -629.200942
Sum of electronic and thermal Free Energies= -629.255015

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.809	49.444	113.806

M062X/6-31++G**	**Job14deko2**

xyz-matrix

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.5829200000	0.2823130000	0.6229720000
H	-1.4493910000	-0.4840630000	1.4468520000
O	-2.2019160000	1.3872310000	0.9624520000
C	-2.1990040000	-0.5085160000	-0.5502490000
C	-3.4187750000	-1.3141410000	-0.2510710000
C	-2.1324250000	-2.0152830000	-0.6028800000
H	-2.1932990000	0.0285270000	-1.4972500000
H	-4.2245390000	-1.3225830000	-0.9762200000
H	-3.7371130000	-1.3344470000	0.7869660000
H	-2.0554160000	-2.5061900000	-1.5680550000
H	-1.6266560000	-2.5327420000	0.2087110000
C	-0.1010290000	0.5348240000	0.1998710000
N	0.4580870000	1.6931870000	-0.1547940000
N	1.7963830000	1.5847030000	-0.4339450000
N	0.9210180000	-0.3439030000	0.1500320000
C	2.0451960000	0.3255320000	-0.2367470000
C	-0.1912050000	2.9997880000	-0.2615000000
C	1.1393980000	-1.7713250000	0.3723740000
C	2.6831860000	-1.8258260000	0.4765570000
C	3.2111190000	-0.6055930000	-0.3249950000
H	-0.2207770000	3.2858630000	-1.3141660000
H	0.4086030000	3.7150100000	0.3019430000
H	-1.1927520000	2.8680430000	0.1633810000
H	0.7499430000	-2.3322570000	-0.4814450000
H	0.6274890000	-2.0993310000	1.2788490000
H	3.0788890000	-2.7724260000	0.1069520000
H	2.9742580000	-1.7213840000	1.5251220000

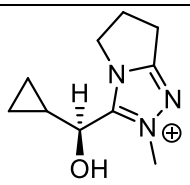
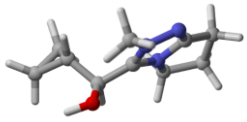
H	4.1220090000	-0.1788990000	0.0959680000
H	3.4044090000	-0.8595170000	-1.3722660000

thermodynamic data

Zero-point correction= 0.248380 (Hartree/Particle)
Thermal correction to Energy= 0.261169
Thermal correction to Enthalpy= 0.262113
Thermal correction to Gibbs Free Energy= 0.208625
Sum of electronic and zero-point Energies= -628.987433
Sum of electronic and thermal Energies= -628.974644
Sum of electronic and thermal Enthalpies= -628.973700
Sum of electronic and thermal Free Energies= -629.027187

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.886	48.944	112.574

B3LYP/6-31G*	**Job14prko2**

xyz-matrix

30

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4340050000	-0.0430560000	0.6813250000
H	-1.2827430000	-0.9564670000	1.2798460000
O	-1.9608780000	0.9988800000	1.4844400000
H	-2.9077230000	0.8182970000	1.6116410000
C	-2.3153980000	-0.3846370000	-0.5061950000
C	-3.5090920000	-1.2932860000	-0.2819740000

C	-2.3337200000	-1.7838400000	-1.0802180000
H	-2.4533830000	0.4373360000	-1.2058630000
H	-4.4294720000	-1.0498890000	-0.8031420000
H	-3.6566350000	-1.7171600000	0.7088430000
H	-2.4383160000	-1.8851860000	-2.1556980000
H	-1.7020850000	-2.5416470000	-0.6227390000
C	-0.0607220000	0.4093390000	0.2427030000
N	0.3328790000	1.6088380000	-0.2070720000
N	1.6616750000	1.6246630000	-0.5531750000
N	1.0429510000	-0.3606900000	0.1885290000
C	2.0657390000	0.4084160000	-0.3034430000
C	-0.4383430000	2.8470530000	-0.3702050000
C	1.4457920000	-1.7513030000	0.4812900000
C	2.9962870000	-1.6369820000	0.4469070000
C	3.3299460000	-0.3801520000	-0.4140070000
H	-0.5878950000	3.0326990000	-1.4361220000
H	0.1433660000	3.6603730000	0.0651720000
H	-1.3850980000	2.7331010000	0.1520290000
H	1.0486520000	-2.4070380000	-0.2986510000
H	1.0572760000	-2.0678640000	1.4512390000
H	3.4498420000	-2.5453100000	0.0468910000
H	3.3706240000	-1.4958430000	1.4644450000
H	4.1984060000	0.1702220000	-0.0454670000
H	3.5207740000	-0.6356610000	-1.4630190000

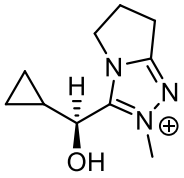
thermodynamic data

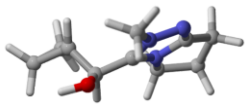
Zero-point correction= 0.261487 (Hartree/Particle)
Thermal correction to Energy= 0.274888
Thermal correction to Enthalpy= 0.275832

Thermal correction to Gibbs Free Energy= 0.220971
Sum of electronic and zero-point Energies= -629.652069
Sum of electronic and thermal Energies= -629.638668
Sum of electronic and thermal Enthalpies= -629.637724
Sum of electronic and thermal Free Energies= -629.692585

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	172.495	50.825	115.466

M062X/6-31++G**	**Job14prko2**





xyz-matrix

30

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4695310000	0.0850940000	0.6194430000
H	-1.3752880000	-0.6851900000	1.4032380000
O	-2.0571910000	1.2557880000	1.1300230000
H	-3.0048100000	1.1051830000	1.2464990000
C	-2.2171660000	-0.5047770000	-0.5536960000
C	-3.4345570000	-1.3416760000	-0.2597050000
C	-2.1882700000	-1.9926780000	-0.7817550000
H	-2.2571170000	0.1360000000	-1.4314930000
H	-4.2830750000	-1.2436360000	-0.9258840000
H	-3.6898830000	-1.5235860000	0.7804550000
H	-2.1789900000	-2.3447300000	-1.8063110000
H	-1.6298110000	-2.6095150000	-0.0835260000

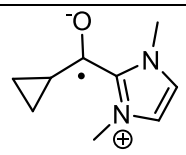
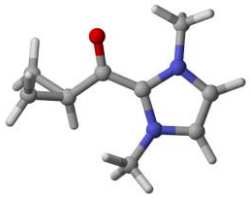
C	-0.0704300000	0.4670130000	0.2211190000
N	0.3821770000	1.6486870000	-0.1961260000
N	1.7109420000	1.6104260000	-0.4968640000
N	0.9896040000	-0.3509230000	0.1838290000
C	2.0565070000	0.3781990000	-0.2610530000
C	-0.3271270000	2.9286750000	-0.3285420000
C	1.3150450000	-1.7659670000	0.4270530000
C	2.8614620000	-1.7082810000	0.4813960000
C	3.2800640000	-0.4714140000	-0.3587050000
H	0.3134650000	3.5621420000	-0.9380420000
H	-0.4814470000	3.3620230000	0.6586360000
H	-1.2873760000	2.7632900000	-0.8116700000
H	0.9413030000	-2.3591090000	-0.4115300000
H	0.8595880000	-2.1118640000	1.3563370000
H	3.3045070000	-2.6323780000	0.1107350000
H	3.1790230000	-1.5700420000	1.5175970000
H	4.1657820000	0.0301770000	0.0319480000
H	3.4666180000	-0.7275220000	-1.4063810000

thermodynamic data

Zero-point correction= 0.263219 (Hartree/Particle)
Thermal correction to Energy= 0.276428
Thermal correction to Enthalpy= 0.277373
Thermal correction to Gibbs Free Energy= 0.223010
Sum of electronic and zero-point Energies= -629.418887
Sum of electronic and thermal Energies= -629.405677
Sum of electronic and thermal Enthalpies= -629.404733
Sum of electronic and thermal Free Energies= -629.459096

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	173.461	50.437	114.416

uB3LYP/6-31G*	**Job8radde**

xyz-matrix

25

XYZ file generated by gabedit : coordinates in Angstrom

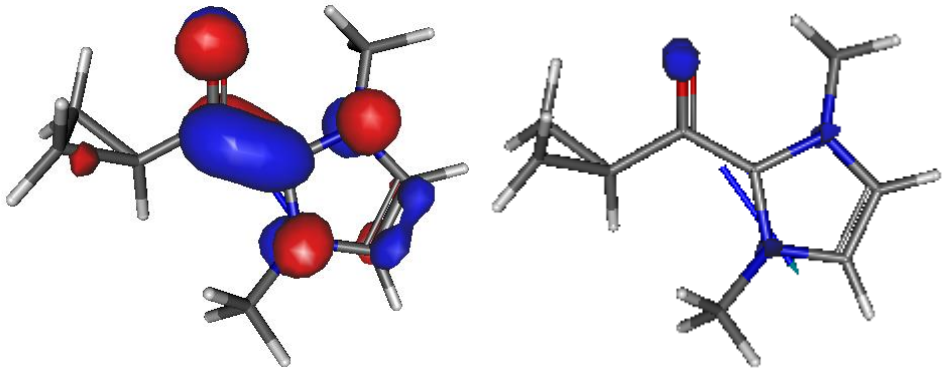
C	0.7818680000	-0.5220100000	0.1040840000
O	1.0201840000	-1.6989930000	0.5022760000
C	1.9355940000	0.3491550000	-0.3137380000
C	3.2013730000	-0.3601640000	-0.7531150000
C	3.1817540000	0.3598270000	0.5612880000
H	1.7060010000	1.2679310000	-0.8431860000
H	3.7617780000	0.0725150000	-1.5776920000
H	3.1618750000	-1.4440830000	-0.7233260000
H	3.7326680000	1.2918630000	0.6616670000
H	3.1345950000	-0.2509460000	1.4582060000
C	-0.5572630000	-0.0359520000	0.0179660000
N	-1.0266990000	1.2803170000	-0.0942050000
C	-2.4184700000	1.2572280000	-0.1516360000
N	-1.7015140000	-0.8342810000	0.0555170000
C	-2.8221530000	-0.0303190000	-0.0767110000
C	-0.2766950000	2.4878380000	0.2096550000
C	-1.7348530000	-2.2842160000	-0.0856390000
H	-1.7050270000	-2.5762940000	-1.1442800000

H	-2.6628340000	-2.6547820000	0.3598580000
H	-0.8651180000	-2.6980200000	0.4204830000
H	-2.9921620000	2.1684290000	-0.2205720000
H	-3.8147050000	-0.4531940000	-0.1055130000
H	-0.9702100000	3.2461380000	0.5831430000
H	0.2343760000	2.8906940000	-0.6723090000
H	0.4678480000	2.2811160000	0.9832030000

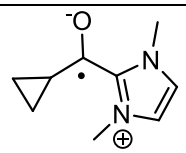
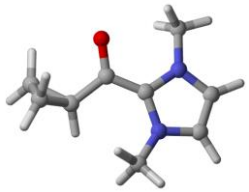
thermodynamic data

Zero-point correction= 0.210857 (Hartree/Particle)
Thermal correction to Energy= 0.223090
Thermal correction to Enthalpy= 0.224034
Thermal correction to Gibbs Free Energy= 0.171461
Sum of electronic and zero-point Energies= -535.217229
Sum of electronic and thermal Energies= -535.204997
Sum of electronic and thermal Enthalpies= -535.204053
Sum of electronic and thermal Free Energies= -535.256625

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.991	45.132	110.648



uM062X/6-31++G**	**Job8radde**

xyz-matrix

25

XYZ file generated by gabedit : coordinates in Angstrom

C	0.7662300000	-0.5463630000	0.0608790000
O	0.9725100000	-1.7276670000	0.4512020000
C	1.9211870000	0.3161040000	-0.3573920000
C	3.2089080000	-0.3946220000	-0.6767000000
C	3.1051660000	0.4070090000	0.5825480000
H	1.6962310000	1.1927170000	-0.9550520000
H	3.8096360000	-0.0002850000	-1.4887760000
H	3.1766090000	-1.4735060000	-0.5752760000
H	3.6370290000	1.3507570000	0.6465700000
H	3.0096070000	-0.1473510000	1.5106780000
C	-0.5576510000	-0.0332110000	0.0005910000
N	-1.0007830000	1.2804720000	-0.0940410000
C	-2.3882880000	1.2830700000	-0.1382190000
N	-1.6994290000	-0.8134270000	0.0399360000
C	-2.8092910000	0.0003060000	-0.0671720000
C	-0.2154890000	2.4649560000	0.1993020000
C	-1.7274360000	-2.2645450000	-0.0524670000
H	-1.1952570000	-2.5933900000	-0.9490170000
H	-2.7734670000	-2.5708390000	-0.1103460000
H	-1.2407310000	-2.7111740000	0.8126910000
H	-2.9495040000	2.2016120000	-0.2013990000
H	-3.8077680000	-0.4071880000	-0.0860110000

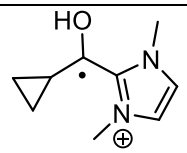
H	-0.8754540000	3.2183760000	0.6342560000
H	0.2493600000	2.8799340000	-0.6998070000
H	0.5650940000	2.2161360000	0.9223870000

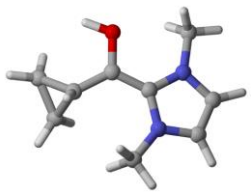
thermodynamic data

Zero-point correction= 0.211822 (Hartree/Particle)
Thermal correction to Energy= 0.223977
Thermal correction to Enthalpy= 0.224921
Thermal correction to Gibbs Free Energy= 0.172545
Sum of electronic and zero-point Energies= -535.017268
Sum of electronic and thermal Energies= -535.005113
Sum of electronic and thermal Enthalpies= -535.004169
Sum of electronic and thermal Free Energies= -535.056545

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	140.548	44.835	110.233

uB3LYP/6-31G*	**Job8radpr**	





xyz-matrix

26

XYZ file generated by gabedit : coordinates in Angstrom

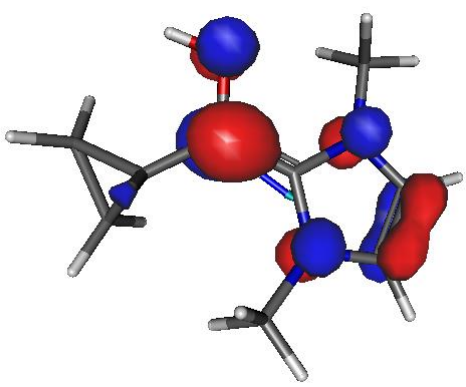
C	0.7282190000	0.6084410000	-0.3426580000
O	0.7138430000	1.9502990000	-0.5438690000
H	1.6311680000	2.2542450000	-0.6609430000
C	2.0354360000	-0.0930690000	-0.3969650000
C	2.6474950000	-0.7525140000	0.8266210000

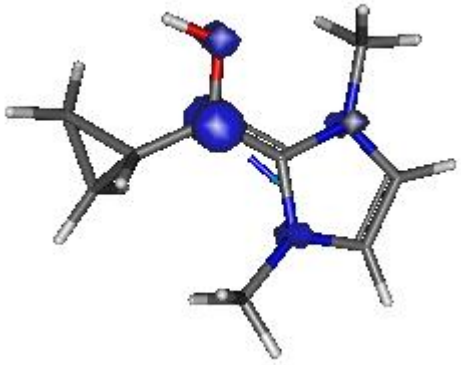
C	3.2256620000	0.5354810000	0.3202200000
H	2.2757200000	-0.5564350000	-1.3543390000
H	3.2092610000	-1.6689390000	0.6721000000
H	2.0899280000	-0.7135160000	1.7582130000
H	4.1820140000	0.5148350000	-0.1920950000
H	3.0618460000	1.4216180000	0.9288380000
C	-0.5390490000	0.0310660000	-0.1237480000
N	-1.7186280000	0.7092990000	0.1085280000
C	-2.7335850000	-0.2040350000	0.2796040000
N	-0.8558410000	-1.3113610000	-0.1010760000
C	-2.2033100000	-1.4498340000	0.1494510000
C	-1.9195150000	2.1610550000	0.2299380000
C	0.0176910000	-2.4461330000	-0.4156720000
H	0.4923390000	-2.2993610000	-1.3876270000
H	-0.6052360000	-3.3396720000	-0.4613750000
H	0.7786560000	-2.5777110000	0.3535440000
H	-3.7469820000	0.1055740000	0.4818990000
H	-2.6727050000	-2.4194430000	0.2057920000
H	-2.9615080000	2.3225960000	0.5068380000
H	-1.7083480000	2.6561630000	-0.7177000000
H	-1.2698820000	2.5693380000	1.0048930000

thermodynamic data

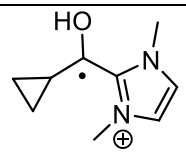
Zero-point correction= 0.224440 (Hartree/Particle)
Thermal correction to Energy= 0.236811
Thermal correction to Enthalpy= 0.237755
Thermal correction to Gibbs Free Energy= 0.184885
Sum of electronic and zero-point Energies= -535.605657
Sum of electronic and thermal Energies= -535.593286
Sum of electronic and thermal Enthalpies= -535.592342
Sum of electronic and thermal Free Energies= -535.645212

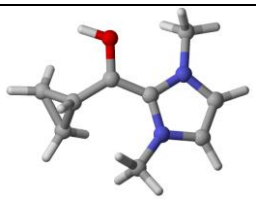
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.601	46.283	111.275





uM062X/6-31++G**	**Job8radpr**





xyz-matrix

26

XYZ file generated by gabedit : coordinates in Angstrom

C	0.7317330000	0.6294980000	-0.4258520000
O	0.6787600000	1.9377780000	-0.7425720000
H	1.5773570000	2.2911720000	-0.8210710000
C	2.0495110000	-0.0382650000	-0.3852430000
C	2.4911960000	-0.8004750000	0.8361170000
C	3.0910400000	0.5407840000	0.5577570000
H	2.4337730000	-0.3831280000	-1.3446550000
H	3.1043990000	-1.6806060000	0.6777590000
H	1.7949910000	-0.8651180000	1.6671050000

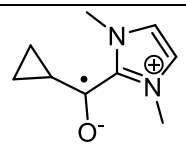
H	4.1118970000	0.5871970000	0.1980640000
H	2.7926690000	1.3586710000	1.2063520000
C	-0.5196570000	0.0344390000	-0.1544350000
N	-1.6822130000	0.6918360000	0.1348340000
C	-2.6753240000	-0.2315290000	0.3506960000
N	-0.8068020000	-1.3012380000	-0.1295360000
C	-2.1337220000	-1.4672430000	0.1879190000
C	-1.8716290000	2.1385400000	0.2882320000
C	0.0697260000	-2.4032920000	-0.5279660000
H	0.6428900000	-2.1146400000	-1.4084870000
H	-0.5629600000	-3.2532410000	-0.7802570000
H	0.7440510000	-2.6755380000	0.2835460000
H	-3.6812370000	0.0644480000	0.6038780000
H	-2.5825480000	-2.4454770000	0.2597180000
H	-2.8781970000	2.2928980000	0.6735320000
H	-1.7569550000	2.6384640000	-0.6722210000
H	-1.1443490000	2.5337550000	0.9968830000

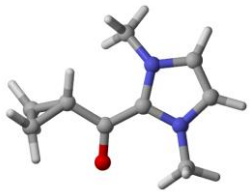
thermodynamic data

Zero-point correction= 0.226352 (Hartree/Particle)
Thermal correction to Energy= 0.238226
Thermal correction to Enthalpy= 0.239170
Thermal correction to Gibbs Free Energy= 0.188139
Sum of electronic and zero-point Energies= -535.400550
Sum of electronic and thermal Energies= -535.388676
Sum of electronic and thermal Enthalpies= -535.387731
Sum of electronic and thermal Free Energies= -535.438762

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	149.489	45.584	107.404

uB3LYP/6-31G*	**Job8raddeko2**





xyz-matrix

25

XYZ file generated by gabedit : coordinates in Angstrom

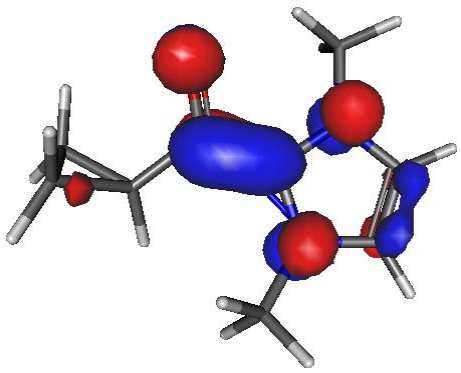
C	0.7818700000	-0.5220150000	0.1040340000
O	1.0201500000	-1.6989820000	0.5021780000
C	1.9355970000	0.3492220000	-0.3136880000
C	3.2014250000	-0.3600780000	-0.7529640000
C	3.1816600000	0.3599610000	0.5614240000
H	1.7059640000	1.2679560000	-0.8431860000
H	3.7619150000	0.0726670000	-1.5774460000
H	3.1619680000	-1.4439990000	-0.7232370000
H	3.7325480000	1.2920260000	0.6616870000
H	3.1345570000	-0.2507480000	1.4583840000
C	-0.5572540000	-0.0359120000	0.0180330000
N	-1.7014280000	-0.8343720000	0.0557940000
C	-2.8221420000	-0.0305290000	-0.0765220000
N	-1.0268200000	1.2802980000	-0.0941300000
C	-2.4185970000	1.2570620000	-0.1514800000
C	-1.7344950000	-2.2842730000	-0.0859090000
C	-0.2768930000	2.4879720000	0.2092580000
H	0.4676480000	2.2816200000	0.9829150000
H	-0.9704790000	3.2463680000	0.5824140000
H	0.2341670000	2.8905310000	-0.6728460000

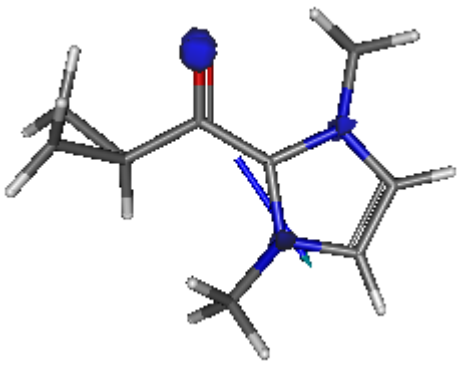
H	-0.8663170000	-2.6985030000	0.4225000000
H	-1.7014760000	-2.5760300000	-1.1445510000
H	-2.6639230000	-2.6547150000	0.3566140000
H	-3.8146720000	-0.4534650000	-0.1051750000
H	-2.9923960000	2.1682060000	-0.2202630000

thermodynamic data

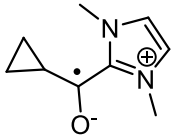
Zero-point correction= 0.210859 (Hartree/Particle)
Thermal correction to Energy= 0.223091
Thermal correction to Enthalpy= 0.224035
Thermal correction to Gibbs Free Energy= 0.171466
Sum of electronic and zero-point Energies= -535.217227
Sum of electronic and thermal Energies= -535.204996
Sum of electronic and thermal Enthalpies= -535.204052
Sum of electronic and thermal Free Energies= -535.256621

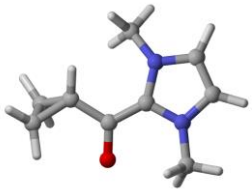
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.991	45.131	110.641





uM062X/6-31++G**	**Job8raddeko2**





xyz-matrix

25

XYZ file generated by gabedit : coordinates in Angstrom

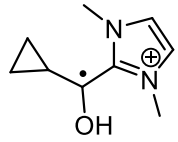
C	0.7662580000	-0.5461730000	0.0609430000
O	0.9724990000	-1.7275510000	0.4511190000
C	1.9212560000	0.3162630000	-0.3572210000
C	3.2088860000	-0.3945490000	-0.6767630000
C	3.1053680000	0.4069470000	0.5825740000
H	1.6963830000	1.1929890000	-0.9547350000
H	3.8096130000	-0.0003530000	-1.4889030000
H	3.1763670000	-1.4734280000	-0.5753220000
H	3.6372600000	1.3506850000	0.6465430000
H	3.0100150000	-0.1474590000	1.5106930000
C	-0.5576700000	-0.0331260000	0.0007730000
N	-1.6993120000	-0.8135220000	0.0398610000
C	-2.8093150000	0.0000500000	-0.0672120000
N	-1.0010190000	1.2804680000	-0.0937090000
C	-2.3884860000	1.2828840000	-0.1380520000
C	-1.7271580000	-2.2646340000	-0.0525640000
C	-0.2157310000	2.4650690000	0.1989520000
H	0.5650530000	2.2165680000	0.9219250000
H	-0.8756050000	3.2186180000	0.6338270000
H	0.2488550000	2.8797640000	-0.7004310000
H	-1.2417650000	-2.7113480000	0.8132990000
H	-1.1936380000	-2.5934430000	-0.9483060000
H	-2.7731010000	-2.5709400000	-0.1119760000
H	-3.8077230000	-0.4076090000	-0.0860330000
H	-2.9498310000	2.2013530000	-0.2011660000

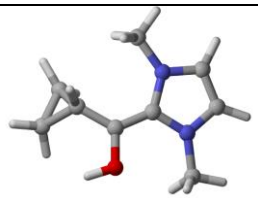
thermodynamic data

Zero-point correction=	0.211818 (Hartree/Particle)
Thermal correction to Energy=	0.223975
Thermal correction to Enthalpy=	0.224920
Thermal correction to Gibbs Free Energy=	0.172532
Sum of electronic and zero-point Energies=	-535.017272
Sum of electronic and thermal Energies=	-535.005115
Sum of electronic and thermal Enthalpies=	-535.004170
Sum of electronic and thermal Free Energies=	-535.056558

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	140.547	44.836	110.258

uB3LYP/6-31G*	**Job8radprko2**





xyz-matrix

26

XYZ file generated by gabedit : coordinates in Angstrom

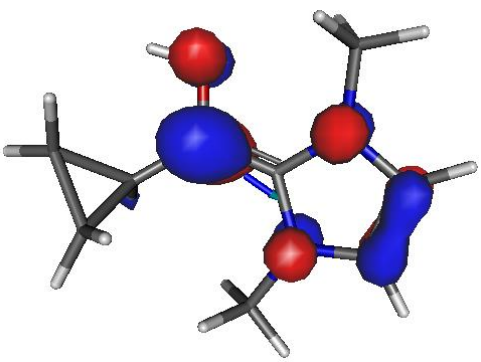
C	0.7282580000	-0.6083150000	-0.3428300000
O	0.7139220000	-1.9501820000	-0.5440240000
H	1.6312310000	-2.2540940000	-0.6612760000
C	2.0354470000	0.0932720000	-0.3969400000
C	3.2257110000	-0.5354090000	0.3201240000
C	2.6474250000	0.7523560000	0.8268940000
H	2.2756490000	0.5570100000	-1.3541490000
H	4.1820810000	-0.5145040000	-0.1921460000
H	3.0619200000	-1.4217630000	0.9284280000

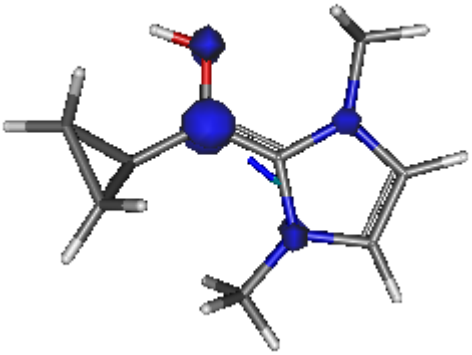
H	3.2091350000	1.6688650000	0.6726500000
H	2.0898050000	0.7131040000	1.7584410000
C	-0.5390280000	-0.0310470000	-0.1236850000
N	-1.7185710000	-0.7093730000	0.1085380000
C	-2.7335910000	0.2038920000	0.2795950000
N	-0.8559090000	1.3113490000	-0.1010200000
C	-2.2034020000	1.4497320000	0.1494490000
C	-1.9193650000	-2.1611440000	0.2300150000
C	0.0175390000	2.4461600000	-0.4157390000
H	0.4911310000	2.2999630000	-1.3883100000
H	0.7793430000	2.5770120000	0.3527590000
H	-0.6052220000	3.3398820000	-0.4600840000
H	-1.2698240000	-2.5693180000	1.0051040000
H	-1.7080020000	-2.6562950000	-0.7175560000
H	-2.9613930000	-2.3227530000	0.5067410000
H	-3.7469730000	-0.1057790000	0.4818770000
H	-2.6728600000	2.4193090000	0.2057890000

thermodynamic data

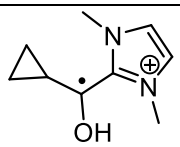
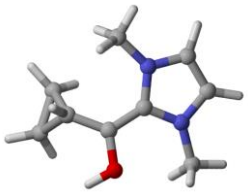
Zero-point correction= 0.224438 (Hartree/Particle)
Thermal correction to Energy= 0.236810
Thermal correction to Enthalpy= 0.237755
Thermal correction to Gibbs Free Energy= 0.184879
Sum of electronic and zero-point Energies= -535.605658
Sum of electronic and thermal Energies= -535.593286
Sum of electronic and thermal Enthalpies= -535.592342
Sum of electronic and thermal Free Energies= -535.645218

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.601	46.283	111.286





uM062X/6-31++G**	**Job8radprko2**

xyz-matrix

26

XYZ file generated by gabedit : coordinates in Angstrom

C	0.7317900000	-0.6290180000	-0.4248430000
O	0.6789640000	-1.9370600000	-0.7426770000
H	1.5776530000	-2.2902570000	-0.8210350000
C	2.0494740000	0.0390110000	-0.3854260000
C	3.0920990000	-0.5406340000	0.5559410000
C	2.4924790000	0.8004420000	0.8359410000
H	2.4324710000	0.3844480000	-1.3451260000
H	4.1125840000	-0.5867080000	0.1951810000
H	2.7944350000	-1.3590110000	1.2042510000
H	3.1055790000	1.6806050000	0.6773020000
H	1.7974180000	0.8646650000	1.6678950000
C	-0.5198440000	-0.0343010000	-0.1539800000
N	-1.6822670000	-0.6923130000	0.1344400000

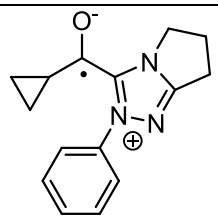
C	-2.6761260000	0.2304350000	0.3492590000
N	-0.8077810000	1.3012920000	-0.1291310000
C	-2.1350810000	1.4664780000	0.1868680000
C	-1.8704710000	-2.1390350000	0.2892920000
C	0.0688230000	2.4037560000	-0.5260830000
H	0.6424120000	2.1160370000	-1.4066530000
H	0.7427080000	2.6752740000	0.2860190000
H	-0.5637680000	3.2539900000	-0.7776490000
H	-1.1422080000	-2.5329410000	0.9976770000
H	-1.7562320000	-2.6397660000	-0.6707890000
H	-2.8765560000	-2.2938220000	0.6756880000
H	-3.6821010000	-0.0661090000	0.6015270000
H	-2.5846330000	2.4444200000	0.2581600000

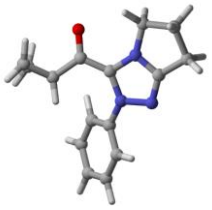
thermodynamic data

Zero-point correction= 0.226352 (Hartree/Particle)
Thermal correction to Energy= 0.238226
Thermal correction to Enthalpy= 0.239170
Thermal correction to Gibbs Free Energy= 0.188137
Sum of electronic and zero-point Energies= -535.400549
Sum of electronic and thermal Energies= -535.388675
Sum of electronic and thermal Enthalpies= -535.387731
Sum of electronic and thermal Free Energies= -535.438764

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	149.489	45.583	107.408

uB3LYP/6-31G*	**Job11radde**





xyz-matrix

35

XYZ file generated by gabedit : coordinates in Angstrom

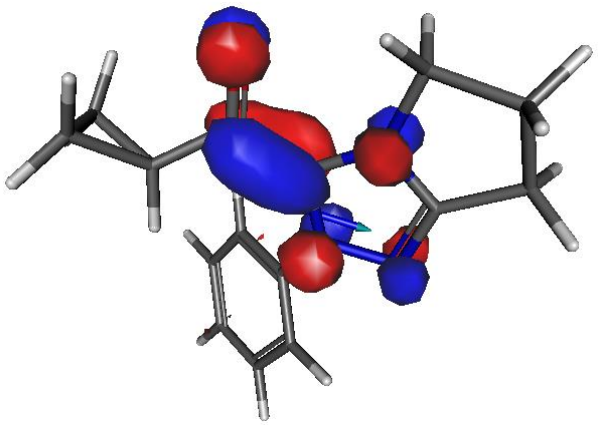
C	-0.5037890000	1.7136470000	0.0173810000
O	-1.4232080000	2.4962920000	0.3749490000
C	0.8012520000	2.2521070000	-0.4774520000
C	1.4006580000	3.4456000000	0.2546270000
C	0.7762290000	3.6392680000	-1.0918760000
H	1.4999650000	1.5426760000	-0.9064470000
H	2.4824070000	3.4903070000	0.3476600000
H	0.8422150000	3.8034050000	1.1147270000
H	1.4219520000	3.8172540000	-1.9473730000
H	-0.1948330000	4.1228260000	-1.1234810000
C	-0.7539900000	0.3071170000	0.0653240000
N	0.0191910000	-0.8346140000	-0.1967230000
N	-0.7842970000	-1.9883830000	-0.3098710000
N	-2.0357750000	-0.2133100000	0.1757720000
C	-1.9840860000	-1.5466230000	-0.0753560000
C	1.4083280000	-1.0319400000	-0.0285310000
C	2.1406130000	-0.2787510000	0.9004750000
C	2.0467620000	-2.0310070000	-0.7790400000
C	3.5071100000	-0.5082230000	1.0506540000

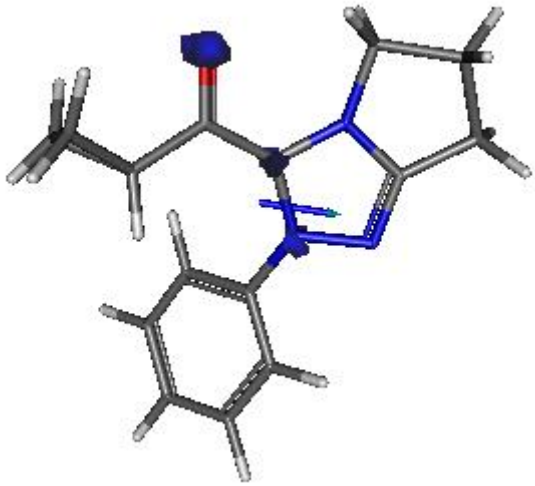
C	3.4097520000	-2.2561560000	-0.6086290000
C	4.1501820000	-1.4937630000	0.2993460000
H	1.6392030000	0.4706510000	1.5029780000
H	1.4642600000	-2.6213150000	-1.4770880000
H	4.0666300000	0.0795410000	1.7734400000
H	3.8975830000	-3.0304010000	-1.1947460000
H	5.2147230000	-1.6702390000	0.4234880000
C	-3.3767990000	0.3022240000	0.4340400000
C	-3.3507430000	-2.1546170000	0.0151430000
C	-4.2624820000	-0.8916480000	-0.0233280000
H	-3.5489380000	1.2213340000	-0.1251360000
H	-3.4881800000	0.5347810000	1.4992870000
H	-3.4541750000	-2.7061470000	0.9577780000
H	-3.5534380000	-2.8554110000	-0.7985540000
H	-4.6002660000	-0.7181970000	-1.0500730000
H	-5.1512430000	-1.0006670000	0.6030290000

thermodynamic data

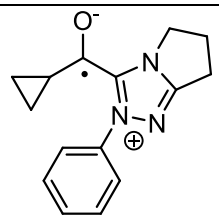
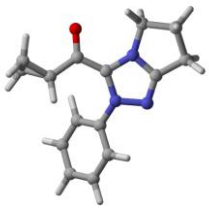
Zero-point correction= 0.288273 (Hartree/Particle)
Thermal correction to Energy= 0.304338
Thermal correction to Enthalpy= 0.305282
Thermal correction to Gibbs Free Energy= 0.243079
Sum of electronic and zero-point Energies= -820.340534
Sum of electronic and thermal Energies= -820.324469
Sum of electronic and thermal Enthalpies= -820.323525
Sum of electronic and thermal Free Energies= -820.385728

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	190.975	62.587	130.918





uM062X/6-31++G**	**Job11radde**

xyz-matrix

35

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.4421730000	1.7095470000	-0.0082680000
O	-1.3010450000	2.5384520000	0.3812700000
C	0.8771560000	2.1577620000	-0.5445290000
C	1.6352380000	3.1976960000	0.2532530000

C	0.9599570000	3.5833280000	-1.0233500000
H	1.4692090000	1.4202400000	-1.0753760000
H	2.7173240000	3.1219860000	0.2724580000
H	1.1628690000	3.5212400000	1.1754350000
H	1.5766910000	3.7780970000	-1.8934690000
H	0.0427960000	4.1557310000	-0.9415840000
C	-0.7627800000	0.3237580000	0.0433020000
N	-0.0350850000	-0.8361960000	-0.2099960000
N	-0.8652590000	-1.9548370000	-0.2959880000
N	-2.0523610000	-0.1436100000	0.1778720000
C	-2.0460090000	-1.4792090000	-0.0546570000
C	1.3482460000	-1.0574440000	-0.0325500000
C	2.0827050000	-0.2878330000	0.8738480000
C	1.9640570000	-2.0859960000	-0.7514760000
C	3.4438760000	-0.5310630000	1.0307870000
C	3.3224800000	-2.3243370000	-0.5745160000
C	4.0710200000	-1.5451890000	0.3087310000
H	1.5903890000	0.4927380000	1.4445660000
H	1.3677360000	-2.6863630000	-1.4293050000
H	4.0124190000	0.0705900000	1.7331660000
H	3.8002690000	-3.1223250000	-1.1341660000
H	5.1318840000	-1.7323490000	0.4382300000
C	-3.3736430000	0.4229800000	0.4128380000
C	-3.4321130000	-2.0319820000	0.0518570000
C	-4.2862680000	-0.7403150000	-0.0510670000
H	-3.5013110000	1.3422770000	-0.1581560000
H	-3.4877460000	0.6631070000	1.4746960000
H	-3.5540680000	-2.5257830000	1.0214320000

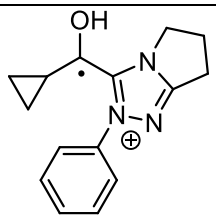
H	-3.6520730000	-2.7593640000	-0.7302740000
H	-4.5673860000	-0.5772870000	-1.0950930000
H	-5.2022030000	-0.7978780000	0.5388550000

thermodynamic data

Zero-point correction= 0.290170 (Hartree/Particle)
Thermal correction to Energy= 0.306074
Thermal correction to Enthalpy= 0.307019
Thermal correction to Gibbs Free Energy= 0.245287
Sum of electronic and zero-point Energies= -820.041696
Sum of electronic and thermal Energies= -820.025791
Sum of electronic and thermal Enthalpies= -820.024847
Sum of electronic and thermal Free Energies= -820.086579

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	192.065	62.057	129.925

uB3LYP/6-31G*	**Job11radpr**

xyz-matrix

36

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.3459800000	1.6451730000	-0.0959280000
O	-1.3188040000	2.5479820000	0.1825600000
H	-1.0531190000	3.4324520000	-0.1218020000
C	1.0131680000	2.0744400000	-0.4382470000
C	1.7935680000	3.0308650000	0.4782360000

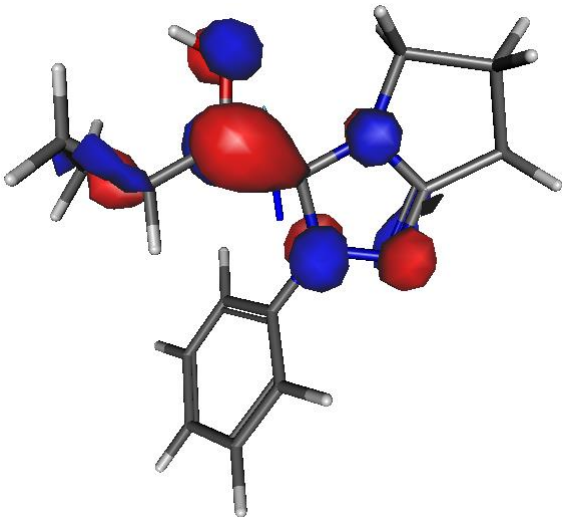
C	1.3227830000	3.5075720000	-0.8552420000
H	1.6092480000	1.3122380000	-0.9252650000
H	2.8466510000	2.8124270000	0.6235540000
H	1.2781620000	3.3972370000	1.3617760000
H	2.0397250000	3.6210480000	-1.6623680000
H	0.5306610000	4.2545920000	-0.8897390000
C	-0.7919020000	0.3129640000	0.0027670000
N	-0.0888460000	-0.8698010000	-0.0315670000
N	-0.9271050000	-1.9671590000	-0.0119910000
N	-2.1021030000	-0.0868220000	0.0779660000
C	-2.1242760000	-1.4506330000	0.0590270000
C	1.3278890000	-1.0951920000	0.0165650000
C	2.0670230000	-0.6224230000	1.1042220000
C	1.9223650000	-1.8444390000	-1.0011000000
C	3.4356650000	-0.8844320000	1.1536710000
C	3.2904850000	-2.1046000000	-0.9343910000
C	4.0468970000	-1.6221600000	0.1367190000
H	1.5757030000	-0.0764490000	1.9035500000
H	1.3189920000	-2.2197970000	-1.8209300000
H	4.0194440000	-0.5285320000	1.9969920000
H	3.7637620000	-2.6861090000	-1.7192920000
H	5.1113720000	-1.8302420000	0.1844390000
C	-3.4440220000	0.5211390000	0.1717340000
C	-3.5213050000	-1.9719250000	0.1570480000
C	-4.3596090000	-0.6939780000	-0.1434120000
H	-3.5451540000	1.3372490000	-0.5431750000
H	-3.5854620000	0.9200260000	1.1803450000
H	-3.7016980000	-2.3581050000	1.1673160000

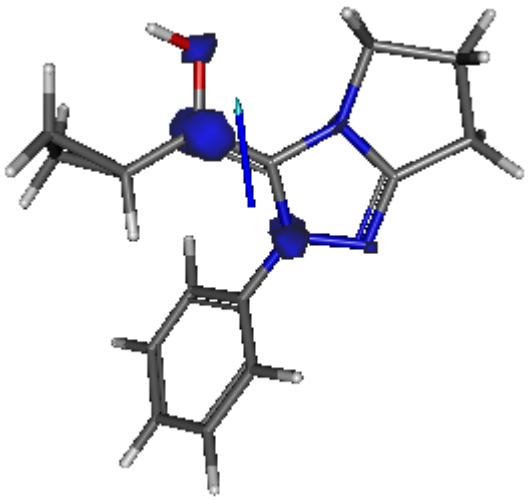
H	-3.7124100000	-2.7866860000	-0.5449150000
H	-4.6342120000	-0.6755160000	-1.2018270000
H	-5.2813380000	-0.6574400000	0.4399820000

thermodynamic data

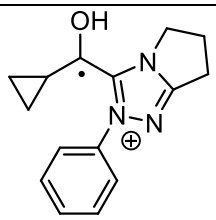
Zero-point correction= 0.300786 (Hartree/Particle)
Thermal correction to Energy= 0.317258
Thermal correction to Enthalpy= 0.318203
Thermal correction to Gibbs Free Energy= 0.254776
Sum of electronic and zero-point Energies= -820.722697
Sum of electronic and thermal Energies= -820.706225
Sum of electronic and thermal Enthalpies= -820.705281
Sum of electronic and thermal Free Energies= -820.768708

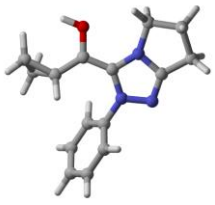
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	199.083	64.256	133.493





uM062X/6-31++G**	**Job11radpr**





xyz-matrix

36

XYZ file generated by gabedit : coordinates in Angstrom

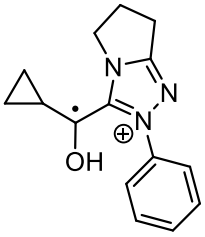
C	-0.2986320000	1.6245920000	-0.1487710000
O	-1.2391670000	2.5619210000	0.0727510000
H	-0.9435340000	3.4276950000	-0.2420300000
C	1.0856730000	1.9841800000	-0.4691790000
C	1.9226010000	2.7665890000	0.5380280000
C	1.4880340000	3.4187270000	-0.7300880000
H	1.6251170000	1.2320150000	-1.0342290000
H	2.9563860000	2.4593830000	0.6474870000
H	1.4254230000	3.0704240000	1.4538710000
H	2.2159020000	3.5689160000	-1.5184050000
H	0.7568070000	4.2202620000	-0.6624420000
C	-0.7962420000	0.3148190000	-0.0144150000
N	-0.1358020000	-0.8787790000	0.0051430000
N	-0.9958270000	-1.9407380000	0.0653130000
N	-2.1108600000	-0.0319750000	0.0649510000
C	-2.1753300000	-1.3921030000	0.1073620000
C	1.2769620000	-1.1178050000	0.0345190000
C	2.0301970000	-0.6203770000	1.0941370000
C	1.8458050000	-1.8719220000	-0.9872260000
C	3.4013050000	-0.8616720000	1.1096150000
C	3.2164670000	-2.1139150000	-0.9538390000
C	3.9924950000	-1.6042980000	0.0871810000
H	1.5481210000	-0.0627240000	1.8919500000
H	1.2204330000	-2.2622110000	-1.7835440000
H	4.0039850000	-0.4866980000	1.9301970000
H	3.6775560000	-2.7005430000	-1.7410260000

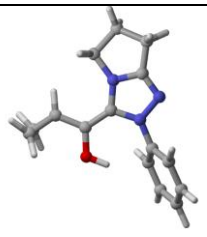
H	5.0598700000	-1.7970940000	0.1085910000
C	-3.4299670000	0.6192090000	0.1209820000
C	-3.5893080000	-1.8565950000	0.2211730000
C	-4.3671540000	-0.5756310000	-0.1785000000
H	-3.4935490000	1.4160450000	-0.6185980000
H	-3.5733350000	1.0438740000	1.1177750000
H	-3.7893840000	-2.1557930000	1.2549940000
H	-3.7998180000	-2.7087120000	-0.4254690000
H	-4.5833480000	-0.6008430000	-1.2491450000
H	-5.3133190000	-0.4817120000	0.3542940000

thermodynamic data

Zero-point correction= 0.302751 (Hartree/Particle)
Thermal correction to Energy= 0.319102
Thermal correction to Enthalpy= 0.320047
Thermal correction to Gibbs Free Energy= 0.256980
Sum of electronic and zero-point Energies= -820.418682
Sum of electronic and thermal Energies= -820.402331
Sum of electronic and thermal Enthalpies= -820.401387
Sum of electronic and thermal Free Energies= -820.464453

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.240	63.782	132.734





xyz-matrix

36

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.6144000000	1.4300150000	-0.1130420000

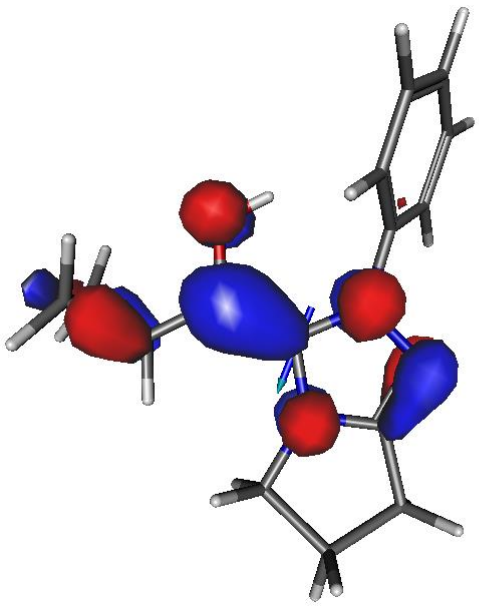
O	0.5266060000	2.1304060000	-0.2238220000
H	1.3278720000	1.5754620000	-0.1523430000
C	-1.8199320000	2.2585280000	-0.1287080000
C	-1.8234540000	3.5745580000	-0.9160070000
C	-1.8077220000	3.6272820000	0.5700170000
H	-2.7602980000	1.7255220000	-0.1034260000
H	-2.7432140000	3.8086150000	-1.4433360000
H	-0.9107110000	3.8266490000	-1.4451280000
H	-2.7143630000	3.8995680000	1.1017590000
H	-0.8820490000	3.9119120000	1.0593010000
C	-0.6184010000	0.0254280000	-0.0046690000
N	0.4602690000	-0.8440410000	-0.0362280000
N	0.0651890000	-2.1666190000	-0.0701980000
N	-1.7041410000	-0.8245850000	0.0435200000
C	-1.2359850000	-2.1072560000	-0.0245810000
C	1.8630390000	-0.5539780000	0.0168140000
C	2.3916600000	0.1372120000	1.1168630000
C	2.6881330000	-1.0250180000	-1.0095980000
C	3.7642710000	0.3921560000	1.1597950000
C	4.0575750000	-0.7775360000	-0.9416010000
C	4.5944790000	-0.0640760000	0.1342610000
H	1.7453870000	0.4394530000	1.9362350000
H	2.2570220000	-1.5772850000	-1.8376840000
H	4.7058550000	-1.1385860000	-1.7337270000
H	5.6619370000	0.1281870000	0.1772770000
H	4.1823910000	0.9263910000	2.0070590000
C	-3.1771610000	-0.7531250000	0.0890410000
C	-2.3533100000	-3.0978940000	-0.0510390000

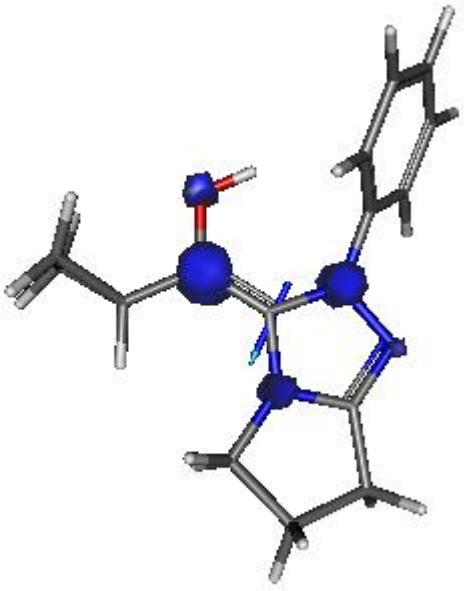
C	-3.5610160000	-2.2268210000	0.3973480000
H	-3.5564380000	-0.4078370000	-0.8783580000
H	-3.5067700000	-0.0659320000	0.8702380000
H	-2.1701810000	-3.9502190000	0.6069890000
H	-2.4788270000	-3.4867480000	-1.0686030000
H	-4.4867330000	-2.5076280000	-0.1078380000
H	-3.7196130000	-2.3408970000	1.4731450000

thermodynamic data

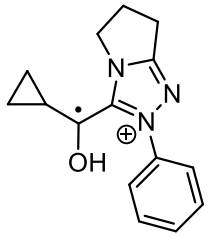
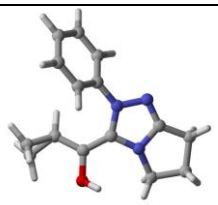
Zero-point correction= 0.301028 (Hartree/Particle)
Thermal correction to Energy= 0.317353
Thermal correction to Enthalpy= 0.318297
Thermal correction to Gibbs Free Energy= 0.255182
Sum of electronic and zero-point Energies= -820.722475
Sum of electronic and thermal Energies= -820.706150
Sum of electronic and thermal Enthalpies= -820.705205
Sum of electronic and thermal Free Energies= -820.768321

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	199.142	64.003	132.838





uM062X/6-31++G**	**Job11radprko2**

xyz-matrix

36

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.2696140000	1.6185700000	0.0085530000
O	-1.0525040000	2.6402780000	0.4138190000
H	-1.6741990000	2.3847460000	1.1070490000
C	1.0225690000	1.9924620000	-0.5444490000
C	1.8834950000	3.0003990000	0.2169250000
C	1.2194700000	3.4165390000	-1.0432190000
H	1.5478300000	1.2085210000	-1.0759600000
H	2.9498850000	2.8057270000	0.2150190000
H	1.4727710000	3.3761020000	1.1480950000
H	1.8205790000	3.5114770000	-1.9398480000
H	0.3693010000	4.0844410000	-0.9729870000
C	-0.7804130000	0.3083510000	0.0503050000
N	-0.1092210000	-0.8784220000	-0.0373650000
N	-0.9620130000	-1.9463370000	-0.1135860000
N	-2.0973320000	-0.0598030000	0.1264090000
C	-2.1451480000	-1.4182270000	-0.0221650000
C	1.2995260000	-1.1134820000	0.0553770000
C	2.0305280000	-0.5198520000	1.0820720000
C	1.8915290000	-1.9597840000	-0.8779020000

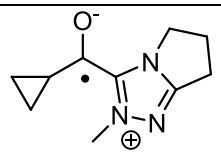
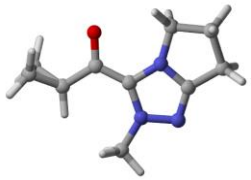
C	3.3987820000	-0.7629520000	1.1544450000
C	3.2591940000	-2.2013250000	-0.7858740000
C	4.0124780000	-1.5996750000	0.2220590000
H	1.5381250000	0.1144950000	1.8133280000
H	1.2861120000	-2.4201250000	-1.6516070000
H	3.7354270000	-2.8594190000	-1.5045210000
H	5.0781880000	-1.7912260000	0.2877930000
H	3.9814290000	-0.3106130000	1.9499070000
C	-3.4205720000	0.5695850000	-0.0223080000
C	-3.5523730000	-1.8996360000	-0.1487670000
C	-4.3558640000	-0.6338140000	0.2418480000
H	-3.5122830000	0.9769450000	-1.0336260000
H	-3.5718820000	1.3717560000	0.7008590000
H	-3.7602570000	-2.7562360000	0.4933550000
H	-3.7343300000	-2.2002400000	-1.1853180000
H	-5.2866670000	-0.5411200000	-0.3173600000
H	-4.6015470000	-0.6684750000	1.3056600000

thermodynamic data

Zero-point correction= 0.302516 (Hartree/Particle)
Thermal correction to Energy= 0.318876
Thermal correction to Enthalpy= 0.319820
Thermal correction to Gibbs Free Energy= 0.257167
Sum of electronic and zero-point Energies= -820.412300
Sum of electronic and thermal Energies= -820.395941
Sum of electronic and thermal Enthalpies= -820.394997
Sum of electronic and thermal Free Energies= -820.457650

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.098	63.952	131.865

uB3LYP/6-31G*	**Job14radde**

xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

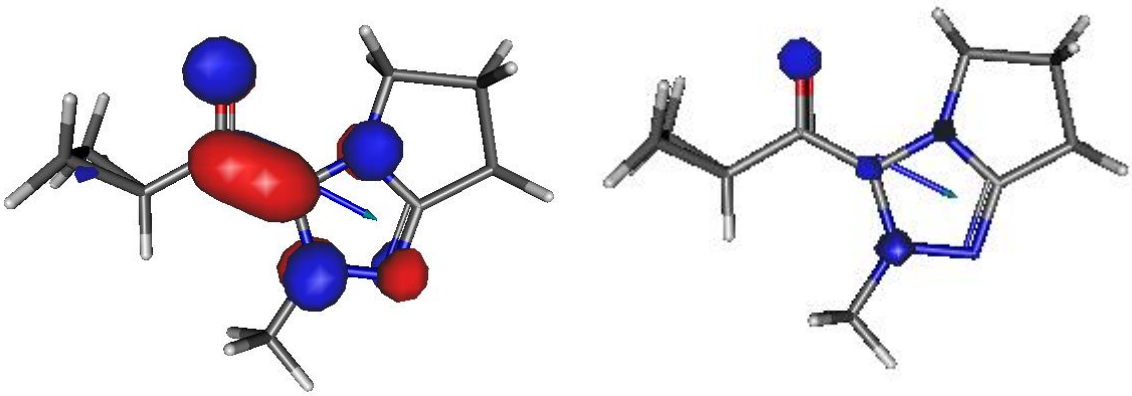
C	1.2766220000	-0.5232300000	0.0019800000
O	1.1954050000	-1.7847720000	0.0505130000
C	2.6248450000	0.1295480000	-0.0454600000
C	3.7334610000	-0.6288960000	-0.7559230000
C	3.7459550000	-0.5337340000	0.7386780000
H	2.6649910000	1.2104740000	-0.1183130000
H	4.4570200000	-0.0522160000	-1.3261070000
H	3.4460720000	-1.5823450000	-1.1877600000
H	4.4787110000	0.1088160000	1.2199210000
H	3.4674540000	-1.4247110000	1.2928200000
C	0.0696280000	0.2304360000	-0.0106380000
N	-0.2453800000	1.5898960000	-0.0221180000
N	-1.6242290000	1.8157510000	-0.0429430000
N	-1.1857890000	-0.3622710000	-0.0095000000
C	-2.1290360000	0.6168810000	-0.0464780000
C	0.6261920000	2.7354910000	0.0982860000
C	-1.7252740000	-1.7154410000	-0.0934720000
C	-3.2238770000	-1.4648970000	0.2338580000
C	-3.5028690000	0.0243220000	-0.1302260000
H	-1.2174580000	-2.3757230000	0.6079540000

H	-1.5730760000	-2.1180320000	-1.1020120000
H	-3.3895650000	-1.6145470000	1.3057090000
H	-3.8790620000	-2.1553260000	-0.3030370000
H	-3.8945780000	0.1262930000	-1.1500220000
H	-4.2153740000	0.5058480000	0.5445560000
H	1.2760430000	2.8418140000	-0.7784420000
H	1.2478970000	2.6694030000	0.9988310000
H	-0.0184120000	3.6119200000	0.1700930000

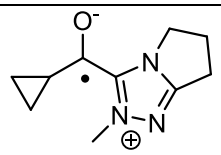
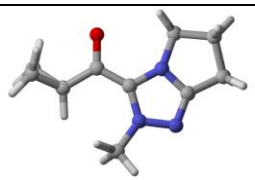
thermodynamic data

Zero-point correction= 0.235662 (Hartree/Particle)
Thermal correction to Energy= 0.248825
Thermal correction to Enthalpy= 0.249769
Thermal correction to Gibbs Free Energy= 0.194195
Sum of electronic and zero-point Energies= -628.653681
Sum of electronic and thermal Energies= -628.640517
Sum of electronic and thermal Enthalpies= -628.639573
Sum of electronic and thermal Free Energies= -628.695148

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.140	49.089	116.967



uM062X/6-31++G**	**Job14radde**

xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

C	1.2642060000	-0.5440430000	-0.0011460000
O	1.1817800000	-1.7901790000	0.1713770000
C	2.5995430000	0.1032980000	-0.1864140000
C	3.7043130000	-0.7775940000	-0.7141980000
C	3.7165640000	-0.3636090000	0.7219380000
H	2.6200090000	1.1402470000	-0.4993470000
H	4.4239580000	-0.3268030000	-1.3885480000
H	3.4174520000	-1.8016350000	-0.9261120000
H	4.4452320000	0.3702250000	1.0491490000
H	3.4369030000	-1.1173910000	1.4504090000
C	0.0651450000	0.2144130000	-0.0158770000
N	-0.2200970000	1.5684780000	-0.0454940000
N	-1.5819180000	1.8171780000	-0.0761320000
N	-1.1887920000	-0.3588990000	0.0165090000
C	-2.1121800000	0.6341710000	-0.0523930000
C	0.6805180000	2.6820190000	0.1373660000
C	-1.7493640000	-1.6983460000	-0.0975920000
C	-3.2348890000	-1.4206820000	0.2364220000
C	-3.4910480000	0.0608190000	-0.1488570000
H	-1.2523880000	-2.3807390000	0.5898160000

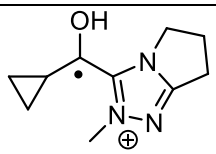
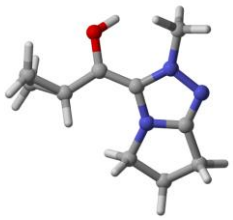
H	-1.6061560000	-2.0721800000	-1.1178810000
H	-3.3871820000	-1.5459230000	1.3120180000
H	-3.9048290000	-2.1082870000	-0.2820680000
H	-3.8532100000	0.1554350000	-1.1778980000
H	-4.2031790000	0.5613530000	0.5086570000
H	1.2378140000	2.9047200000	-0.7782360000
H	1.3821850000	2.4687970000	0.9489550000
H	0.0679490000	3.5436320000	0.4003960000

thermodynamic data

Zero-point correction= 0.236806 (Hartree/Particle)
Thermal correction to Energy= 0.249875
Thermal correction to Enthalpy= 0.250819
Thermal correction to Gibbs Free Energy= 0.195357
Sum of electronic and zero-point Energies= -628.419946
Sum of electronic and thermal Energies= -628.406877
Sum of electronic and thermal Enthalpies= -628.405933
Sum of electronic and thermal Free Energies= -628.461395

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.799	48.823	116.729

uB3LYP/6-31G*	**Job14radpr**

xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

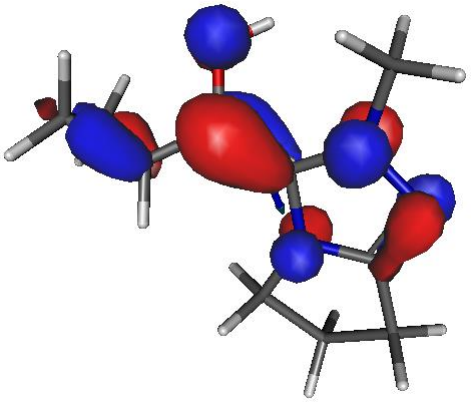
C	1.4093120000	0.3059960000	0.0692030000
O	2.2430270000	1.3164800000	0.4197610000
H	1.8105250000	1.9795750000	0.9810990000
C	2.0731150000	-0.9443630000	-0.2825880000
C	3.2149860000	-1.4868400000	0.5985130000
C	3.5378280000	-0.9266030000	-0.7388350000
H	1.4433000000	-1.6830800000	-0.7642160000
H	3.2359900000	-2.5626210000	0.7446880000
H	3.4715270000	-0.8975790000	1.4733050000
H	3.7823100000	-1.6052390000	-1.5501030000
H	4.0250190000	0.0412370000	-0.7848330000
C	0.0170780000	0.5094620000	-0.0063750000
N	-0.6792530000	1.6968370000	-0.0235680000
N	-2.0388450000	1.5031130000	-0.0664680000
N	-0.9728180000	-0.4424480000	-0.0533390000
C	-2.1754440000	0.2048680000	-0.0862590000
C	-0.1770310000	3.0679630000	-0.0848340000
C	-1.1040010000	-1.9115600000	-0.0302790000
C	-2.6128690000	-2.0875540000	0.2975020000
C	-3.3112270000	-0.7641600000	-0.1334660000
H	-0.4456250000	-2.3441400000	0.7255790000
H	-0.8372020000	-2.3156100000	-1.0121390000
H	-2.7344470000	-2.2348090000	1.3742330000
H	-3.0285940000	-2.9606620000	-0.2082820000
H	-3.7104880000	-0.8206130000	-1.1532650000
H	-4.1319710000	-0.4760410000	0.5269140000
H	-0.9719160000	3.6759230000	-0.5159170000
H	0.7060910000	3.1147090000	-0.7243960000

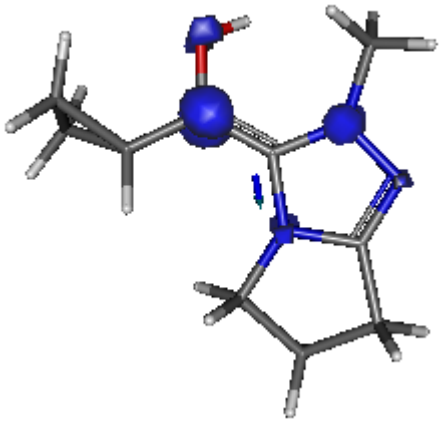
H 0.0471900000 3.4513400000 0.9173910000

thermodynamic data

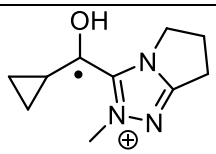
Zero-point correction= 0.248455 (Hartree/Particle)
Thermal correction to Energy= 0.261801
Thermal correction to Enthalpy= 0.262745
Thermal correction to Gibbs Free Energy= 0.207711
Sum of electronic and zero-point Energies= -629.030175
Sum of electronic and thermal Energies= -629.016830
Sum of electronic and thermal Enthalpies= -629.015885
Sum of electronic and thermal Free Energies= -629.070919

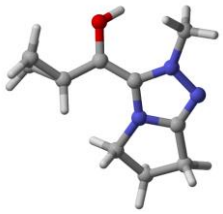
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.282	50.805	115.829





uM062X/6-31++G**	**Job14radpr**





xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

C 1.4048920000 0.3138290000 0.0615380000

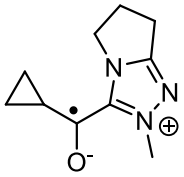
O	2.2352790000	1.2999120000	0.4492400000
H	1.8145710000	1.9568780000	1.0188820000
C	2.0508090000	-0.9353240000	-0.3191000000
C	3.1380800000	-1.5125710000	0.5888130000
C	3.5212660000	-0.9106160000	-0.7116450000
H	1.4251210000	-1.6407810000	-0.8521690000
H	3.1505220000	-2.5911380000	0.6951790000
H	3.3574660000	-0.9477910000	1.4883620000
H	3.7974420000	-1.5666220000	-1.5286130000
H	4.0109860000	0.0559090000	-0.6976770000
C	0.0144840000	0.5179680000	-0.0136670000
N	-0.6781120000	1.6944160000	-0.0173550000
N	-2.0271960000	1.4987760000	-0.0591750000
N	-0.9602880000	-0.4354810000	-0.0678220000
C	-2.1633740000	0.2053820000	-0.0915580000
C	-0.1673810000	3.0590300000	-0.0938260000
C	-1.0830900000	-1.9008020000	-0.0430730000
C	-2.5769790000	-2.0730880000	0.3241080000
C	-3.2878660000	-0.7744080000	-0.1377650000
H	-0.4028900000	-2.3286080000	0.6953500000
H	-0.8465800000	-2.2995660000	-1.0340220000
H	-2.6700070000	-2.1742510000	1.4080260000
H	-2.9988160000	-2.9659700000	-0.1370320000
H	-3.6626050000	-0.8521440000	-1.1634610000
H	-4.1171940000	-0.4835350000	0.5071170000
H	-0.9574250000	3.6637000000	-0.5361270000
H	0.7154060000	3.0849510000	-0.7338040000
H	0.0559020000	3.4492960000	0.9035890000

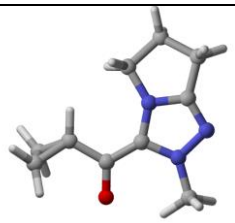
thermodynamic data

Zero-point correction= 0.249997 (Hartree/Particle)
Thermal correction to Energy= 0.263153
Thermal correction to Enthalpy= 0.264097
Thermal correction to Gibbs Free Energy= 0.209358
Sum of electronic and zero-point Energies= -628.791288
Sum of electronic and thermal Energies= -628.778132
Sum of electronic and thermal Enthalpies= -628.777188
Sum of electronic and thermal Free Energies= -628.831926

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	165.131	50.339	115.207

uB3LYP/6-31G*	**Job14raddeko2**





xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4694320000	0.3963490000	0.0298760000
O	-2.2133710000	1.4032800000	0.1992900000
C	-2.1013270000	-0.9559610000	-0.1459920000
C	-3.4930260000	-0.9912040000	-0.7507970000
C	-3.3173460000	-1.2788840000	0.7089020000
H	-1.4559060000	-1.7902960000	-0.4008930000
H	-3.7323660000	-1.8117170000	-1.4221270000
H	-3.9105140000	-0.0256500000	-1.0175490000

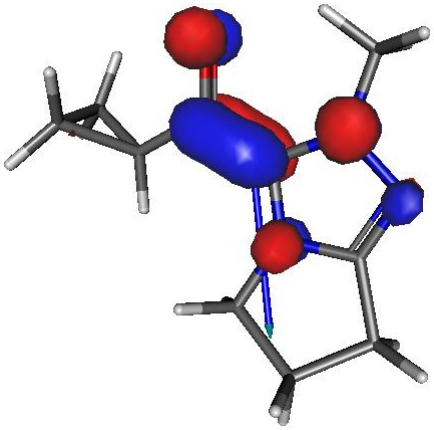
H	-3.4368130000	-2.2993040000	1.0642210000
H	-3.6207460000	-0.5031060000	1.4053460000
C	-0.0516060000	0.5246500000	0.0006370000
N	0.6850530000	1.7063460000	0.0482870000
N	2.0540200000	1.4876160000	-0.0207790000
N	0.9510370000	-0.4454310000	-0.0557280000
C	2.1595760000	0.1959520000	-0.0748080000
C	0.2021870000	3.0729140000	0.0025770000
C	1.0650730000	-1.8989090000	-0.0515650000
C	2.5741420000	-2.1069560000	0.2597190000
C	3.2839910000	-0.7880790000	-0.1576080000
H	0.3995100000	3.5141650000	-0.9824960000
H	0.7245790000	3.6598560000	0.7640200000
H	-0.8694300000	3.0455730000	0.1938840000
H	0.7800620000	-2.3121320000	-1.0279000000
H	0.4191290000	-2.3436490000	0.7102210000
H	2.9758650000	-2.9833430000	-0.2547120000
H	2.6999410000	-2.2652370000	1.3354320000
H	4.1215690000	-0.5280980000	0.4942520000
H	3.6679140000	-0.8422570000	-1.1841220000

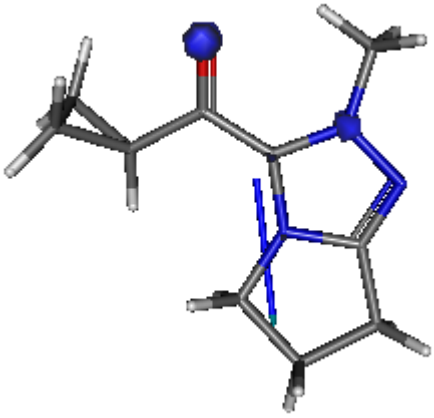
thermodynamic data

Zero-point correction= 0.235633 (Hartree/Particle)
Thermal correction to Energy= 0.248848
Thermal correction to Enthalpy= 0.249792
Thermal correction to Gibbs Free Energy= 0.193853
Sum of electronic and zero-point Energies= -628.653426
Sum of electronic and thermal Energies= -628.640211
Sum of electronic and thermal Enthalpies= -628.639267
Sum of electronic and thermal Free Energies= -628.695206

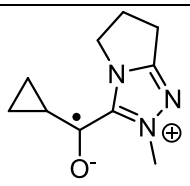
	E (Thermal)	CV	S

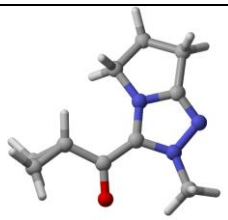
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	156.154	49.053	117.733





uM062X/6-31++G**	**Job14raddeko2**





xyz-matrix

28

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4628070000	0.4070260000	0.0368430000
O	-2.1964480000	1.3945060000	0.2969410000
C	-2.0803840000	-0.9324530000	-0.2312700000
C	-3.5094010000	-0.9276970000	-0.7113750000
C	-3.2050190000	-1.3619400000	0.6862940000
H	-1.4424190000	-1.7136510000	-0.6298820000
H	-3.7970960000	-1.6820210000	-1.4353400000
H	-3.9502180000	0.0553640000	-0.8339160000
H	-3.2853000000	-2.4146330000	0.9355880000
H	-3.4470270000	-0.6627560000	1.4797930000

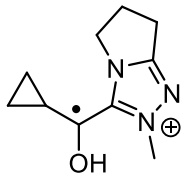
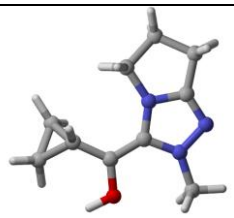
C	-0.0497550000	0.5333420000	0.0035600000
N	0.6826550000	1.7024690000	0.0985920000
N	2.0406310000	1.4795870000	0.0024090000
N	0.9352820000	-0.4388690000	-0.0824500000
C	2.1440300000	0.1940400000	-0.0863580000
C	0.1988580000	3.0606310000	-0.0528330000
C	1.0384930000	-1.8900820000	-0.0644410000
C	2.5338930000	-2.0954140000	0.2824940000
C	3.2562070000	-0.8010520000	-0.1683150000
H	0.1327480000	3.3260260000	-1.1144280000
H	0.9151790000	3.7173890000	0.4415410000
H	-0.7870900000	3.1307080000	0.4006840000
H	0.7795710000	-2.3044940000	-1.0460700000
H	0.3695220000	-2.3185190000	0.6858630000
H	2.9400050000	-2.9917760000	-0.1886810000
H	2.6343970000	-2.2064090000	1.3655660000
H	4.1016530000	-0.5362240000	0.4672300000
H	3.6129880000	-0.8757680000	-1.2009220000

thermodynamic data

Zero-point correction= 0.236916 (Hartree/Particle)
Thermal correction to Energy= 0.249989
Thermal correction to Enthalpy= 0.250933
Thermal correction to Gibbs Free Energy= 0.195863
Sum of electronic and zero-point Energies= -628.419199
Sum of electronic and thermal Energies= -628.406126
Sum of electronic and thermal Enthalpies= -628.405182
Sum of electronic and thermal Free Energies= -628.460252

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	156.871	48.780	115.905

uB3LYP/6-31G*	**Job14radprko2**

xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

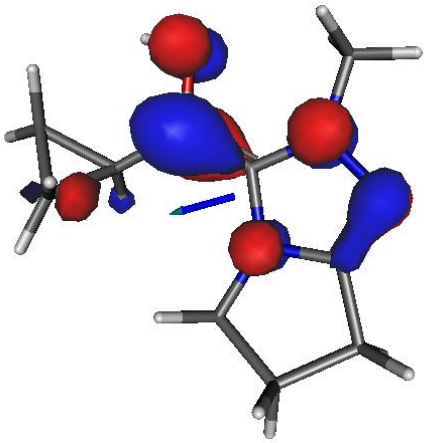
C	-1.4553950000	0.4256280000	-0.2210180000
O	-2.1697440000	1.5708800000	-0.1570440000
H	-3.1000890000	1.3756500000	-0.3672070000
C	-2.1320320000	-0.8729900000	-0.4433900000
C	-3.5620470000	-1.0759890000	0.0276170000
C	-2.4554940000	-1.8167660000	0.7150420000
H	-1.8767730000	-1.3636330000	-1.3823270000
H	-4.2281390000	-1.6191890000	-0.6346330000
H	-4.0502060000	-0.2885940000	0.5978580000
H	-2.3502090000	-2.8819760000	0.5318080000
H	-2.1873470000	-1.4967130000	1.7176780000
C	-0.0626860000	0.5802650000	-0.0945750000
N	0.6554030000	1.7378170000	0.0650190000
N	2.0036070000	1.5015310000	0.1401500000
N	0.8947710000	-0.4024750000	-0.1052040000
C	2.1110880000	0.2041350000	0.0275670000
C	0.1848920000	3.1205900000	0.1792960000
C	0.9949950000	-1.8626400000	-0.2964840000

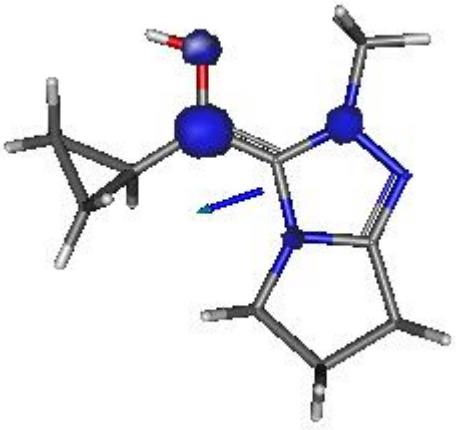
C	2.4605820000	-2.1335430000	0.1414600000
C	3.2254230000	-0.7887760000	-0.0329000000
H	-0.3558100000	3.4106800000	-0.7228390000
H	1.0775360000	3.7325890000	0.2987660000
H	-0.4672710000	3.2281440000	1.0476410000
H	0.8175730000	-2.1008240000	-1.3503050000
H	0.2598230000	-2.3842740000	0.3161110000
H	2.9044980000	-2.9427800000	-0.4409110000
H	2.4742700000	-2.4317590000	1.1934920000
H	3.9783230000	-0.6197900000	0.7402930000
H	3.7293610000	-0.7221620000	-1.0045110000

thermodynamic data

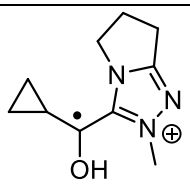
Zero-point correction= 0.248576 (Hartree/Particle)
Thermal correction to Energy= 0.261966
Thermal correction to Enthalpy= 0.262910
Thermal correction to Gibbs Free Energy= 0.207196
Sum of electronic and zero-point Energies= -629.035697
Sum of electronic and thermal Energies= -629.022308
Sum of electronic and thermal Enthalpies= -629.021363
Sum of electronic and thermal Free Energies= -629.077078

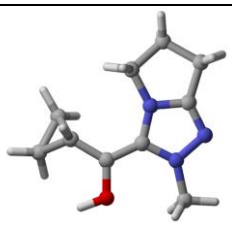
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.386	50.534	117.261





uM062X/6-31++G**	**Job14radprko2**





xyz-matrix

29

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4785270000	0.3912080000	-0.2892040000
O	-2.2028090000	1.5192830000	-0.3557500000
H	-3.1355890000	1.3028190000	-0.5037540000
C	-2.1260640000	-0.9269370000	-0.4540760000
C	-3.4382610000	-1.1718860000	0.2595860000
C	-2.2075900000	-1.8946480000	0.7055380000
H	-2.0334630000	-1.3687790000	-1.4455760000
H	-4.1993460000	-1.7241650000	-0.2777910000
H	-3.8160040000	-0.3998310000	0.9235660000
H	-2.1235120000	-2.9512060000	0.4764840000
H	-1.7670070000	-1.5859210000	1.6484860000
C	-0.0951190000	0.5766170000	-0.1104160000

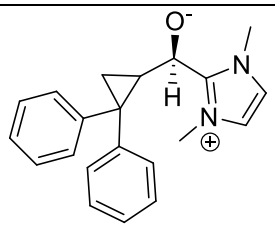
N	0.5746510000	1.7422090000	0.0949100000
N	1.9162390000	1.5471410000	0.2058930000
N	0.8782650000	-0.3774490000	-0.1038190000
C	2.0697960000	0.2609840000	0.0731560000
C	0.0453690000	3.0988730000	0.2364350000
C	1.0358580000	-1.8128360000	-0.3915020000
C	2.4832950000	-2.0578680000	0.0954710000
C	3.2129660000	-0.6946140000	-0.0105640000
H	-0.4607900000	3.3987990000	-0.6805020000
H	0.9069400000	3.7356230000	0.4254780000
H	-0.6502780000	3.1406190000	1.0747510000
H	0.9155290000	-1.9735200000	-1.4672610000
H	0.2970440000	-2.4009710000	0.1498440000
H	2.9714010000	-2.8388690000	-0.4873040000
H	2.4587580000	-2.3790160000	1.1394720000
H	3.9478750000	-0.5365810000	0.7791640000
H	3.7164950000	-0.5699300000	-0.9744790000

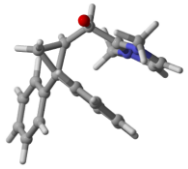
thermodynamic data

Zero-point correction= 0.250144 (Hartree/Particle)
Thermal correction to Energy= 0.263400
Thermal correction to Enthalpy= 0.264344
Thermal correction to Gibbs Free Energy= 0.209132
Sum of electronic and zero-point Energies= -628.797818
Sum of electronic and thermal Energies= -628.784562
Sum of electronic and thermal Enthalpies= -628.783618
Sum of electronic and thermal Free Energies= -628.838830

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	165.286	50.144	116.204

M062X/6-31++G**	**Job9de**





xyz-matrix

46

XYZ file generated by gabedit : coordinates in Angstrom

C	1.1568900000	-1.4985500000	-1.4282630000
H	1.2565420000	-2.6177400000	-1.5299230000
O	1.7793700000	-0.7995430000	-2.3568450000
C	-0.3954010000	-1.2802730000	-1.3587420000
C	-0.9525640000	-0.3506680000	-2.3757550000
C	-0.9935860000	0.0537150000	-0.9160660000
H	-0.9705550000	-2.1706790000	-1.1253300000
H	-1.9128530000	-0.5758770000	-2.8285110000
H	-0.1877760000	0.0788540000	-3.0166080000
C	1.7517870000	-1.2623590000	-0.0058450000
N	1.2953080000	-1.7753130000	1.1565810000
C	2.1030750000	-1.3716240000	2.2000610000
N	2.8570990000	-0.5622590000	0.2964130000
C	3.0828710000	-0.6105850000	1.6554990000
C	-2.3693340000	0.0698930000	-0.2922270000
C	-2.9021290000	1.2727860000	0.1970070000
C	-4.1862220000	1.3326010000	0.7302200000
C	-4.9813820000	0.1889850000	0.7893740000
C	-4.4750790000	-1.0097350000	0.2956070000

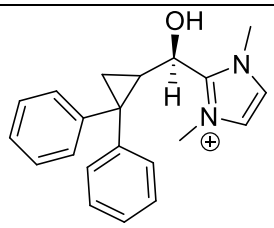
C	-3.1883910000	-1.0662260000	-0.2398260000
H	-2.3008210000	2.1757120000	0.1572060000
H	-4.5678270000	2.2806340000	1.0976670000
H	-5.9826450000	0.2347750000	1.2058670000
H	-5.0821240000	-1.9099580000	0.3203930000
H	-2.8368240000	-2.0152830000	-0.6326130000
C	-0.0373300000	1.0846860000	-0.3745330000
C	0.7297650000	1.9128810000	-1.1973500000
C	1.6131940000	2.8428160000	-0.6482310000
C	1.7592860000	2.9513710000	0.7331000000
C	1.0068630000	2.1225860000	1.5665800000
C	0.1172510000	1.2054620000	1.0145570000
H	0.6518280000	1.8183240000	-2.2739130000
H	2.1961090000	3.4788920000	-1.3081640000
H	2.4470900000	3.6773400000	1.1569580000
H	1.1074250000	2.1943690000	2.6460310000
H	-0.4829260000	0.5778220000	1.6711970000
C	3.7591760000	0.1456210000	-0.6257230000
C	0.1038420000	-2.5986230000	1.3180540000
H	1.9048090000	-1.6566030000	3.2209600000
H	4.7080710000	-0.3949050000	-0.6588630000
H	3.9078400000	1.1543780000	-0.2374990000
H	3.2721670000	0.1443310000	-1.6040550000
H	3.9142510000	-0.0933020000	2.1072430000
H	-0.7985090000	-1.9843260000	1.2564060000
H	0.1589790000	-3.0817920000	2.2938690000
H	0.0804450000	-3.3641780000	0.5404830000

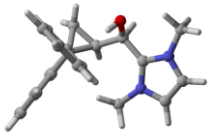
thermodynamic data

Zero-point correction= 0.387599 (Hartree/Particle)
Thermal correction to Energy= 0.408075
Thermal correction to Enthalpy= 0.409019
Thermal correction to Gibbs Free Energy= 0.338693
Sum of electronic and zero-point Energies= -997.373574
Sum of electronic and thermal Energies= -997.353099
Sum of electronic and thermal Enthalpies= -997.352155
Sum of electronic and thermal Free Energies= -997.422481

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	256.071	82.277	148.014

B3LYP/6-31G*	**Job9pr**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	1.5919310000	-0.2041960000	-1.3155930000
H	2.0733220000	-0.6051080000	-2.2192060000
O	1.8519800000	1.1850900000	-1.3664320000
H	1.3102680000	1.6275420000	-0.6844790000
C	0.1182900000	-0.5785870000	-1.4165480000
C	-0.7730420000	0.2007780000	-2.3371900000
C	-1.0798000000	0.2119530000	-0.8484410000
H	-0.0294330000	-1.6559160000	-1.4362870000

H	-1.4377340000	-0.3401750000	-3.0034370000
H	-0.3611840000	1.1147170000	-2.7546800000
C	2.3729460000	-0.8282920000	-0.1500400000
N	1.9862610000	-1.6532950000	0.8530990000
C	3.0871770000	-1.9660230000	1.6316120000
N	3.7037960000	-0.6292920000	-0.0036420000
C	4.1578540000	-1.3247850000	1.0966820000
C	-2.2497560000	-0.6235780000	-0.3524070000
C	-2.9558980000	-0.2660110000	0.8068750000
C	-4.0258230000	-1.0383050000	1.2658930000
C	-4.4147640000	-2.1867830000	0.5795850000
C	-3.7242420000	-2.5551580000	-0.5765710000
C	-2.6577960000	-1.7842880000	-1.0355800000
H	-2.6842160000	0.6304760000	1.3530270000
H	-4.5576020000	-0.7309380000	2.1619590000
H	-5.2494060000	-2.7841290000	0.9342210000
H	-4.0211690000	-3.4408910000	-1.1311920000
H	-2.1573400000	-2.0946990000	-1.9489450000
C	-0.8627230000	1.5244070000	-0.1239310000
C	-1.4503350000	2.6972960000	-0.6226530000
C	-1.3083910000	3.9120140000	0.0479260000
C	-0.5731400000	3.9804320000	1.2335790000
C	0.0125850000	2.8239150000	1.7486160000
C	-0.1366320000	1.6058070000	1.0777250000
H	-2.0253250000	2.6520280000	-1.5430960000
H	-1.7716880000	4.8068340000	-0.3572540000
H	-0.4604950000	4.9271360000	1.7533220000
H	0.5780550000	2.8643200000	2.6753560000

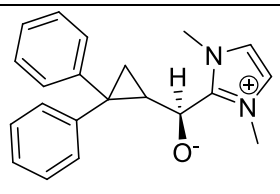
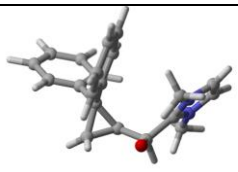
H	0.3015150000	0.7082670000	1.5083770000
C	4.5801430000	0.1428860000	-0.9024480000
C	0.6631710000	-2.2494560000	1.1159650000
H	3.0065200000	-2.6088470000	2.4940100000
H	4.8621470000	-0.4744160000	-1.7599890000
H	5.4754600000	0.4189930000	-0.3448550000
H	4.0515320000	1.0333250000	-1.2358480000
H	5.1919040000	-1.2973470000	1.4031270000
H	-0.1286770000	-1.5125140000	1.0112930000
H	0.6722140000	-2.6237580000	2.1398650000
H	0.4845720000	-3.0816600000	0.4316380000

thermodynamic data

Zero-point correction= 0.400008 (Hartree/Particle)
Thermal correction to Energy= 0.421219
Thermal correction to Enthalpy= 0.422163
Thermal correction to Gibbs Free Energy= 0.349289
Sum of electronic and zero-point Energies= -998.161608
Sum of electronic and thermal Energies= -998.140397
Sum of electronic and thermal Enthalpies= -998.139452
Sum of electronic and thermal Free Energies= -998.212327

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.319	84.095	153.377

B3LYP/6-31G*	**Job9deko2**

xyz-matrix

46

XYZ file generated by gabedit : coordinates in Angstrom

C	1.4993860000	-0.5927540000	1.6369480000
H	1.8448290000	-1.4811920000	2.2605460000
O	1.8311900000	0.5782240000	2.1216620000
C	-0.0337390000	-0.8668200000	1.4778070000
C	-1.0251900000	0.1267720000	0.8603140000
C	-0.9247330000	-0.0500140000	2.3638380000
H	-0.3094930000	-1.9139180000	1.3494600000
H	-1.7601400000	-0.5248280000	2.8719070000
H	-0.3846580000	0.7048110000	2.9273750000
C	2.2005250000	-0.9307860000	0.2659860000
N	2.8947050000	-0.0748760000	-0.5104650000
C	3.4811020000	-0.7594750000	-1.5617270000
N	2.3646110000	-2.1624940000	-0.2874080000
C	3.1524160000	-2.0685970000	-1.4244720000
C	-0.5840870000	1.4086100000	0.1812130000
C	-0.5356970000	1.4655050000	-1.2217200000
C	-0.1947080000	2.6429070000	-1.8912250000
C	0.1038370000	3.7985980000	-1.1678280000
C	0.0599280000	3.7568130000	0.2276630000
C	-0.2791120000	2.5784980000	0.8922030000
H	-0.7918420000	0.5818450000	-1.7998030000
H	-0.1767050000	2.6572520000	-2.9786980000
H	0.3600480000	4.7208270000	-1.6833900000
H	0.2879760000	4.6487380000	0.8060920000
H	-0.2961510000	2.5658670000	1.9747650000
C	-2.2572470000	-0.4823630000	0.2193390000

C	-3.5171790000	0.0879740000	0.4584450000
C	-4.6680600000	-0.4360860000	-0.1277890000
C	-4.5835460000	-1.5444840000	-0.9746080000
C	-3.3384250000	-2.1190110000	-1.2279790000
C	-2.1889690000	-1.5904200000	-0.6348270000
H	-3.5871130000	0.9522000000	1.1142500000
H	-5.6335600000	0.0198770000	0.0769900000
H	-5.4803160000	-1.9554700000	-1.4309040000
H	-3.2593110000	-2.9802360000	-1.8872310000
H	-1.2217160000	-2.0434280000	-0.8402810000
C	1.8101410000	-3.4085590000	0.2314590000
C	3.0316320000	1.3746870000	-0.2883510000
H	1.8277970000	-3.3826050000	1.3231250000
H	2.4266810000	-4.2379520000	-0.1211810000
H	0.7805660000	-3.5515970000	-0.1076940000
H	4.0761240000	1.6470320000	-0.4635780000
H	2.7171160000	1.5380900000	0.7501030000
H	2.3771870000	1.9097220000	-0.9794250000
H	4.0807960000	-0.2522560000	-2.3010780000
H	3.4075050000	-2.9329390000	-2.0176750000

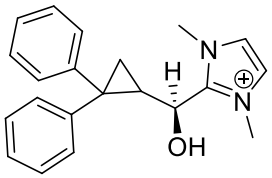
thermodynamic data

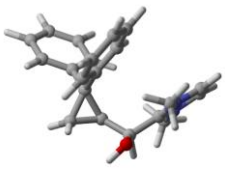
Zero-point correction= 0.384006 (Hartree/Particle)
Thermal correction to Energy= 0.405118
Thermal correction to Enthalpy= 0.406062
Thermal correction to Gibbs Free Energy= 0.333060
Sum of electronic and zero-point Energies= -997.726547
Sum of electronic and thermal Energies= -997.705435
Sum of electronic and thermal Enthalpies= -997.704491
Sum of electronic and thermal Free Energies= -997.777493

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	254.215	83.351	153.646

B3LYP/6-31G*	**Job9prko2**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	1.3885930000	-0.8476030000	1.6403980000
H	1.6396960000	-1.7246150000	2.2612890000
O	1.9787620000	0.3074680000	2.1970070000
H	1.6877650000	0.3757280000	3.1197000000
C	-0.1461830000	-0.8263090000	1.5459120000
C	-1.0239430000	0.2253540000	0.8616100000
C	-0.9510310000	0.1500160000	2.3705520000
H	-0.5572320000	-1.8324770000	1.5114850000
H	-1.8126840000	-0.2284740000	2.9115840000
H	-0.4121700000	0.9386660000	2.8864760000
C	2.0752580000	-1.0826550000	0.3097310000
N	2.8318260000	-0.2354270000	-0.4145220000
C	3.2629550000	-0.8865430000	-1.5564750000
N	2.0356620000	-2.2609470000	-0.3530770000
C	2.7662370000	-2.1494220000	-1.5219480000

C	-0.4299770000	1.4138990000	0.1293840000
C	-0.1564500000	1.3122240000	-1.2454550000
C	0.3266560000	2.4043080000	-1.9658570000
C	0.5428240000	3.6279700000	-1.3265130000
C	0.2652620000	3.7468110000	0.0355110000
C	-0.2207920000	2.6508790000	0.7541660000
H	-0.3585990000	0.3786960000	-1.7638720000
H	0.5146700000	2.3057590000	-3.0317350000
H	0.9064440000	4.4835870000	-1.8881660000
H	0.4088100000	4.6978180000	0.5406900000
H	-0.4599810000	2.7758820000	1.8056390000
C	-2.2984980000	-0.2995750000	0.2275970000
C	-3.5142810000	0.3480840000	0.4865860000
C	-4.6962900000	-0.0933650000	-0.1064740000
C	-4.6813790000	-1.1886620000	-0.9733230000
C	-3.4770230000	-1.8378940000	-1.2438420000
C	-2.2957300000	-1.3933970000	-0.6461050000
H	-3.5321240000	1.2034910000	1.1571000000
H	-5.6302800000	0.4177690000	0.1086280000
H	-5.6026340000	-1.5333300000	-1.4336210000
H	-3.4560050000	-2.6894960000	-1.9182630000
H	-1.3593280000	-1.9007730000	-0.8706410000
C	1.3517250000	-3.4880520000	0.0739490000
C	3.2191220000	1.1562860000	-0.1018820000
H	0.2798280000	-3.4210710000	-0.1234370000
H	1.5226900000	-3.6609750000	1.1381440000
H	1.7727520000	-4.3225900000	-0.4870960000
H	3.9492080000	1.1571930000	0.7071820000

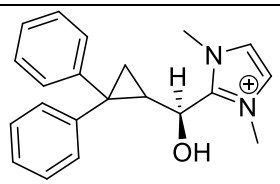
H	2.3433250000	1.7303580000	0.1862220000
H	3.6566110000	1.5755600000	-1.0074670000
H	3.8866840000	-0.3940620000	-2.2854930000
H	2.8677300000	-2.9719060000	-2.2123400000

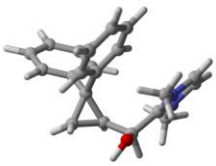
thermodynamic data

Zero-point correction= 0.399210 (Hartree/Particle)
Thermal correction to Energy= 0.420826
Thermal correction to Enthalpy= 0.421771
Thermal correction to Gibbs Free Energy= 0.347869
Sum of electronic and zero-point Energies= -998.160870
Sum of electronic and thermal Energies= -998.139253
Sum of electronic and thermal Enthalpies= -998.138309
Sum of electronic and thermal Free Energies= -998.212210

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.073	84.742	155.538

M062X/6-31++G**	**Job9prko2**	





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	1.2735360000	-0.9619700000	1.7087940000
H	1.4807600000	-1.8727280000	2.2929560000
O	1.9467500000	0.1313000000	2.2774270000
H	1.7295850000	0.1825520000	3.2162680000
C	-0.2479990000	-0.8173970000	1.6320800000

C	-0.9796990000	0.2807770000	0.8831840000
C	-0.9408310000	0.2894520000	2.3848020000
H	-0.7659390000	-1.7733520000	1.6515700000
H	-1.8489940000	0.0389810000	2.9216840000
H	-0.3146560000	1.0379850000	2.8587880000
C	1.8974430000	-1.1854080000	0.3518810000
N	2.7370210000	-0.3962560000	-0.3292960000
C	3.0196970000	-0.9900300000	-1.5402210000
N	1.6642030000	-2.2796250000	-0.3934150000
C	2.3508690000	-2.1703330000	-1.5834710000
C	-0.2206500000	1.3329270000	0.1090230000
C	0.1644870000	1.0717910000	-1.2126240000
C	0.7989040000	2.0454080000	-1.9791750000
C	1.0506810000	3.3074520000	-1.4375430000
C	0.6616190000	3.5829270000	-0.1287530000
C	0.0288470000	2.6020880000	0.6373060000
H	-0.0512340000	0.0995890000	-1.6528890000
H	1.0770600000	1.8272880000	-3.0062870000
H	1.5305790000	4.0741170000	-2.0373060000
H	0.8351580000	4.5664770000	0.2960270000
H	-0.2907050000	2.8397530000	1.6473830000
C	-2.2902340000	-0.1034660000	0.2403030000
C	-3.4402440000	0.6353880000	0.5283510000
C	-4.6519420000	0.3262040000	-0.0847480000
C	-4.7263810000	-0.7252550000	-0.9972980000
C	-3.5834730000	-1.4643350000	-1.2960710000
C	-2.3740200000	-1.1512590000	-0.6786090000
H	-3.3816700000	1.4584780000	1.2365460000

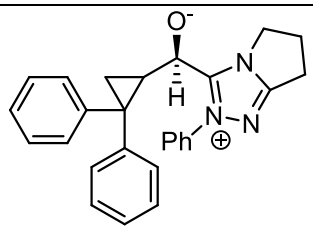
H	-5.5387430000	0.9054680000	0.1510020000
H	-5.6706170000	-0.9674250000	-1.4737050000
H	-3.6349690000	-2.2821840000	-2.0078970000
H	-1.4796320000	-1.7206270000	-0.9241660000
C	0.8653580000	-3.4426880000	0.0008100000
C	3.2876300000	0.9155610000	0.0571680000
H	-0.1983220000	-3.2457650000	-0.1366090000
H	1.0659630000	-3.6896580000	1.0442190000
H	1.1664250000	-4.2838080000	-0.6219390000
H	3.9876410000	0.7871080000	0.8806050000
H	2.4787460000	1.5812290000	0.3513390000
H	3.7953780000	1.3117230000	-0.8207580000
H	3.6733590000	-0.5225470000	-2.2592770000
H	2.3106720000	-2.9388890000	-2.3391310000

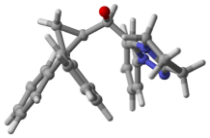
thermodynamic data

Zero-point correction= 0.401940 (Hartree/Particle)
Thermal correction to Energy= 0.422947
Thermal correction to Enthalpy= 0.423892
Thermal correction to Gibbs Free Energy= 0.352392
Sum of electronic and zero-point Energies= -997.804100
Sum of electronic and thermal Energies= -997.783093
Sum of electronic and thermal Enthalpies= -997.782148
Sum of electronic and thermal Free Energies= -997.853648

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	265.404	83.826	150.483

B3LYP/6-31G*	**Job12de**





xyz-matrix

56

XYZ file generated by gabedit : coordinates in Angstrom

C	0.6697410000	-0.4964590000	-2.0019450000
H	0.3575130000	-1.3509400000	-2.6804880000
O	1.6397780000	0.2565420000	-2.4396510000
C	-0.6901020000	0.2083030000	-1.6795080000
C	-0.8938590000	1.4970280000	-2.4062300000
C	-0.7825760000	1.5220920000	-0.8862770000
H	-1.5343980000	-0.4676160000	-1.5712660000
H	-1.8643300000	1.7381460000	-2.8317470000
H	-0.0196730000	1.8044350000	-2.9742500000
C	1.1637690000	-1.2784190000	-0.7000610000
N	0.6282390000	-2.1636110000	0.1785570000
N	1.5216520000	-2.5487510000	1.1735430000
N	2.4235570000	-1.1238100000	-0.2583770000
C	2.6011100000	-1.8871760000	0.8605770000
C	-2.0786270000	1.8173780000	-0.1510600000
C	-2.1447360000	2.8432280000	0.8084090000
C	-3.3382190000	3.1602470000	1.4579460000
C	-4.5101810000	2.4629940000	1.1674620000
C	-4.4690900000	1.4502270000	0.2090510000

C	-3.2751720000	1.1360150000	-0.4396980000
H	-1.2504300000	3.4068430000	1.0495320000
H	-3.3472210000	3.9616040000	2.1929710000
H	-5.4401550000	2.7074690000	1.6740270000
H	-5.3717060000	0.8969960000	-0.0395870000
H	-3.2894500000	0.3485970000	-1.1863620000
C	0.4593220000	2.0655600000	-0.2205510000
C	1.2434100000	3.0729590000	-0.7970070000
C	2.3483610000	3.5987970000	-0.1265730000
C	2.6909070000	3.1328470000	1.1454030000
C	1.9148930000	2.1336380000	1.7379800000
C	0.8136190000	1.6078310000	1.0591670000
H	0.9860700000	3.4445230000	-1.7832070000
H	2.9398690000	4.3802240000	-0.5971650000
H	3.5436600000	3.5528130000	1.6731780000
H	2.1561660000	1.7738100000	2.7359860000
H	0.2001090000	0.8476030000	1.5374420000
C	-0.6865760000	-2.7287530000	0.1950820000
C	-1.2740140000	-3.1689890000	-0.9920570000
C	-1.3458710000	-2.8626330000	1.4186710000
C	-2.5519230000	-3.7264280000	-0.9516590000
C	-2.6173360000	-3.4324040000	1.4462230000
C	-3.2250150000	-3.8601520000	0.2638350000
H	-0.8605400000	-2.5273900000	2.3282060000
H	-3.0141020000	-4.0665710000	-1.8737480000
H	-3.1356770000	-3.5351030000	2.3950310000
H	-4.2183440000	-4.2987480000	0.2904410000
H	-0.7380920000	-3.0766760000	-1.9310010000

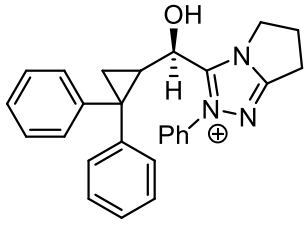
C	3.6222960000	-0.3562660000	-0.6484610000
C	4.5028720000	-0.4984170000	0.6234690000
C	3.9957440000	-1.7609700000	1.3858880000
H	3.3293300000	0.6572590000	-0.9049290000
H	4.0558180000	-0.8190430000	-1.5373360000
H	4.3616910000	0.3858090000	1.2514460000
H	5.5641190000	-0.5684570000	0.3732160000
H	4.5747890000	-2.6568630000	1.1295110000
H	4.0261330000	-1.6503460000	2.4727940000

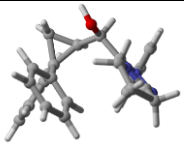
thermodynamic data

Zero-point correction= 0.460969 (Hartree/Particle)
Thermal correction to Energy= 0.486275
Thermal correction to Enthalpy= 0.487219
Thermal correction to Gibbs Free Energy= 0.402638
Sum of electronic and zero-point Energies= -1282.839158
Sum of electronic and thermal Energies= -1282.813852
Sum of electronic and thermal Enthalpies= -1282.812908
Sum of electronic and thermal Free Energies= -1282.897489

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	305.142	101.170	178.016

B3LYP/6-31G*		**Job12pr**





xyz-matrix

57

XYZ file generated by gabedit : coordinates in Angstrom

C	0.5475660000	-0.7536760000	-1.8502280000
H	0.1924990000	-1.6048510000	-2.4527820000
O	1.6481050000	-0.1354670000	-2.4897030000
H	1.3807420000	0.0888000000	-3.3944820000
C	-0.6808290000	0.1402760000	-1.6232020000
C	-0.8426340000	1.4051270000	-2.4205550000
C	-0.7063440000	1.5004640000	-0.9098240000
H	-1.5725120000	-0.4634130000	-1.4884510000
H	-1.8132040000	1.6227690000	-2.8555790000
H	-0.0001210000	1.7397740000	-3.0184370000
C	1.1248240000	-1.3474990000	-0.5850630000
N	0.4950410000	-2.1357430000	0.3027730000
N	1.3238380000	-2.5155970000	1.3396430000
N	2.3797870000	-1.2310350000	-0.1253760000
C	2.4611840000	-1.9479880000	1.0422630000
C	-1.9784440000	1.8547830000	-0.1489050000
C	-1.9651440000	2.8376730000	0.8530040000
C	-3.1337210000	3.2013300000	1.5248190000
C	-4.3484960000	2.5950840000	1.2108630000
C	-4.3825600000	1.6261510000	0.2074690000
C	-3.2152480000	1.2642810000	-0.4637790000
H	-1.0379900000	3.3361090000	1.1106150000
H	-3.0882700000	3.9681260000	2.2931000000
H	-5.2578000000	2.8793860000	1.7321660000
H	-5.3222190000	1.1522350000	-0.0628920000
H	-3.2939890000	0.5211560000	-1.2522460000

C	0.5776990000	2.0457280000	-0.3264810000
C	1.3312730000	3.0308570000	-0.9768130000
C	2.4836570000	3.5602150000	-0.3902250000
C	2.8945770000	3.1244400000	0.8704410000
C	2.1437780000	2.1533620000	1.5397870000
C	1.0018390000	1.6172010000	0.9427950000
H	1.0070960000	3.4068650000	-1.9425950000
H	3.0473670000	4.3287300000	-0.9114350000
H	3.7773440000	3.5527270000	1.3367510000
H	2.4332540000	1.8318610000	2.5372460000
H	0.4035090000	0.8898380000	1.4869970000
C	-0.8655440000	-2.6139630000	0.2613860000
C	-1.2195350000	-3.5695050000	-0.6924910000
C	-1.7804180000	-2.1306220000	1.1962700000
C	-2.5343970000	-4.0352530000	-0.7198210000
C	-3.0893060000	-2.6099480000	1.1608480000
C	-3.4659190000	-3.5558820000	0.2040480000
H	-1.4730670000	-1.3962340000	1.9331490000
H	-2.8243630000	-4.7814820000	-1.4527920000
H	-3.8131600000	-2.2417150000	1.8807060000
H	-4.4864090000	-3.9259010000	0.1827570000
H	-0.4771870000	-3.9585160000	-1.3831910000
C	3.6503610000	-0.5636700000	-0.4934170000
C	4.4813500000	-0.7291020000	0.8083170000
C	3.8395140000	-1.8970670000	1.6161640000
H	3.4569640000	0.4735270000	-0.7592190000
H	4.0763780000	-1.0829230000	-1.3546530000
H	4.4183330000	0.1953950000	1.3872140000

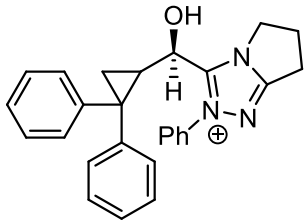
H	5.5333160000	-0.9153340000	0.5845920000
H	4.3489110000	-2.8521110000	1.4414870000
H	3.8345570000	-1.7212260000	2.6943020000

thermodynamic data

Zero-point correction= 0.476163 (Hartree/Particle)
Thermal correction to Energy= 0.501690
Thermal correction to Enthalpy= 0.502634
Thermal correction to Gibbs Free Energy= 0.418481
Sum of electronic and zero-point Energies= -1283.275141
Sum of electronic and thermal Energies= -1283.249615
Sum of electronic and thermal Enthalpies= -1283.248670
Sum of electronic and thermal Free Energies= -1283.332824

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	314.815	102.280	177.115

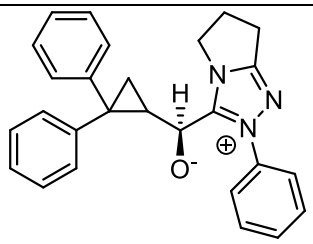
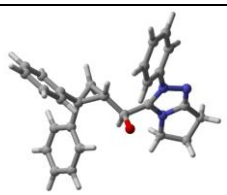
M062X/6-31++G**	**Job12pr**

xyz-matrix

thermodynamic data

B3LYP/6-31G*	**Job12deko2**

xyz-matrix

56

XYZ file generated by gabedit : coordinates in Angstrom

C	0.5372470000	-0.7079930000	0.2967480000
H	0.2898410000	-1.7441790000	-0.0562170000
O	0.6402070000	-0.5682970000	1.6276210000
C	-0.4512640000	0.2034600000	-0.4316830000
C	-1.9103230000	-0.1947420000	-0.5809470000
C	-1.0055360000	-0.1339240000	-1.7974000000
H	-0.3118030000	1.2617670000	-0.2331400000
H	-1.1401930000	0.6702740000	-2.5162270000
H	-0.7159780000	-1.0858900000	-2.2388310000
C	2.0012800000	-0.5463230000	-0.1371150000
N	2.8400660000	0.5219990000	-0.1803940000
N	4.1807210000	0.1477970000	-0.3029490000
N	2.8390830000	-1.6042260000	-0.2513200000
C	4.1259300000	-1.1496910000	-0.3408100000
C	-2.4119960000	-1.5495980000	-0.1192840000
C	-2.1229590000	-2.0467160000	1.1608270000
C	-2.6626310000	-3.2644780000	1.5819350000
C	-3.5018840000	-3.9983670000	0.7422380000
C	-3.7918790000	-3.5121770000	-0.5344650000
C	-3.2493650000	-2.2992300000	-0.9585580000
H	-1.4306640000	-1.4993020000	1.7982600000

H	-2.4222510000	-3.6403180000	2.5737740000
H	-3.9235290000	-4.9432560000	1.0764560000
H	-4.4406420000	-4.0766850000	-1.2000840000
H	-3.4801390000	-1.9236670000	-1.9528730000
C	-2.9261660000	0.9106690000	-0.3856180000
C	-3.7799380000	1.3157860000	-1.4185810000
C	-4.7350440000	2.3128330000	-1.2084950000
C	-4.8509310000	2.9188370000	0.0429470000
C	-4.0042640000	2.5223070000	1.0812400000
C	-3.0509000000	1.5273680000	0.8676760000
H	-3.6930600000	0.8486150000	-2.3965330000
H	-5.3873080000	2.6160900000	-2.0239030000
H	-5.5927710000	3.6960420000	0.2080490000
H	-4.0854860000	2.9910430000	2.0589370000
H	-2.3859570000	1.2216720000	1.6718300000
C	2.5525420000	1.9058210000	0.0532110000
C	1.6870600000	2.2612800000	1.0906130000
C	3.1978120000	2.8658170000	-0.7294430000
C	1.4504320000	3.6177670000	1.3199240000
C	2.7192140000	-3.0602790000	-0.1861230000
C	4.1981860000	-3.4817680000	0.0549260000
C	5.0830320000	-2.2958110000	-0.4408760000
H	2.3150160000	-3.4477720000	-1.1267420000
H	2.0504310000	-3.3384420000	0.6310210000
H	4.4384450000	-4.4196040000	-0.4508240000
H	4.3579910000	-3.6294890000	1.1270440000
H	5.9786610000	-2.1502570000	0.1674190000
H	5.4059000000	-2.4352680000	-1.4800020000

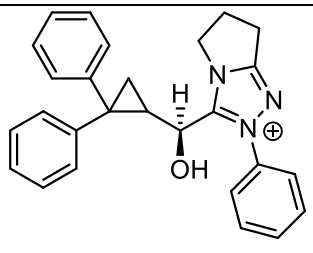
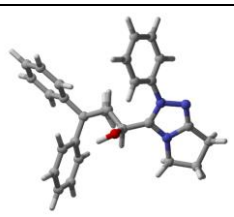
C	2.9576920000	4.2146580000	-0.4757660000
C	2.0811730000	4.5927080000	0.5448620000
H	1.2135680000	1.4666450000	1.6711650000
H	3.8791930000	2.5538680000	-1.5136890000
H	0.7745280000	3.9103180000	2.1185760000
H	3.4527590000	4.9700640000	-1.0794560000
H	1.8935690000	5.6458360000	0.7357700000

thermodynamic data

Zero-point correction= 0.461923 (Hartree/Particle)
Thermal correction to Energy= 0.487299
Thermal correction to Enthalpy= 0.488243
Thermal correction to Gibbs Free Energy= 0.403930
Sum of electronic and zero-point Energies= -1282.843542
Sum of electronic and thermal Energies= -1282.818166
Sum of electronic and thermal Enthalpies= -1282.817222
Sum of electronic and thermal Free Energies= -1282.901535

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	305.784	100.698	177.452

B3LYP/6-31G*	**Job12prko2**

xyz-matrix

57

XYZ file generated by gabedit : coordinates in Angstrom

C	0.5609520000	-0.7463770000	0.3760130000

H	0.3898310000	-1.7990180000	0.1089410000
O	0.4148180000	-0.5772100000	1.7809710000
H	-0.4623240000	-0.9367230000	2.0122060000
C	-0.3785570000	0.1057220000	-0.4547200000
C	-1.8262480000	-0.3546400000	-0.6447970000
C	-0.8501690000	-0.4020580000	-1.7984050000
H	-0.2355610000	1.1762780000	-0.3518290000
H	-0.9742610000	0.3228690000	-2.5966320000
H	-0.4858550000	-1.3705750000	-2.1319800000
C	2.0198840000	-0.4933370000	0.0712120000
N	2.7252960000	0.6531020000	0.0247090000
N	4.0392340000	0.4369180000	-0.3387380000
N	2.9087460000	-1.4546440000	-0.2437550000
C	4.1129730000	-0.8565060000	-0.4966780000
C	-2.2644850000	-1.6442180000	0.0214780000
C	-2.6906390000	-1.6118940000	1.3630110000
C	-3.0886310000	-2.7776050000	2.0178450000
C	-3.0802010000	-3.9998520000	1.3405840000
C	-2.6820190000	-4.0417260000	0.0049950000
C	-2.2762600000	-2.8738710000	-0.6485680000
H	-2.7595030000	-0.6554970000	1.8777000000
H	-3.4201210000	-2.7290340000	3.0513040000
H	-3.3971550000	-4.9071020000	1.8462870000
H	-2.6949010000	-4.9830710000	-0.5374460000
H	-1.9908300000	-2.9220190000	-1.6956370000
C	-2.8843940000	0.7279020000	-0.6707920000
C	-3.9263910000	0.6486640000	-1.6054790000
C	-4.9335750000	1.6117950000	-1.6288390000

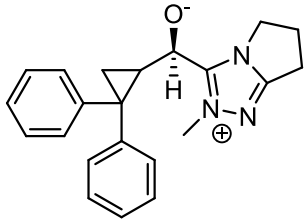
C	-4.9159060000	2.6678160000	-0.7140650000
C	-3.8855890000	2.7537560000	0.2219100000
C	-2.8759120000	1.7885710000	0.2429640000
H	-3.9467450000	-0.1735680000	-2.3164450000
H	-5.7325900000	1.5389000000	-2.3611980000
H	-5.7005940000	3.4185550000	-0.7325740000
H	-3.8651200000	3.5715920000	0.9368790000
H	-2.0738100000	1.8647600000	0.9734060000
C	2.3153510000	2.0072120000	0.3062130000
C	1.6263030000	2.3010470000	1.4842630000
C	2.6814100000	3.0002670000	-0.6051970000
C	1.2763350000	3.6285740000	1.7344490000
C	2.9357500000	-2.9213990000	-0.4047170000
C	4.4658210000	-3.1974470000	-0.4467900000
C	5.1460460000	-1.8642310000	-0.8855130000
H	2.4282910000	-3.1884690000	-1.3364550000
H	2.4310960000	-3.4067870000	0.4323520000
H	4.7003280000	-4.0233900000	-1.1203720000
H	4.8097830000	-3.4731510000	0.5537940000
H	6.1045980000	-1.6918380000	-0.3911460000
H	5.3194190000	-1.8251930000	-1.9674690000
C	2.3288980000	4.3201930000	-0.3337840000
C	1.6252130000	4.6348630000	0.8317760000
H	1.3689930000	1.5117340000	2.1807690000
H	3.2352220000	2.7408040000	-1.5007090000
H	0.7438100000	3.8747200000	2.6478570000
H	2.6054180000	5.1020520000	-1.0340020000
H	1.3553400000	5.6658810000	1.0388890000

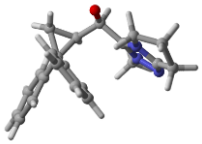
thermodynamic data

Zero-point correction= 0.476093 (Hartree/Particle)
Thermal correction to Energy= 0.501688
Thermal correction to Enthalpy= 0.502633
Thermal correction to Gibbs Free Energy= 0.417843
Sum of electronic and zero-point Energies= -1283.281355
Sum of electronic and thermal Energies= -1283.255760
Sum of electronic and thermal Enthalpies= -1283.254816
Sum of electronic and thermal Free Energies= -1283.339605

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	314.814	102.055	178.454

B3LYP/6-31G*	**Job15de**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7161610000	-1.1175050000	1.7705850000
H	-0.8209890000	-2.1517700000	2.2385000000
O	-1.2364630000	-0.1211000000	2.4380470000
C	0.8223880000	-1.0476820000	1.4686270000
C	1.5710830000	-0.0977800000	2.3419270000
C	1.5063490000	0.1837360000	0.8462430000
H	1.2805300000	-2.0068160000	1.2311030000
H	2.5396960000	-0.3688910000	2.7528520000

H	0.9071840000	0.4749900000	2.9851440000
C	-1.5014550000	-1.3248640000	0.4284230000
N	-1.4707550000	-2.2730850000	-0.5276880000
N	-2.4681340000	-2.1244580000	-1.4776640000
N	-2.5583040000	-0.5671010000	0.0914240000
C	-3.1067860000	-1.0647280000	-1.0558990000
C	0.6455700000	1.3077720000	0.3209950000
C	0.3940040000	2.4686300000	1.0624850000
C	-0.3497820000	3.5202450000	0.5251730000
C	-0.8585370000	3.4352630000	-0.7731330000
C	-0.6183710000	2.2834660000	-1.5267000000
C	0.1246930000	1.2342550000	-0.9818330000
H	0.7858490000	2.5473370000	2.0709770000
H	-0.5275370000	4.4113270000	1.1219930000
H	-1.4281080000	4.2595570000	-1.1952010000
H	-0.9961580000	2.2064950000	-2.5439760000
H	0.3295340000	0.3526350000	-1.5851250000
C	2.8006470000	-0.0499580000	0.0871240000
C	3.2916240000	0.8951910000	-0.8306250000
C	4.4990520000	0.7015840000	-1.5033800000
C	5.2614000000	-0.4436370000	-1.2786210000
C	4.8011440000	-1.3864720000	-0.3590630000
C	3.5952270000	-1.1902400000	0.3129980000
H	2.7263730000	1.8005060000	-1.0199750000
H	4.8433090000	1.4576690000	-2.2049690000
H	6.2005610000	-0.5959990000	-1.8037580000
H	5.3839880000	-2.2820640000	-0.1571940000
H	3.2840980000	-1.9379840000	1.0358970000

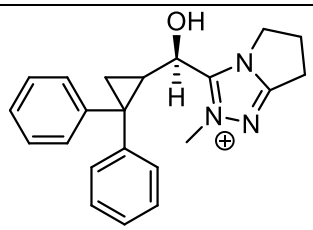
C	-0.5288540000	-3.3765210000	-0.6423040000
C	-3.2470260000	0.6222340000	0.6186430000
C	-4.5776480000	0.5704400000	-0.1813090000
C	-4.2814890000	-0.2406390000	-1.4822070000
H	0.4109940000	-3.0381400000	-1.0871580000
H	-0.9882330000	-4.1346390000	-1.2764320000
H	-0.3357930000	-3.7860760000	0.3521240000
H	-2.6438300000	1.5030150000	0.3919630000
H	-3.3238150000	0.5272960000	1.6993810000
H	-4.9566910000	1.5716210000	-0.3990670000
H	-5.3392080000	0.0461410000	0.4054470000
H	-5.1263650000	-0.8483080000	-1.8156130000
H	-3.9957800000	0.4166660000	-2.3126960000

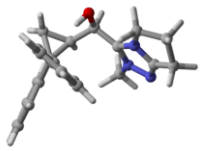
thermodynamic data

Zero-point correction= 0.408895 (Hartree/Particle)
Thermal correction to Energy= 0.431002
Thermal correction to Enthalpy= 0.431946
Thermal correction to Gibbs Free Energy= 0.356372
Sum of electronic and zero-point Energies= -1091.156859
Sum of electronic and thermal Energies= -1091.134752
Sum of electronic and thermal Enthalpies= -1091.133808
Sum of electronic and thermal Free Energies= -1091.209382

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	270.458	87.433	159.060

B3LYP/6-31G*	**Job15pr**





xyz-matrix

50

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7592840000	-0.6507060000	1.8172390000
H	-1.0012150000	-1.3509920000	2.6301310000
O	-1.2951270000	0.5862500000	2.2263100000
H	-0.8789390000	1.2945480000	1.6988710000
C	0.7597010000	-0.6859560000	1.6345540000
C	1.6261730000	0.3018470000	2.3574810000
C	1.5639770000	0.3543600000	0.8377140000
H	1.1396260000	-1.7013110000	1.5899190000
H	2.5454180000	-0.0588540000	2.8084510000
H	1.1261720000	1.0791420000	2.9268720000
C	-1.5430820000	-1.1417600000	0.5992970000
N	-1.3212030000	-2.2094450000	-0.1859710000
N	-2.2977080000	-2.3674760000	-1.1424630000
N	-2.6997510000	-0.6190500000	0.1490400000
C	-3.1193880000	-1.3797730000	-0.9110290000
C	0.7942180000	1.4893580000	0.1961880000
C	0.7986790000	2.7841940000	0.7393270000
C	0.0917040000	3.8236860000	0.1257710000
C	-0.6204170000	3.5898940000	-1.0505440000

C	-0.6181130000	2.3103540000	-1.6155770000
C	0.0801040000	1.2722960000	-0.9974170000
H	1.3723690000	2.9851260000	1.6394880000
H	0.1132910000	4.8178450000	0.5623700000
H	-1.1583110000	4.4001140000	-1.5339640000
H	-1.1425560000	2.1275700000	-2.5498920000
H	0.1109570000	0.2913660000	-1.4658300000
C	2.7793740000	-0.1440080000	0.0728000000
C	3.2600640000	0.5501390000	-1.0476700000
C	4.3915400000	0.1105780000	-1.7373760000
C	5.0717140000	-1.0336240000	-1.3246200000
C	4.6143210000	-1.7290690000	-0.2046260000
C	3.4857800000	-1.2882900000	0.4858400000
H	2.7572960000	1.4492820000	-1.3853250000
H	4.7409470000	0.6723630000	-2.5989840000
H	5.9517400000	-1.3751770000	-1.8612390000
H	5.1402800000	-2.6143970000	0.1414880000
H	3.1812030000	-1.8410070000	1.3708130000
C	-0.2344090000	-3.1948910000	-0.1466730000
C	-3.5883100000	0.5376370000	0.4137540000
C	-4.8542770000	0.1421710000	-0.3918370000
C	-4.3825280000	-0.8435930000	-1.5024560000
H	0.7062910000	-2.7368230000	-0.4588740000
H	-0.5142980000	-3.9836950000	-0.8432330000
H	-0.1413000000	-3.6095670000	0.8591810000
H	-3.0990480000	1.4361070000	0.0277370000
H	-3.7540120000	0.6518110000	1.4830320000
H	-5.3517440000	1.0220090000	-0.8038630000

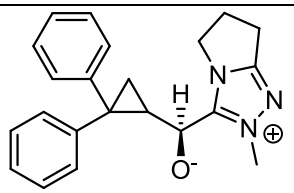
H	-5.5637880000	-0.3625990000	0.2700370000
H	-5.1096400000	-1.6301580000	-1.7164110000
H	-4.1643360000	-0.3299640000	-2.4463400000

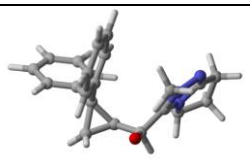
thermodynamic data

Zero-point correction= 0.424477 (Hartree/Particle)
Thermal correction to Energy= 0.446513
Thermal correction to Enthalpy= 0.447457
Thermal correction to Gibbs Free Energy= 0.371800
Sum of electronic and zero-point Energies= -1091.591785
Sum of electronic and thermal Energies= -1091.569748
Sum of electronic and thermal Enthalpies= -1091.568804
Sum of electronic and thermal Free Energies= -1091.644461

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	280.191	88.111	159.233

B3LYP/6-31G*		**Job15deko2**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.0383980000	-0.4614030000	1.8879440000
H	-1.6567150000	0.1446290000	2.6305540000
O	-0.8329300000	-1.7097700000	2.2106160000
C	0.2315930000	0.4320000000	1.6878240000
C	1.4452260000	-0.0036150000	0.8594560000

C	1.4680500000	-0.0649490000	2.3744030000
H	0.0533040000	1.5086740000	1.7123670000
H	2.1111760000	0.6377720000	2.8976030000
H	1.3277430000	-1.0338500000	2.8443950000
C	-1.9439670000	-0.2729960000	0.6125980000
N	-2.4118240000	-1.2183080000	-0.2127790000
N	-3.3235470000	-0.7362410000	-1.1379360000
N	-2.5888060000	0.8508420000	0.2089440000
C	-3.4034750000	0.5303280000	-0.8434510000
C	1.4320480000	-1.2616990000	0.0130660000
C	1.1862620000	-1.1628680000	-1.3662800000
C	1.2179730000	-2.2878200000	-2.1931220000
C	1.5037290000	-3.5436390000	-1.6555650000
C	1.7509960000	-3.6567560000	-0.2855160000
C	1.7147070000	-2.5311080000	0.5370180000
H	0.9900610000	-0.1879930000	-1.8048140000
H	1.0314470000	-2.1776060000	-3.2588870000
H	1.5391300000	-4.4215510000	-2.2957460000
H	1.9759580000	-4.6278780000	0.1484400000
H	1.8987500000	-2.6423340000	1.5985660000
C	2.2659610000	1.1123270000	0.2429970000
C	3.6666000000	1.0664080000	0.3182520000
C	4.4516160000	2.0660950000	-0.2538080000
C	3.8506040000	3.1366570000	-0.9212050000
C	2.4601180000	3.1942740000	-1.0102730000
C	1.6793630000	2.1903060000	-0.4319080000
H	4.1381870000	0.2339420000	0.8343420000
H	5.5347680000	2.0112120000	-0.1782550000

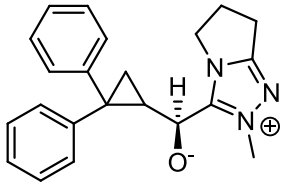
H	4.4613750000	3.9177870000	-1.3662230000
H	1.9809760000	4.0213670000	-1.5289240000
H	0.5954190000	2.2415000000	-0.5068570000
C	-2.6579050000	2.2578000000	0.6049020000
C	-3.9338400000	2.7316520000	-0.1477580000
C	-4.1366930000	1.7389500000	-1.3342150000
C	-2.0629370000	-2.6394390000	-0.2030890000
H	-1.5429490000	-2.7952240000	0.7509500000
H	-1.4066820000	-2.8527030000	-1.0492560000
H	-2.9890070000	-3.2120240000	-0.2859050000
H	-1.7540420000	2.7808430000	0.2771060000
H	-2.7349420000	2.3442970000	1.6915160000
H	-3.8433560000	3.7677320000	-0.4813830000
H	-4.7929860000	2.6723700000	0.5273680000
H	-5.1900480000	1.5379840000	-1.5437260000
H	-3.6806620000	2.1121260000	-2.2593860000

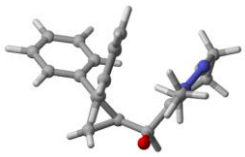
thermodynamic data

Zero-point correction= 0.408555 (Hartree/Particle)
Thermal correction to Energy= 0.430553
Thermal correction to Enthalpy= 0.431498
Thermal correction to Gibbs Free Energy= 0.356166
Sum of electronic and zero-point Energies= -1091.156708
Sum of electronic and thermal Energies= -1091.134710
Sum of electronic and thermal Enthalpies= -1091.133766
Sum of electronic and thermal Free Energies= -1091.209098

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	270.176	87.336	158.549

M062X/6-31++G**	**Job15deko2**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.0846760000	-0.4705130000	2.0122080000
H	-1.6787430000	0.1299220000	2.7622170000
O	-0.9461180000	-1.7470730000	2.2928110000
C	0.2316650000	0.3401960000	1.8335000000
C	1.3359800000	-0.1340070000	0.9033660000
C	1.4618710000	-0.2942930000	2.3975260000
H	0.1413900000	1.4230770000	1.9320220000
H	2.1952660000	0.3282330000	2.9000820000
H	1.2740650000	-1.2776140000	2.8174020000
C	-1.8835210000	-0.2028830000	0.7103360000
N	-2.3109590000	-1.0671780000	-0.2070360000
N	-2.9983540000	-0.4680370000	-1.2311760000
N	-2.3268550000	0.9923410000	0.2654470000
C	-2.9895150000	0.7899580000	-0.9091890000
C	1.1641840000	-1.3279890000	-0.0099560000
C	0.9287300000	-1.1177600000	-1.3754550000
C	0.8559390000	-2.1842260000	-2.2715270000
C	1.0233810000	-3.4903010000	-1.8155540000
C	1.2395350000	-3.7137320000	-0.4556410000
C	1.3032760000	-2.6463610000	0.4373350000

H	0.8307100000	-0.1020640000	-1.7513270000
H	0.6808570000	-1.9896870000	-3.3255940000
H	0.9825970000	-4.3241710000	-2.5097960000
H	1.3588540000	-4.7267910000	-0.0831640000
H	1.4418850000	-2.8393890000	1.4942890000
C	2.1994370000	0.9417430000	0.2917940000
C	3.5904910000	0.7937810000	0.2956920000
C	4.4130900000	1.7510760000	-0.2914350000
C	3.8559420000	2.8771670000	-0.8985630000
C	2.4722280000	3.0343910000	-0.9148570000
C	1.6551210000	2.0712390000	-0.3226030000
H	4.0218040000	-0.0873240000	0.7647840000
H	5.4908680000	1.6199650000	-0.2755450000
H	4.4966450000	3.6254030000	-1.3547630000
H	2.0287470000	3.9055200000	-1.3884470000
H	0.5736850000	2.1893430000	-0.3443580000
C	-2.3292460000	2.3825240000	0.7138410000
C	-3.4325820000	2.9886920000	-0.1900650000
C	-3.5044620000	2.0841620000	-1.4510300000
C	-2.1236960000	-2.5177170000	-0.2244910000
H	-1.6734020000	-2.7743750000	0.7389510000
H	-1.4620210000	-2.7660100000	-1.0556230000
H	-3.1041720000	-2.9743980000	-0.3656320000
H	-1.3468690000	2.8301940000	0.5400400000
H	-2.5589310000	2.4376780000	1.7797400000
H	-3.2255350000	4.0312550000	-0.4338720000
H	-4.3887090000	2.9465060000	0.3380220000
H	-4.5124280000	1.9973740000	-1.8573210000

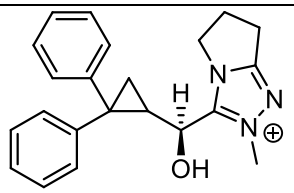
H -2.8434680000 2.4431590000 -2.2466270000

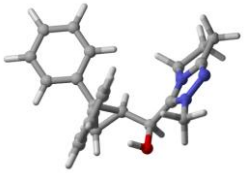
thermodynamic data

Zero-point correction= 0.412387 (Hartree/Particle)
Thermal correction to Energy= 0.433765
Thermal correction to Enthalpy= 0.434709
Thermal correction to Gibbs Free Energy= 0.361896
Sum of electronic and zero-point Energies= -1090.769407
Sum of electronic and thermal Energies= -1090.748029
Sum of electronic and thermal Enthalpies= -1090.747085
Sum of electronic and thermal Free Energies= -1090.819898

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.192	86.207	153.249

B3LYP/6-31G*	**Job15prko2**





xyz-matrix

50

XYZ file generated by gabedit : coordinates in Angstrom

C -0.9728780000 -0.6980970000 1.6986430000

H -1.5498100000 -0.4719620000 2.6082120000

O -0.5621140000 -2.0320630000 1.8399530000

H 0.2170560000 -2.1880520000 1.2721150000

C 0.1514350000 0.3387060000 1.6123670000

C 1.4636450000 0.1553030000 0.8472160000

C	1.4360980000	0.1054990000	2.3616650000
H	-0.2209700000	1.3602160000	1.6371110000
H	1.8637950000	0.9407920000	2.9073040000
H	1.5493230000	-0.8562440000	2.8523820000
C	-1.9740880000	-0.5469620000	0.5545990000
N	-2.4211820000	-1.4569900000	-0.3232240000
N	-3.3798490000	-0.9408280000	-1.1667510000
N	-2.6798740000	0.5715700000	0.2791520000
C	-3.5156150000	0.2944180000	-0.7713740000
C	1.7301540000	-1.1148950000	0.0582370000
C	1.2559450000	-1.2292860000	-1.2618420000
C	1.5276000000	-2.3641740000	-2.0256660000
C	2.2787650000	-3.4132260000	-1.4852530000
C	2.7650220000	-3.3099520000	-0.1830700000
C	2.4995170000	-2.1678510000	0.5800770000
H	0.7046720000	-0.4040410000	-1.7052220000
H	1.1676290000	-2.4236020000	-3.0492990000
H	2.4941010000	-4.2948380000	-2.0815560000
H	3.3657510000	-4.1093190000	0.2408070000
H	2.9103040000	-2.0907890000	1.5825770000
C	2.0492630000	1.3983830000	0.2082470000
C	3.4109830000	1.6849670000	0.3755680000
C	3.9819780000	2.8036310000	-0.2298620000
C	3.2002230000	3.6528900000	-1.0165060000
C	1.8449580000	3.3754100000	-1.1947340000
C	1.2763860000	2.2547900000	-0.5854030000
H	4.0252800000	1.0268850000	0.9847450000
H	5.0380170000	3.0133340000	-0.0864650000

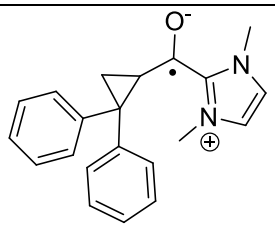
H	3.6451410000	4.5248250000	-1.4867380000
H	1.2308600000	4.0297940000	-1.8073400000
H	0.2195720000	2.0414560000	-0.7368680000
C	-2.8166540000	1.9556990000	0.7799330000
C	-4.1460190000	2.3988910000	0.1073840000
C	-4.3310370000	1.4896500000	-1.1448300000
C	-2.0562330000	-2.8723050000	-0.5013900000
H	-1.0944870000	-2.9401170000	-1.0144820000
H	-2.8412250000	-3.3086200000	-1.1170000000
H	-2.0014130000	-3.3568050000	0.4705320000
H	-1.9557070000	2.5428670000	0.4485410000
H	-2.8594400000	1.9679830000	1.8708710000
H	-4.1246910000	3.4595170000	-0.1487720000
H	-4.9742870000	2.2390760000	0.8032160000
H	-5.3758740000	1.2377490000	-1.3388730000
H	-3.9270200000	1.9511990000	-2.0536730000

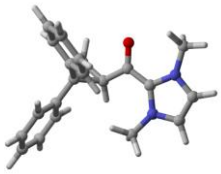
thermodynamic data

Zero-point correction= 0.423956 (Hartree/Particle)
Thermal correction to Energy= 0.446170
Thermal correction to Enthalpy= 0.447114
Thermal correction to Gibbs Free Energy= 0.371201
Sum of electronic and zero-point Energies= -1091.592062
Sum of electronic and thermal Energies= -1091.569848
Sum of electronic and thermal Enthalpies= -1091.568904
Sum of electronic and thermal Free Energies= -1091.644816

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	279.976	88.289	159.771

uB3LYP/6-31G*	**Job9radde**





xyz-matrix

45

XYZ file generated by gabedit : coordinates in Angstrom

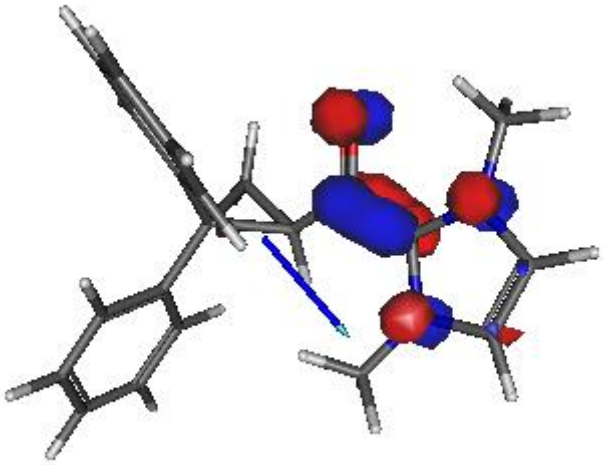
C	-1.5373430000	0.0127670000	0.9721260000
O	-1.8553550000	1.1116640000	1.5119790000
C	-0.1732290000	-0.5718120000	1.2190110000
C	0.6936910000	0.0924030000	2.2441860000
C	1.1306330000	0.1779980000	0.7967610000
H	-0.0884160000	-1.6509310000	1.1467640000
H	1.2764280000	-0.5201080000	2.9267670000
H	0.2652350000	0.9932440000	2.6727000000
C	-2.4719120000	-0.6696030000	0.1372750000
N	-2.3256180000	-1.7916090000	-0.6877580000
C	-3.5528660000	-2.0911580000	-1.2696560000
N	-3.8096130000	-0.2957450000	0.0072270000
C	-4.4539330000	-1.1788320000	-0.8408330000
C	2.2737900000	-0.6985620000	0.3397880000
C	3.0785080000	-0.3380770000	-0.7546560000
C	4.1270720000	-1.1529830000	-1.1850130000
C	4.4053340000	-2.3544140000	-0.5350260000
C	3.6185840000	-2.7290400000	0.5555650000
C	2.5721040000	-1.9147720000	0.9848460000

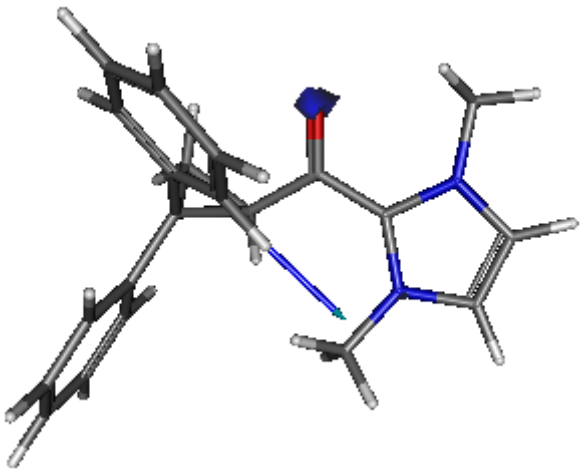
H	2.8880390000	0.5948620000	-1.2731600000
H	4.7300850000	-0.8392390000	-2.0336270000
H	5.2230890000	-2.9875530000	-0.8686690000
H	3.8213500000	-3.6590230000	1.0812740000
H	1.9868010000	-2.2370210000	1.8414520000
C	1.0054350000	1.5173520000	0.1140840000
C	1.5895410000	2.6560720000	0.6838090000
C	1.5268380000	3.8932390000	0.0421010000
C	0.8765040000	4.0125590000	-1.1873000000
C	0.2920290000	2.8858600000	-1.7680270000
C	0.3594960000	1.6506270000	-1.1225810000
H	2.0946080000	2.5678480000	1.6421480000
H	1.9840690000	4.7646510000	0.5040190000
H	0.8230270000	4.9761850000	-1.6873660000
H	-0.2211770000	2.9685000000	-2.7229300000
H	-0.1052260000	0.7804080000	-1.5782940000
C	-4.4863050000	0.7764440000	0.7273470000
C	-1.1024710000	-2.4950810000	-1.0335220000
H	-3.6646760000	-2.9223890000	-1.9480880000
H	-5.5191400000	0.8103140000	0.3689950000
H	-3.9886140000	1.7286480000	0.5523300000
H	-4.4792680000	0.5876190000	1.8042930000
H	-5.5034460000	-1.0749320000	-1.0685240000
H	-0.2768120000	-1.7947330000	-1.1741930000
H	-1.2696570000	-3.0291020000	-1.9724330000
H	-0.8158450000	-3.2250090000	-0.2672770000

thermodynamic data

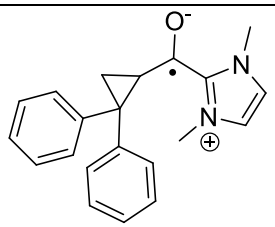
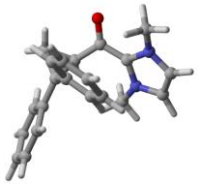
Zero-point correction= 0.372781 (Hartree/Particle)
Thermal correction to Energy= 0.394205
Thermal correction to Enthalpy= 0.395149
Thermal correction to Gibbs Free Energy= 0.319675
Sum of electronic and zero-point Energies= -997.155858
Sum of electronic and thermal Energies= -997.134435
Sum of electronic and thermal Enthalpies= -997.133491
Sum of electronic and thermal Free Energies= -997.208964

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	247.367	83.279	158.848





uM062X/6-31++G**	**Job9radde**

xyz-matrix

45

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2001880000	-0.7830940000	1.4930510000
O	-1.8891790000	-0.1754110000	2.3566540000
C	0.3057470000	-0.7783190000	1.5720050000
C	0.9296130000	0.2973150000	2.3895130000
C	1.0381930000	0.3906260000	0.8835190000
H	0.8247330000	-1.7300410000	1.5304730000
H	1.8409180000	0.0789400000	2.9364750000
H	0.2233350000	0.9542710000	2.8871880000
C	-1.8163840000	-1.2993220000	0.3198330000
N	-1.3030280000	-2.1268930000	-0.6645990000
C	-2.2373900000	-2.2532850000	-1.6806790000
N	-3.0818860000	-0.9457850000	-0.1056880000
C	-3.3191500000	-1.5165300000	-1.3410000000
C	2.3708760000	0.0944000000	0.2516190000
C	2.8161150000	0.8038770000	-0.8716650000
C	4.0500050000	0.5263580000	-1.4582150000
C	4.8738370000	-0.4669530000	-0.9371660000
C	4.4504090000	-1.1752110000	0.1865550000
C	3.2186570000	-0.8968020000	0.7725100000

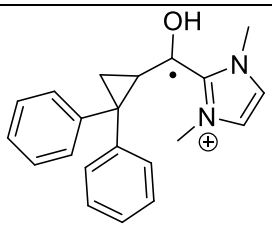
H	2.1948650000	1.5876460000	-1.2916120000
H	4.3657180000	1.0969550000	-2.3265680000
H	5.8348930000	-0.6820780000	-1.3933580000
H	5.0836300000	-1.9464660000	0.6151530000
H	2.9261390000	-1.4584810000	1.6557900000
C	0.1621420000	1.3865360000	0.1722480000
C	-0.1204830000	2.6369640000	0.7203860000
C	-0.9504180000	3.5404170000	0.0532300000
C	-1.5108660000	3.2012080000	-1.1748510000
C	-1.2313960000	1.9538370000	-1.7381190000
C	-0.4015970000	1.0597030000	-1.0689980000
H	0.3092540000	2.9055230000	1.6809350000
H	-1.1581070000	4.5087150000	0.4983660000
H	-2.1592760000	3.9016120000	-1.6925210000
H	-1.6618730000	1.6759480000	-2.6959810000
H	-0.1837230000	0.0903230000	-1.5129720000
C	-3.8505240000	0.1728800000	0.4278520000
C	-0.0684950000	-2.8830170000	-0.6051870000
H	-2.0528000000	-2.8754260000	-2.5419460000
H	-4.7414140000	0.2817920000	-0.1935800000
H	-3.2508760000	1.0881700000	0.3812720000
H	-4.1205620000	-0.0122370000	1.4648890000
H	-4.2466440000	-1.3560340000	-1.8673710000
H	0.8092240000	-2.2302930000	-0.6557070000
H	-0.0510960000	-3.5651120000	-1.4560780000
H	-0.0307220000	-3.4712290000	0.3172810000

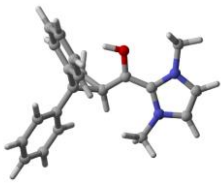
thermodynamic data

Zero-point correction= 0.375653 (Hartree/Particle)
Thermal correction to Energy= 0.396329
Thermal correction to Enthalpy= 0.397273
Thermal correction to Gibbs Free Energy= 0.324761
Sum of electronic and zero-point Energies= -996.795241
Sum of electronic and thermal Energies= -996.774565
Sum of electronic and thermal Enthalpies= -996.773621
Sum of electronic and thermal Free Energies= -996.846132

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	248.700	82.049	152.613

uB3LYP/6-31G*	**Job9radpr**





xyz-matrix

46

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4880960000	0.1005920000	0.5888670000
O	-1.6621130000	1.4178310000	0.8578000000
H	-0.7912840000	1.8672950000	0.8707510000
C	-0.2370820000	-0.5639040000	0.9583720000
C	0.6023850000	-0.0483430000	2.1133540000
C	1.1879300000	0.0839790000	0.7355880000
H	-0.2394770000	-1.6381160000	0.8450740000
H	1.0216520000	-0.7880180000	2.7884570000
H	0.2495340000	0.8496340000	2.6128500000

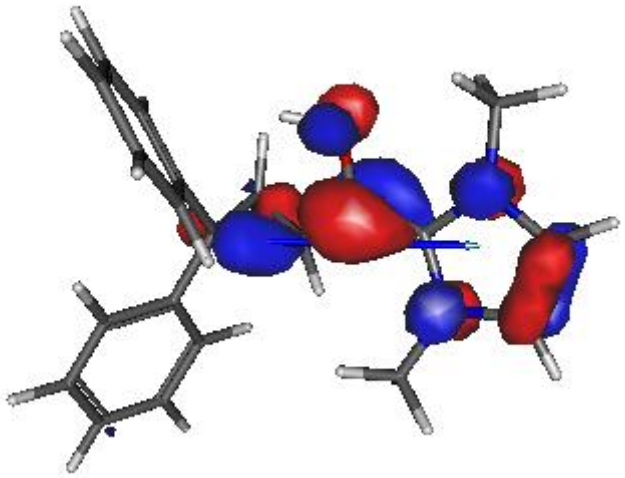
C	-2.6250900000	-0.5390390000	0.0417990000
N	-2.7023380000	-1.7784010000	-0.5626810000
C	-4.0111220000	-2.0170310000	-0.9332610000
N	-3.9051040000	-0.0227360000	0.0207420000
C	-4.7489980000	-0.9357360000	-0.5736060000
C	2.2811260000	-0.8777030000	0.3181620000
C	3.2647060000	-0.4947010000	-0.6061930000
C	4.2796870000	-1.3764770000	-0.9823740000
C	4.3354620000	-2.6613520000	-0.4458990000
C	3.3672350000	-3.0559090000	0.4793290000
C	2.3558040000	-2.1752340000	0.8570830000
H	3.2520050000	0.5027830000	-1.0299110000
H	5.0307380000	-1.0493930000	-1.6956790000
H	5.1261200000	-3.3460180000	-0.7377580000
H	3.4021920000	-4.0498060000	0.9164990000
H	1.6315240000	-2.5140500000	1.5938010000
C	1.2204170000	1.4666180000	0.1280240000
C	1.6531590000	2.5711310000	0.8810600000
C	1.7190690000	3.8443000000	0.3073540000
C	1.3577230000	4.0303280000	-1.0269370000
C	0.9278470000	2.9396490000	-1.7885660000
C	0.8596300000	1.6706780000	-1.2164090000
H	1.9590870000	2.4293410000	1.9140880000
H	2.0614540000	4.6851490000	0.9032520000
H	1.4109160000	5.0188450000	-1.4733280000
H	0.6472710000	3.0787060000	-2.8286210000
H	0.5325490000	0.8247640000	-1.8157820000
C	-4.3804910000	1.2396480000	0.6039900000

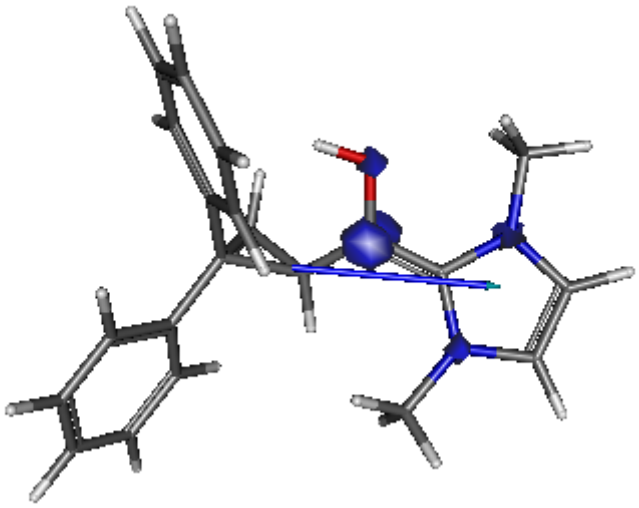
C	-1.6052840000	-2.6762850000	-0.9306500000
H	-4.3001940000	-2.9290280000	-1.4313550000
H	-4.0899720000	1.3043250000	1.6530320000
H	-5.4681850000	1.2433850000	0.5271090000
H	-3.9674280000	2.0908990000	0.0633560000
H	-5.8037310000	-0.7404550000	-0.6874640000
H	-0.7553250000	-2.1032540000	-1.3041620000
H	-1.9618620000	-3.3319640000	-1.7260960000
H	-1.2946910000	-3.2909810000	-0.0814720000

thermodynamic data

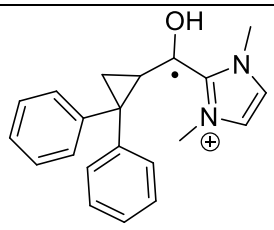
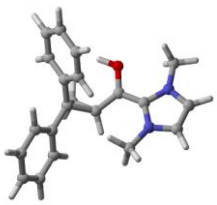
Zero-point correction= 0.386690 (Hartree/Particle)
Thermal correction to Energy= 0.407949
Thermal correction to Enthalpy= 0.408893
Thermal correction to Gibbs Free Energy= 0.334780
Sum of electronic and zero-point Energies= -997.552214
Sum of electronic and thermal Energies= -997.530954
Sum of electronic and thermal Enthalpies= -997.530010
Sum of electronic and thermal Free Energies= -997.604123

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	255.992	84.243	155.984





uM062X/6-31++G**	**Job9radpr**

xyz-matrix

46

XYZ file generated by gabedit : coordinates in Angstrom

C -1.4554920000 0.0300980000 0.8139640000

O	-1.8458600000	1.2789630000	1.1305440000
H	-1.0781830000	1.8626230000	1.2547310000
C	-0.1510750000	-0.4966260000	1.2103650000
C	0.7095320000	0.1757550000	2.2475160000
C	1.1662120000	0.2336790000	0.8212590000
H	-0.0847200000	-1.5768400000	1.1917150000
H	1.2414280000	-0.4754830000	2.9328260000
H	0.3364680000	1.0883520000	2.7037700000
C	-2.4113840000	-0.7295530000	0.0996200000
N	-2.1924440000	-1.8659940000	-0.6311880000
C	-3.3925520000	-2.3003110000	-1.1491860000
N	-3.7471090000	-0.4594040000	0.0138910000
C	-4.3528250000	-1.4276020000	-0.7512090000
C	2.2956500000	-0.6532210000	0.3654870000
C	3.1505640000	-0.2507750000	-0.6660100000
C	4.1911660000	-1.0764510000	-1.0914660000
C	4.3959290000	-2.3171410000	-0.4961710000
C	3.5540500000	-2.7265020000	0.5376510000
C	2.5168830000	-1.9030550000	0.9636280000
H	3.0177640000	0.7180130000	-1.1358110000
H	4.8457520000	-0.7398520000	-1.8889150000
H	5.2075940000	-2.9569370000	-0.8258720000
H	3.7099910000	-3.6859300000	1.0204790000
H	1.8911740000	-2.2456340000	1.7848280000
C	0.9877430000	1.5471950000	0.1098260000
C	1.3387370000	2.7503890000	0.7293040000
C	1.1587540000	3.9674750000	0.0677610000
C	0.6282120000	3.9901150000	-1.2191270000

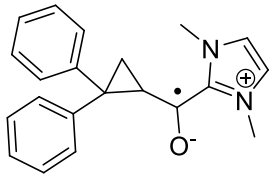
C	0.2828860000	2.7929360000	-1.8493630000
C	0.4614280000	1.5820800000	-1.1877150000
H	1.7723340000	2.7339970000	1.7261070000
H	1.4408940000	4.8933450000	0.5584260000
H	0.4881960000	4.9354820000	-1.7328100000
H	-0.1226620000	2.8059130000	-2.8559510000
H	0.1995830000	0.6498020000	-1.6843530000
C	-4.4782330000	0.6110900000	0.6989080000
C	-0.9091630000	-2.4766580000	-0.9867200000
H	-3.4558190000	-3.1818480000	-1.7673910000
H	-4.2454030000	0.5947080000	1.7635030000
H	-5.5404700000	0.4209900000	0.5533110000
H	-4.2088380000	1.5801710000	0.2819340000
H	-5.4137820000	-1.4163910000	-0.9446580000
H	-0.1448720000	-1.7075870000	-1.1050240000
H	-1.0419280000	-2.9934710000	-1.9367200000
H	-0.5928710000	-3.1948370000	-0.2273270000

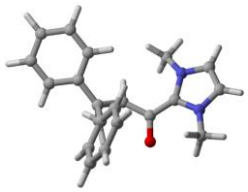
thermodynamic data

Zero-point correction= 0.388862 (Hartree/Particle)
Thermal correction to Energy= 0.409926
Thermal correction to Enthalpy= 0.410870
Thermal correction to Gibbs Free Energy= 0.337741
Sum of electronic and zero-point Energies= -997.185161
Sum of electronic and thermal Energies= -997.164098
Sum of electronic and thermal Enthalpies= -997.163153
Sum of electronic and thermal Free Energies= -997.236282

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	257.232	83.688	153.912

uB3LYP/6-31G*	**Job9raddeko2**





xyz-matrix

45

XYZ file generated by gabedit : coordinates in Angstrom

C	1.4632050000	0.0046170000	1.0577360000
O	1.6238310000	1.1596560000	1.5451760000
C	0.1298970000	-0.6727910000	1.2129830000
C	-1.1544070000	0.0595880000	0.7609890000
C	-0.8326010000	-0.1014330000	2.2251030000
H	0.0792560000	-1.7442760000	1.0647100000
H	-1.4347060000	-0.7912130000	2.8107300000
H	-0.4608850000	0.7715140000	2.7524100000
C	2.5055680000	-0.5832510000	0.2766810000
N	3.6088660000	0.1301980000	-0.1915870000
C	4.4376110000	-0.7224680000	-0.8997350000
N	2.7077540000	-1.9011410000	-0.1533930000
C	3.9025430000	-1.9632000000	-0.8676100000
C	-1.0654670000	1.4221320000	0.1138150000
C	-0.6400140000	1.5440970000	-1.2172190000
C	-0.6043290000	2.7873110000	-1.8479410000
C	-1.0016540000	3.9352930000	-1.1588100000
C	-1.4319930000	3.8260070000	0.1639500000
C	-1.4630860000	2.5801090000	0.7916610000
H	-0.3356890000	0.6551050000	-1.7634680000

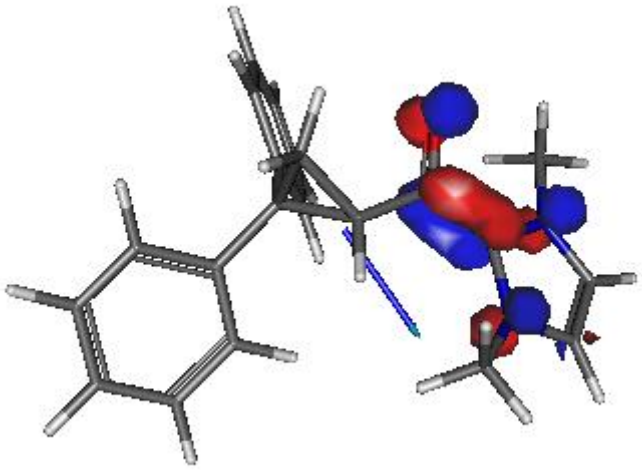
H	-0.2693440000	2.8593560000	-2.8800040000
H	-0.9762510000	4.9051400000	-1.6490440000
H	-1.7433520000	4.7123760000	0.7111040000
H	-1.7940970000	2.5049700000	1.8235650000
C	-2.2521210000	-0.8121540000	0.1894860000
C	-3.5634320000	-0.7007890000	0.6735870000
C	-4.5942980000	-1.4729330000	0.1385250000
C	-4.3327410000	-2.3733760000	-0.8966430000
C	-3.0331840000	-2.4931180000	-1.3902800000
C	-2.0043320000	-1.7189300000	-0.8500560000
H	-3.7721170000	0.0000630000	1.4780270000
H	-5.6032820000	-1.3720590000	0.5305750000
H	-5.1349100000	-2.9767320000	-1.3134210000
H	-2.8182280000	-3.1904370000	-2.1963520000
H	-0.9939980000	-1.8171460000	-1.2403920000
C	2.0279020000	-3.0863380000	0.3350910000
C	3.7546480000	1.5817870000	-0.1848220000
H	1.9293700000	-3.0519740000	1.4258690000
H	2.6256390000	-3.9605450000	0.0670020000
H	1.0321750000	-3.2016230000	-0.1068940000
H	4.7041110000	1.8206170000	-0.6719490000
H	3.7365130000	1.9606710000	0.8349250000
H	2.9332470000	2.0533070000	-0.7338900000
H	5.3401250000	-0.3652070000	-1.3711110000
H	4.2631480000	-2.8935180000	-1.2778880000

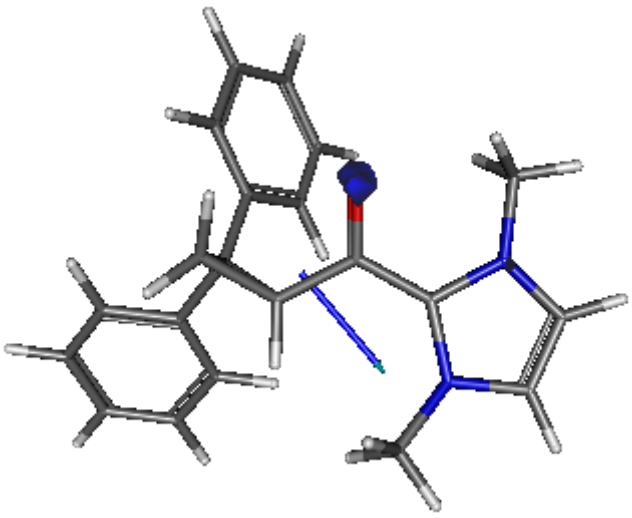
thermodynamic data

Zero-point correction= 0.372497 (Hartree/Particle)

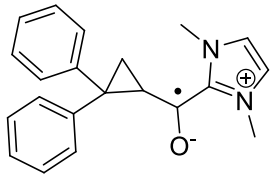
Thermal correction to Energy= 0.394055
Thermal correction to Enthalpy= 0.395000
Thermal correction to Gibbs Free Energy= 0.318366
Sum of electronic and zero-point Energies= -997.154291
Sum of electronic and thermal Energies= -997.132732
Sum of electronic and thermal Enthalpies= -997.131788
Sum of electronic and thermal Free Energies= -997.208422

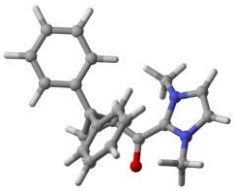
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	247.273	83.285	161.289





uM062X/6-31++G**	**Job9raddeko2**





xyz-matrix

45

XYZ file generated by gabedit : coordinates in Angstrom

C	1.2887850000	-0.3664620000	1.4481810000
O	1.7934640000	0.5883940000	2.0974380000
C	-0.1848900000	-0.6605710000	1.5488690000
C	-1.1141430000	0.3198850000	0.8309470000
C	-1.0108710000	0.3176240000	2.3302250000
H	-0.5240980000	-1.6911740000	1.5451720000
H	-1.8595930000	-0.0648080000	2.8877760000
H	-0.4390750000	1.1099970000	2.8023170000
C	2.0496460000	-1.0110760000	0.4342610000
N	3.1895700000	-0.4765820000	-0.1304700000
C	3.6434250000	-1.3245370000	-1.1202560000
N	1.8219080000	-2.2135910000	-0.2200580000
C	2.8219640000	-2.3968990000	-1.1696770000
C	-0.4732650000	1.4317300000	0.0413330000
C	0.0923230000	1.1551860000	-1.2096750000
C	0.6870180000	2.1636390000	-1.9631340000
C	0.7302340000	3.4693020000	-1.4717670000
C	0.1734410000	3.7534240000	-0.2271190000
C	-0.4239140000	2.7397730000	0.5224500000
H	0.0701960000	0.1373310000	-1.5926270000

H	1.1213440000	1.9305240000	-2.9311670000
H	1.1962180000	4.2576980000	-2.0550400000
H	0.2057960000	4.7653250000	0.1651730000
H	-0.8478750000	2.9638360000	1.4969940000
C	-2.3660360000	-0.2392800000	0.2100490000
C	-3.6120810000	0.3080350000	0.5285280000
C	-4.7764240000	-0.1785180000	-0.0616180000
C	-4.7102150000	-1.2233450000	-0.9827610000
C	-3.4732230000	-1.7747120000	-1.3110690000
C	-2.3117310000	-1.2837230000	-0.7172660000
H	-3.6611960000	1.1232830000	1.2464080000
H	-5.7366060000	0.2571030000	0.1981320000
H	-5.6172880000	-1.6056650000	-1.4404550000
H	-3.4121660000	-2.5876560000	-2.0285680000
H	-1.3452040000	-1.7098160000	-0.9779550000
C	1.0184140000	-3.3032720000	0.3014610000
C	3.6611270000	0.8875490000	0.0718820000
H	1.1500350000	-3.3706850000	1.3866920000
H	1.3621430000	-4.2329370000	-0.1546610000
H	-0.0438160000	-3.1737870000	0.0786700000
H	4.4480490000	1.0731280000	-0.6615300000
H	4.0392800000	1.0151890000	1.0850270000
H	2.8371960000	1.5903970000	-0.0800240000
H	4.5129670000	-1.0855840000	-1.7120650000
H	2.8581220000	-3.2801400000	-1.7871340000

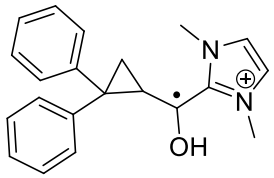
thermodynamic data

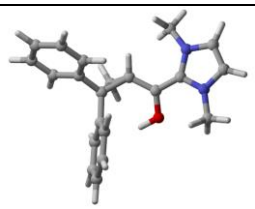
Zero-point correction= 0.374832 (Hartree/Particle)

Thermal correction to Energy= 0.395959
Thermal correction to Enthalpy= 0.396903
Thermal correction to Gibbs Free Energy= 0.321898
Sum of electronic and zero-point Energies= -996.792287
Sum of electronic and thermal Energies= -996.771160
Sum of electronic and thermal Enthalpies= -996.770216
Sum of electronic and thermal Free Energies= -996.845221

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	248.468	82.454	157.861

uB3LYP/6-31G*	**Job9radprko2**





xyz-matrix

46

XYZ file generated by gabedit : coordinates in Angstrom

C	1.4899960000	0.2070100000	0.4996760000
O	1.4238880000	1.5463020000	0.6660720000
H	0.4881860000	1.8442640000	0.6219830000
C	0.3185130000	-0.6410240000	0.7521770000
C	-1.1505490000	-0.1397420000	0.6406370000
C	-0.5608360000	-0.4375370000	1.9870540000
H	0.4315470000	-1.6661810000	0.4250370000
H	-0.8901150000	-1.3302490000	2.5106210000
H	-0.2910010000	0.3933460000	2.6331010000
C	2.7601170000	-0.2651920000	0.0952510000
N	3.7423540000	0.4871010000	-0.5155950000

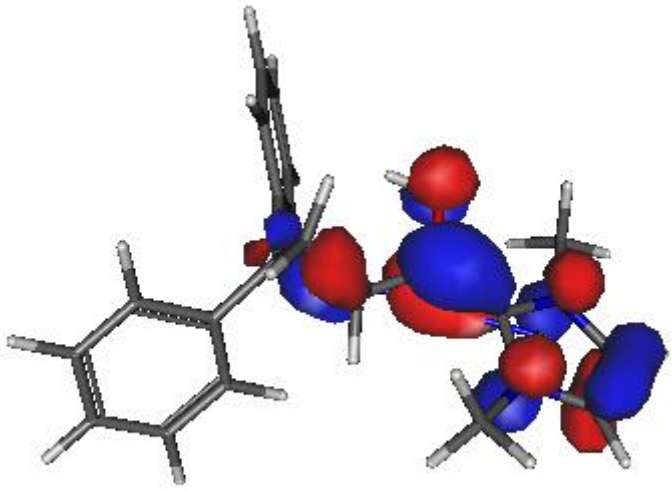
C	4.8361760000	-0.3148320000	-0.7588160000
N	3.2809640000	-1.5353390000	0.2366300000
C	4.5535010000	-1.5612750000	-0.2986830000
C	-1.4495320000	1.2953070000	0.2535410000
C	-1.3986370000	1.6853940000	-1.0985450000
C	-1.7270240000	2.9848370000	-1.4781800000
C	-2.1175040000	3.9211980000	-0.5160280000
C	-2.1782750000	3.5486180000	0.8261510000
C	-1.8495120000	2.2452050000	1.2093530000
H	-1.1175060000	0.9573480000	-1.8545660000
H	-1.6862880000	3.2659960000	-2.5265370000
H	-2.3773380000	4.9326730000	-0.8136410000
H	-2.4913320000	4.2659450000	1.5790350000
H	-1.9213760000	1.9617740000	2.2555390000
C	-2.1264390000	-1.1484630000	0.0699400000
C	-3.3508240000	-1.3594510000	0.7187430000
C	-4.2848860000	-2.2526900000	0.1956960000
C	-4.0083050000	-2.9462830000	-0.9847580000
C	-2.7932580000	-2.7412070000	-1.6387570000
C	-1.8584410000	-1.8464640000	-1.1139670000
H	-3.5734140000	-0.8196020000	1.6357410000
H	-5.2285630000	-2.4077550000	0.7106830000
H	-4.7357390000	-3.6427500000	-1.3911520000
H	-2.5709550000	-3.2765600000	-2.5575240000
H	-0.9140800000	-1.6935240000	-1.6319580000
C	2.7083430000	-2.6607670000	0.9786270000
C	3.6533850000	1.8838480000	-0.9591220000
H	2.0063290000	-3.2280940000	0.3613090000

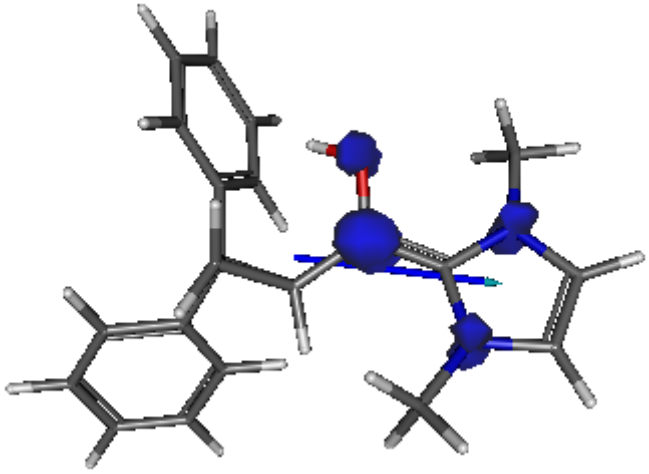
H	2.2044240000	-2.2969960000	1.8751460000
H	3.5263400000	-3.3179040000	1.2770740000
H	3.6124900000	2.5568510000	-0.1029570000
H	2.7626600000	2.0273120000	-1.5726020000
H	4.5414100000	2.0941820000	-1.5560930000
H	5.7220310000	0.0669620000	-1.2417320000
H	5.1519060000	-2.4587230000	-0.2922760000

thermodynamic data

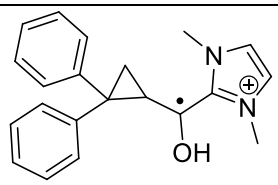
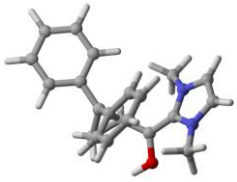
Zero-point correction= 0.386508 (Hartree/Particle)
Thermal correction to Energy= 0.407855
Thermal correction to Enthalpy= 0.408799
Thermal correction to Gibbs Free Energy= 0.334148
Sum of electronic and zero-point Energies= -997.554840
Sum of electronic and thermal Energies= -997.533494
Sum of electronic and thermal Enthalpies= -997.532550
Sum of electronic and thermal Free Energies= -997.607201

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	255.933	84.076	157.117





uM062X/6-31++G**	**Job9radprko2**

xyz-matrix

46

XYZ file generated by gabedit : coordinates in Angstrom

C	1.1784080000	-0.6601010000	1.5616320000
O	1.8985620000	0.0661580000	2.4380220000
H	1.3318000000	0.3738890000	3.1596070000

C	-0.2997580000	-0.6959610000	1.6180680000
C	-1.0901990000	0.3424830000	0.8033700000
C	-1.0222070000	0.4435300000	2.2974660000
H	-0.7743010000	-1.6701740000	1.7115990000
H	-1.9071850000	0.1841990000	2.8672920000
H	-0.4424000000	1.2611580000	2.7173090000
C	1.9329260000	-1.1022950000	0.4357740000
N	3.0084750000	-0.4806970000	-0.1043800000
C	3.4172880000	-1.1830110000	-1.2134630000
N	1.6792700000	-2.2009340000	-0.3176910000
C	2.5924220000	-2.2552250000	-1.3485360000
C	-0.2818050000	1.3195960000	-0.0178000000
C	0.2713460000	0.9132290000	-1.2402080000
C	1.0048090000	1.7998510000	-2.0231200000
C	1.1967960000	3.1156220000	-1.5964310000
C	0.6446260000	3.5333420000	-0.3884650000
C	-0.0906850000	2.6400220000	0.3942820000
H	0.1156530000	-0.1045610000	-1.5919080000
H	1.4141230000	1.4682270000	-2.9728200000
H	1.7603650000	3.8116560000	-2.2093030000
H	0.7726830000	4.5584430000	-0.0559780000
H	-0.5360860000	2.9871170000	1.3225160000
C	-2.4041780000	-0.0818080000	0.1993510000
C	-3.5814520000	0.5557290000	0.5983510000
C	-4.8045140000	0.2080700000	0.0290070000
C	-4.8634570000	-0.7833820000	-0.9480710000
C	-3.6937480000	-1.4206200000	-1.3582190000
C	-2.4729470000	-1.0678970000	-0.7881120000

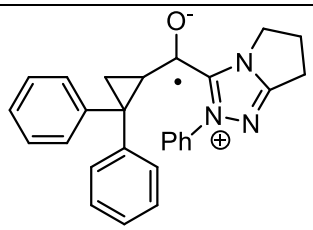
H	-3.5383380000	1.3337280000	1.3565730000
H	-5.7107260000	0.7119800000	0.3490890000
H	-5.8158090000	-1.0576240000	-1.3897080000
H	-3.7332980000	-2.1903860000	-2.1224130000
H	-1.5637230000	-1.5579590000	-1.1269740000
C	0.7322030000	-3.2616780000	0.0209250000
C	3.5215140000	0.8371220000	0.2827690000
H	-0.2930600000	-2.9537980000	-0.1885430000
H	0.8369670000	-3.5097810000	1.0792750000
H	0.9782670000	-4.1377340000	-0.5773620000
H	4.0364620000	0.7738310000	1.2402470000
H	2.6866700000	1.5391460000	0.3484120000
H	4.2075700000	1.1627340000	-0.4978200000
H	4.2565620000	-0.8638230000	-1.8111040000
H	2.5907720000	-3.0578300000	-2.0690970000

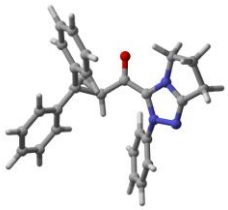
thermodynamic data

Zero-point correction= 0.388844 (Hartree/Particle)
Thermal correction to Energy= 0.409870
Thermal correction to Enthalpy= 0.410814
Thermal correction to Gibbs Free Energy= 0.337816
Sum of electronic and zero-point Energies= -997.180999
Sum of electronic and thermal Energies= -997.159973
Sum of electronic and thermal Enthalpies= -997.159028
Sum of electronic and thermal Free Energies= -997.232027

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	257.197	83.519	153.639

uB3LYP/6-31G*	**Job12radde**





xyz-matrix

55

XYZ file generated by gabedit : coordinates in Angstrom

C	0.5978990000	-0.6955840000	1.1873500000
O	0.4543260000	-1.7851640000	1.8008570000
C	-0.5004970000	0.3212140000	1.1607500000
C	-1.6036170000	0.1798090000	2.1702770000
C	-1.9347700000	-0.1083630000	0.7225140000
H	-0.2328970000	1.3176810000	0.8336010000
H	-2.0272250000	1.0725950000	2.6219270000
H	-1.4993540000	-0.6780890000	2.8280740000
C	1.8060710000	-0.4943980000	0.4478860000
N	2.3620070000	0.5796940000	-0.2614170000
N	3.4555990000	0.1676620000	-1.0515480000
N	2.6489940000	-1.5447750000	0.1185880000
C	3.5676800000	-1.0976230000	-0.7762670000
C	-2.7415640000	0.9362680000	-0.0209990000
C	-3.6893290000	0.5684240000	-0.9899170000
C	-4.4496420000	1.5272070000	-1.6619750000
C	-4.2858860000	2.8832640000	-1.3855540000
C	-3.3513570000	3.2676620000	-0.4227180000
C	-2.5944140000	2.3098510000	0.2490940000

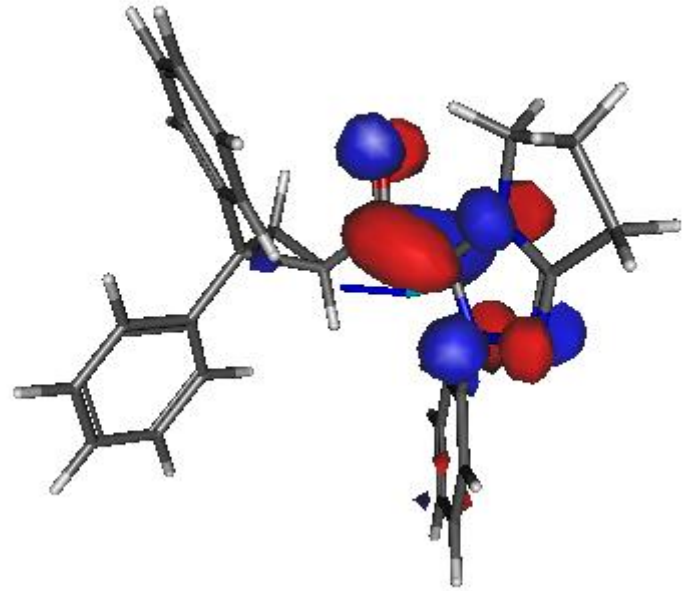
H	-3.8400080000	-0.4798000000	-1.2210060000
H	-5.1749480000	1.2049980000	-2.4050820000
H	-4.8768250000	3.6298050000	-1.9094100000
H	-3.2078070000	4.3198660000	-0.1899470000
H	-1.8785530000	2.6497120000	0.9917780000
C	-2.1591300000	-1.5381010000	0.3005970000
C	-2.9886470000	-2.3889250000	1.0394170000
C	-3.2331280000	-3.6967200000	0.6169620000
C	-2.6525760000	-4.1739880000	-0.5587040000
C	-1.8279470000	-3.3326540000	-1.3094080000
C	-1.5867580000	-2.0268950000	-0.8829390000
H	-3.4434280000	-2.0226600000	1.9558950000
H	-3.8777640000	-4.3425470000	1.2078130000
H	-2.8416900000	-5.1922740000	-0.8886990000
H	-1.3742330000	-3.6932270000	-2.2295630000
H	-0.9477610000	-1.3730130000	-1.4714180000
C	2.2176430000	1.9690630000	-0.0410570000
C	1.9400300000	2.4744370000	1.2370120000
C	2.4030140000	2.8486120000	-1.1175360000
C	1.8186610000	3.8508450000	1.4238000000
C	2.2916490000	4.2208830000	-0.9129880000
C	1.9917050000	4.7304890000	0.3536000000
H	2.6391090000	2.4449500000	-2.0955130000
H	1.6057710000	4.2348060000	2.4178720000
H	2.4337910000	4.8966250000	-1.7519490000
H	1.8997750000	5.8020820000	0.5052310000
H	1.8373230000	1.7928030000	2.0751260000
C	2.7205240000	-2.9769720000	0.3963800000

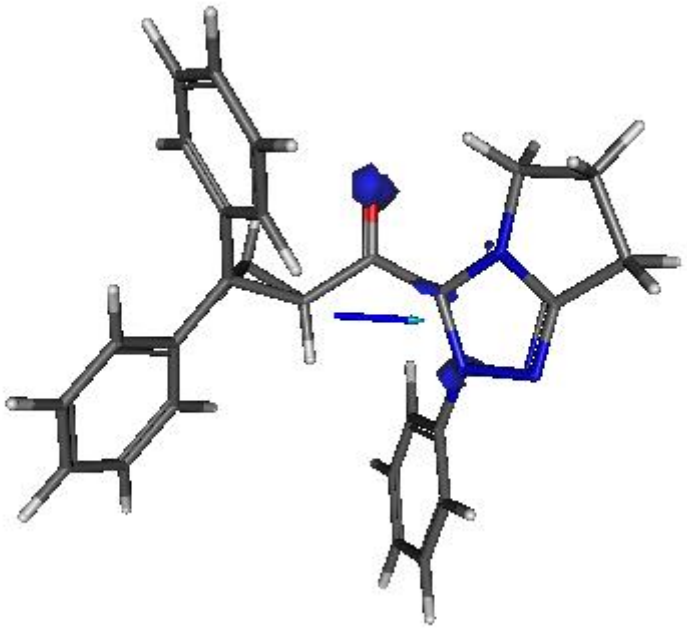
C	3.6848240000	-3.4646190000	-0.7226990000
C	4.4773720000	-2.2103960000	-1.1997760000
H	1.7281180000	-3.4247510000	0.3505730000
H	3.1145970000	-3.1409790000	1.4051700000
H	3.0979650000	-3.8623580000	-1.5568350000
H	4.3428730000	-4.2633640000	-0.3718020000
H	5.4451420000	-2.1191720000	-0.6912690000
H	4.6703490000	-2.2071810000	-2.2753850000

thermodynamic data

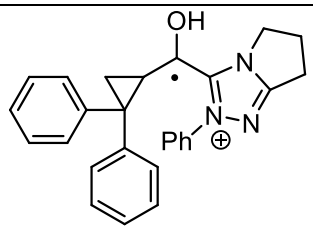
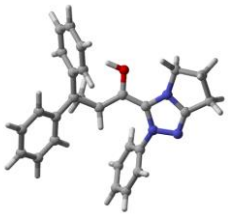
Zero-point correction= 0.450108 (Hartree/Particle)
Thermal correction to Energy= 0.475387
Thermal correction to Enthalpy= 0.476331
Thermal correction to Gibbs Free Energy= 0.391613
Sum of electronic and zero-point Energies= -1282.276526
Sum of electronic and thermal Energies= -1282.251247
Sum of electronic and thermal Enthalpies= -1282.250303
Sum of electronic and thermal Free Energies= -1282.335021

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.310	100.683	178.303





uB3LYP/6-31G*	**Job12radpr**

xyz-matrix

56

XYZ file generated by gabedit : coordinates in Angstrom

C	0.6295830000	-0.7877350000	0.6510020000
O	0.3981040000	-2.0524470000	1.0707420000
H	-0.5673090000	-2.2326260000	1.0562490000
C	-0.3986090000	0.2470380000	0.7212650000
C	-1.3438280000	0.3315930000	1.9099810000
C	-1.9428150000	-0.0421470000	0.5844140000
H	-0.1027850000	1.1861740000	0.2744680000
H	-1.5524480000	1.3167410000	2.3157960000
H	-1.2377620000	-0.4475020000	2.6606280000
C	1.9455370000	-0.6001720000	0.1789920000
N	2.6468480000	0.5473000000	-0.1207050000
N	3.8971220000	0.2664140000	-0.6428320000
N	2.8203310000	-1.6080600000	-0.1427560000
C	3.9583040000	-1.0367480000	-0.6315540000
C	-2.7302790000	1.0194500000	-0.1612640000
C	-3.8267350000	0.6706050000	-0.9636850000
C	-4.5700610000	1.6469620000	-1.6294720000
C	-4.2349730000	2.9939740000	-1.5103470000
C	-3.1491610000	3.3571800000	-0.7117300000
C	-2.4086910000	2.3837770000	-0.0446840000
H	-4.1170760000	-0.3684390000	-1.0660850000
H	-5.4166700000	1.3462010000	-2.2399680000
H	-4.8135720000	3.7530970000	-2.0281730000
H	-2.8778580000	4.4033490000	-0.6020030000
H	-1.5761930000	2.7098380000	0.5733540000
C	-2.3907040000	-1.4714120000	0.3862030000

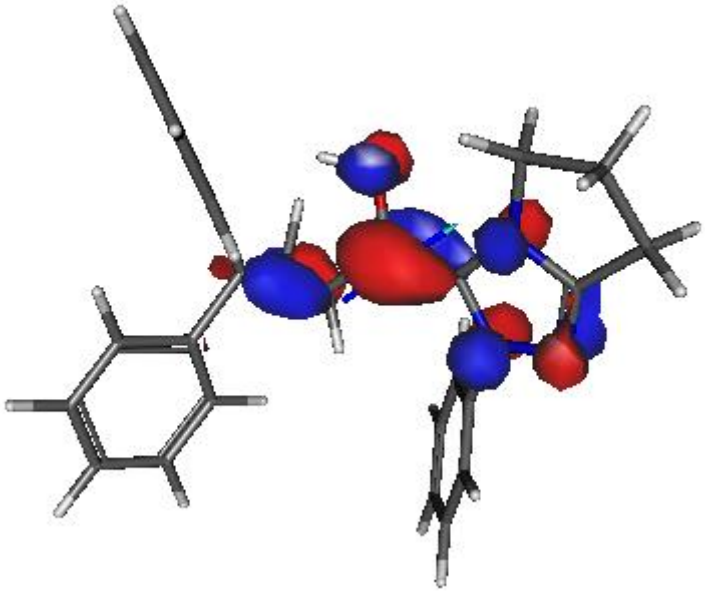
C	-3.1159570000	-2.1420920000	1.3854880000
C	-3.5800460000	-3.4435100000	1.1786770000
C	-3.3301260000	-4.0923810000	-0.0310650000
C	-2.6122580000	-3.4370720000	-1.0356750000
C	-2.1474630000	-2.1386370000	-0.8301090000
H	-3.3322050000	-1.6349990000	2.3216840000
H	-4.1432270000	-3.9440590000	1.9607230000
H	-3.6934830000	-5.1029400000	-0.1925230000
H	-2.4195480000	-3.9357230000	-1.9812470000
H	-1.6001990000	-1.6262880000	-1.6175460000
C	2.3207840000	1.9185800000	0.1447780000
C	2.0473950000	2.3257490000	1.4537860000
C	2.3475060000	2.8311660000	-0.9116830000
C	1.7675090000	3.6697630000	1.6982270000
C	2.0757130000	4.1736080000	-0.6510220000
C	1.7809330000	4.5924260000	0.6487180000
H	2.5847990000	2.4911250000	-1.9141300000
H	1.5597780000	3.9979820000	2.7120670000
H	2.0952990000	4.8914130000	-1.4650660000
H	1.5725670000	5.6395270000	0.8462650000
H	2.0675150000	1.6054480000	2.2657520000
C	2.8638510000	-3.0815870000	-0.1188200000
C	4.1130070000	-3.3722600000	-0.9969410000
C	4.9728970000	-2.0734670000	-0.9917010000
H	1.9418750000	-3.4976310000	-0.5244130000
H	2.9718800000	-3.4200770000	0.9154830000
H	3.7938050000	-3.5970680000	-2.0186180000
H	4.6669770000	-4.2359980000	-0.6247950000

H	5.7598090000	-2.1016400000	-0.2287010000
H	5.4532190000	-1.8717990000	-1.9517610000

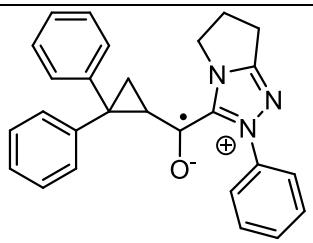
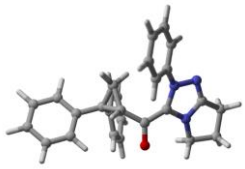
thermodynamic data

Zero-point correction= 0.463164 (Hartree/Particle)
Thermal correction to Energy= 0.488629
Thermal correction to Enthalpy= 0.489573
Thermal correction to Gibbs Free Energy= 0.404144
Sum of electronic and zero-point Energies= -1282.670540
Sum of electronic and thermal Energies= -1282.645075
Sum of electronic and thermal Enthalpies= -1282.644131
Sum of electronic and thermal Free Energies= -1282.729559

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	306.619	101.837	179.799



uB3LYP/6-31G*	**Job12raddeko2**

xyz-matrix

55

XYZ file generated by gabedit : coordinates in Angstrom

C	0.3822100000	-0.2113270000	1.2812700000
O	0.0892320000	-1.0351890000	2.1905000000
C	-0.6833810000	0.7226270000	0.7821040000
C	-1.7754450000	0.1892030000	-0.1536820000
C	-0.8116400000	1.2560290000	-0.6217520000
H	-1.0742610000	1.3690710000	1.5666070000
H	-1.1730840000	2.2735540000	-0.7409690000
H	-0.0618720000	0.9619640000	-1.3501470000
C	1.6952090000	-0.2531110000	0.7244850000
N	2.4389290000	0.5970790000	-0.1013810000
N	3.6128190000	-0.0321990000	-0.5653010000
N	2.5163860000	-1.3608400000	0.8447750000
C	3.5878770000	-1.1902010000	0.0240780000
C	-1.6463020000	-1.1949180000	-0.7554430000
C	-1.7902150000	-2.3399670000	0.0436980000
C	-1.7220310000	-3.6138020000	-0.5202300000
C	-1.5168110000	-3.7686400000	-1.8938760000
C	-1.3778200000	-2.6378880000	-2.6985940000
C	-1.4430430000	-1.3631940000	-2.1314180000

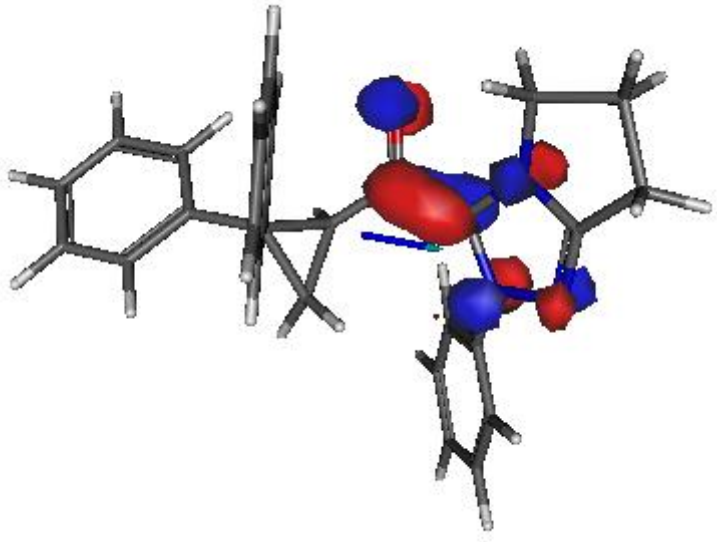
H	-1.9246170000	-2.2248660000	1.1137720000
H	-1.8324970000	-4.4888360000	0.1157160000
H	-1.4678110000	-4.7623070000	-2.3321490000
H	-1.2209000000	-2.7445740000	-3.7691580000
H	-1.3362010000	-0.4872930000	-2.7662780000
C	-3.1983400000	0.5814000000	0.1774970000
C	-4.0550560000	1.0708390000	-0.8176900000
C	-5.3773150000	1.4017490000	-0.5209720000
C	-5.8654600000	1.2432690000	0.7779920000
C	-5.0221250000	0.7521960000	1.7758270000
C	-3.6986360000	0.4240480000	1.4766800000
H	-3.6797420000	1.1938900000	-1.8307860000
H	-6.0267260000	1.7851640000	-1.3040710000
H	-6.8952000000	1.5024310000	1.0100840000
H	-5.3931020000	0.6254120000	2.7897970000
H	-3.0393120000	0.0439960000	2.2532290000
C	2.3629540000	2.0034650000	-0.2274110000
C	1.8092940000	2.7927680000	0.7896070000
C	2.8879990000	2.6096190000	-1.3785030000
C	1.7584260000	4.1770420000	0.6376910000
C	2.3757070000	-2.7201970000	1.3600750000
C	3.8098690000	-3.2725450000	1.1382970000
C	4.4126800000	-2.4406790000	-0.0330480000
H	1.6167650000	-3.2599950000	0.7807380000
H	2.0556300000	-2.7017980000	2.4010340000
H	3.8047150000	-4.3446900000	0.9278400000
H	4.4040260000	-3.1132700000	2.0438340000
H	5.4831610000	-2.2496410000	0.0789860000

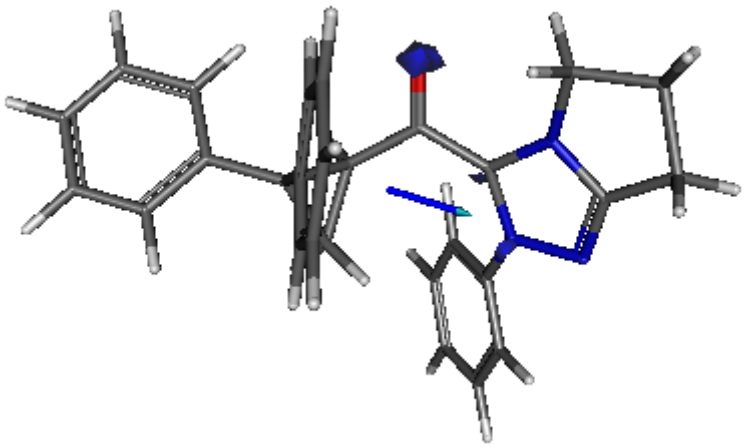
H	4.2656720000	-2.9358040000	-1.0007500000
C	2.8382600000	3.9944770000	-1.5110480000
C	2.2678470000	4.7863230000	-0.5106850000
H	1.4389380000	2.3252600000	1.6950560000
H	3.3352990000	1.9891270000	-2.1464480000
H	1.3295490000	4.7818520000	1.4321190000
H	3.2454780000	4.4571230000	-2.4060730000
H	2.2270220000	5.8659640000	-0.6223310000

thermodynamic data

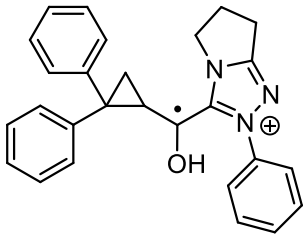
Zero-point correction= 0.449897 (Hartree/Particle)
Thermal correction to Energy= 0.475238
Thermal correction to Enthalpy= 0.476182
Thermal correction to Gibbs Free Energy= 0.391145
Sum of electronic and zero-point Energies= -1282.275811
Sum of electronic and thermal Energies= -1282.250470
Sum of electronic and thermal Enthalpies= -1282.249526
Sum of electronic and thermal Free Energies= -1282.334563

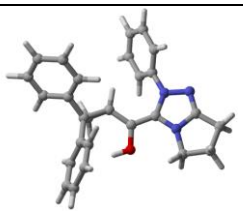
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.216	100.648	178.976





uB3LYP/6-31G*	**Job12radprko2**





xyz-matrix

56

XYZ file generated by gabedit : coordinates in Angstrom

C	0.6306480000	-0.7820700000	-0.5894630000
O	0.3694170000	-2.0579510000	-0.9476240000
H	-0.6012920000	-2.2149380000	-0.9486570000
C	-0.3938630000	0.2615390000	-0.6491100000
C	-1.9182060000	-0.0259880000	-0.5445570000
C	-1.3238800000	0.3842190000	-1.8579770000
H	-0.0939470000	1.2001820000	-0.2018410000
H	-1.5130350000	1.3896080000	-2.2215550000
H	-1.2055520000	-0.3651730000	-2.6360340000
C	1.9663030000	-0.5928060000	-0.1783240000

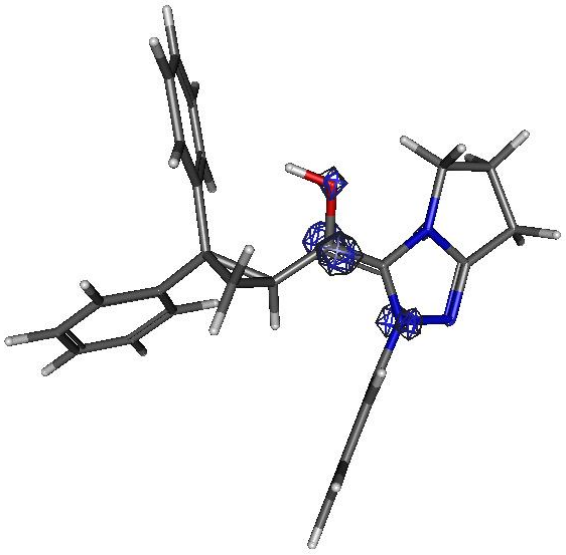
N	2.6859460000	0.5567450000	0.0641740000
N	3.9509660000	0.2798270000	0.5519910000
N	2.8438210000	-1.5990790000	0.1422330000
C	4.0015370000	-1.0236540000	0.5765580000
C	-2.4200570000	-1.4448720000	-0.3616140000
C	-2.4053540000	-2.0355600000	0.9164250000
C	-2.9134250000	-3.3168860000	1.1147260000
C	-3.4499550000	-4.0353790000	0.0415770000
C	-3.4760360000	-3.4628040000	-1.2291140000
C	-2.9675450000	-2.1757880000	-1.4302970000
H	-2.0091980000	-1.4751270000	1.7587640000
H	-2.8982510000	-3.7541890000	2.1088930000
H	-3.8495240000	-5.0328050000	0.1988160000
H	-3.9016940000	-4.0081470000	-2.0662950000
H	-3.0158570000	-1.7309900000	-2.4202350000
C	-2.7178320000	1.0117140000	0.2161840000
C	-3.9297550000	1.4677050000	-0.3207660000
C	-4.7099040000	2.3902810000	0.3746600000
C	-4.2896070000	2.8685840000	1.6180580000
C	-3.0857230000	2.4192730000	2.1607250000
C	-2.3049340000	1.4951450000	1.4634040000
H	-4.2634100000	1.0955880000	-1.2862160000
H	-5.6456670000	2.7363800000	-0.0547900000
H	-4.8971130000	3.5880970000	2.1590920000
H	-2.7518410000	2.7869900000	3.1268920000
H	-1.3666690000	1.1533320000	1.8942950000
C	2.3627350000	1.9213910000	-0.2357170000
C	2.4505730000	2.8710570000	0.7843760000

C	2.0335790000	2.2851710000	-1.5445580000
C	2.1831700000	4.2067270000	0.4875180000
C	2.8765450000	-3.0731620000	0.1563710000
C	4.1525330000	-3.3500790000	0.9996010000
C	5.0200130000	-2.0580700000	0.9324420000
H	2.9479260000	-3.4395720000	-0.8716170000
H	1.9659730000	-3.4714780000	0.6032350000
H	4.6882700000	-4.2269520000	0.6315120000
H	3.8662290000	-3.5467280000	2.0367000000
H	5.5313660000	-1.8343860000	1.8713940000
H	5.7828170000	-2.1119230000	0.1466620000
C	1.7598660000	3.6232070000	-1.8245470000
C	1.8331430000	4.5824830000	-0.8116200000
H	2.7325020000	2.5640200000	1.7859750000
H	2.0070560000	1.5361210000	-2.3298490000
H	2.2493660000	4.9532650000	1.2727710000
H	1.5072700000	3.9175100000	-2.8385660000
H	1.6264020000	5.6242020000	-1.0369200000

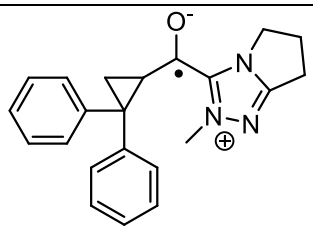
thermodynamic data

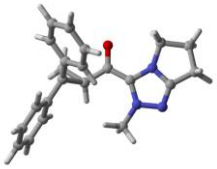
Zero-point correction= 0.462909 (Hartree/Particle)
Thermal correction to Energy= 0.488465
Thermal correction to Enthalpy= 0.489409
Thermal correction to Gibbs Free Energy= 0.403854
Sum of electronic and zero-point Energies= -1282.672476
Sum of electronic and thermal Energies= -1282.646920
Sum of electronic and thermal Enthalpies= -1282.645976
Sum of electronic and thermal Free Energies= -1282.731531

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	306.516	101.836	180.066



uB3LYP/6-31G*	**Job15radde**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9728350000	-0.0735740000	1.1573290000
O	-1.3276780000	0.9823090000	1.7549160000
C	0.4196880000	-0.6139300000	1.3068620000
C	1.3334130000	0.0759980000	2.2721640000
C	1.6547220000	0.1930300000	0.7964090000
H	0.5324980000	-1.6884060000	1.2059830000
H	1.9955720000	-0.5187740000	2.8951910000
H	0.9001400000	0.9493820000	2.7500540000
C	-1.9174380000	-0.7246730000	0.3140150000

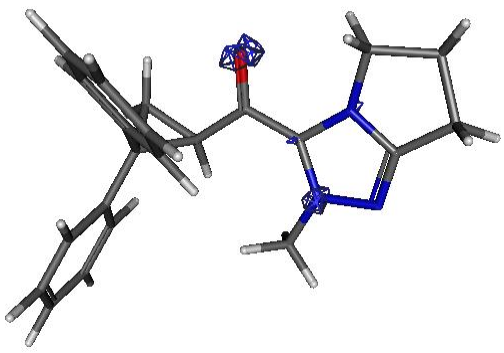
N	-1.8795740000	-1.8343960000	-0.5279340000
N	-3.1123440000	-2.0798120000	-1.1371790000
N	-3.2254680000	-0.2901780000	0.1737860000
C	-3.8675470000	-1.1172810000	-0.6949730000
C	1.4043470000	1.5190530000	0.1241090000
C	1.8828070000	2.7088360000	0.6859620000
C	1.6921640000	3.9332790000	0.0439260000
C	1.0187540000	3.9864780000	-1.1773360000
C	0.5388120000	2.8072240000	-1.7506080000
C	0.7319450000	1.5859290000	-1.1047760000
H	2.4069360000	2.6721240000	1.6372200000
H	2.0690960000	4.8456280000	0.4991290000
H	0.8674260000	4.9393310000	-1.6780490000
H	0.0116480000	2.8381980000	-2.7010320000
H	0.3559650000	0.6713690000	-1.5560840000
C	2.8065700000	-0.6251840000	0.2567950000
C	3.5732600000	-0.1784980000	-0.8323920000
C	4.6366580000	-0.9337330000	-1.3298510000
C	4.9672530000	-2.1594550000	-0.7540030000
C	4.2196030000	-2.6184310000	0.3316640000
C	3.1590060000	-1.8630290000	0.8286910000
H	3.3399360000	0.7737810000	-1.2948250000
H	5.2089520000	-0.5546900000	-2.1729670000
H	5.7954290000	-2.7469780000	-1.1409880000
H	4.4637390000	-3.5687680000	0.8001200000
H	2.6065120000	-2.2481590000	1.6810150000
C	-0.8253240000	-2.8048540000	-0.7261750000
C	-4.0258600000	0.8453960000	0.6225410000

C	-5.4545130000	0.3879010000	0.2158260000
C	-5.2687170000	-0.6442400000	-0.9368280000
H	0.1284370000	-2.3076100000	-0.9205060000
H	-1.1059020000	-3.4012050000	-1.5950760000
H	-0.7134060000	-3.4701370000	0.1402500000
H	-3.7048390000	1.7560690000	0.1042710000
H	-3.8971440000	1.0089820000	1.6915320000
H	-6.0834670000	1.2318540000	-0.0778300000
H	-5.9336650000	-0.1027000000	1.0692840000
H	-6.0012310000	-1.4550820000	-0.9095180000
H	-5.3401190000	-0.1694440000	-1.9233360000

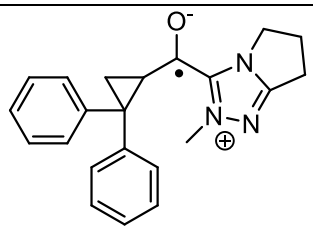
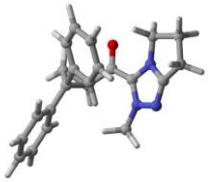
thermodynamic data

Zero-point correction= 0.397652 (Hartree/Particle)
Thermal correction to Energy= 0.419921
Thermal correction to Enthalpy= 0.420865
Thermal correction to Gibbs Free Energy= 0.343034
Sum of electronic and zero-point Energies= -1090.592085
Sum of electronic and thermal Energies= -1090.569816
Sum of electronic and thermal Enthalpies= -1090.568872
Sum of electronic and thermal Free Energies= -1090.646703

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	263.504	87.137	163.809



uM062X/6-31++G**	**Job15radde**

xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.6484450000	-0.7115440000	1.7310050000
O	-1.2686280000	-0.0758250000	2.6245430000
C	0.8564710000	-0.7399890000	1.6777710000
C	1.5570700000	0.3578080000	2.3974110000
C	1.5194790000	0.4060460000	0.8853880000
H	1.3438280000	-1.7076060000	1.6062890000
H	2.5235760000	0.1571790000	2.8478850000
H	0.9033710000	1.0207660000	2.9548820000
C	-1.3633010000	-1.2145820000	0.6165020000
N	-0.9842480000	-1.9771060000	-0.4657250000
N	-1.9453280000	-1.9831840000	-1.4610410000
N	-2.6486060000	-0.8432170000	0.3048370000
C	-2.9111280000	-1.2771150000	-0.9582810000
C	0.5559100000	1.3397810000	0.2005210000
C	0.1120370000	2.5249360000	0.7852690000
C	-0.8351590000	3.3282180000	0.1446930000
C	-1.3538350000	2.9543300000	-1.0915670000
C	-0.9130920000	1.7717180000	-1.6918650000
C	0.0339730000	0.9801830000	-1.0515210000

H	0.4993550000	2.8226110000	1.7545390000
H	-1.1673000000	4.2468090000	0.6189570000
H	-2.0902240000	3.5793080000	-1.5882110000
H	-1.3015100000	1.4667480000	-2.6596970000
H	0.3767230000	0.0641690000	-1.5276050000
C	2.8016070000	0.1043330000	0.1562700000
C	3.2057350000	0.8689380000	-0.9464550000
C	4.3976460000	0.5960730000	-1.6157260000
C	5.2202180000	-0.4465540000	-1.1990080000
C	4.8403290000	-1.2070430000	-0.0944730000
C	3.6501710000	-0.9328850000	0.5738270000
H	2.5858000000	1.6921670000	-1.2853330000
H	4.6818250000	1.2073680000	-2.4669800000
H	6.1470240000	-0.6606160000	-1.7215050000
H	5.4735950000	-2.0179020000	0.2529460000
H	3.3927300000	-1.5369050000	1.4396420000
C	0.2258500000	-2.7452650000	-0.6419360000
C	-3.5485160000	0.2143120000	0.7515850000
C	-4.7639440000	-0.0387800000	-0.1697450000
C	-4.1933710000	-0.6881720000	-1.4584730000
H	1.1046800000	-2.0990990000	-0.7542740000
H	0.0924760000	-3.3387110000	-1.5456940000
H	0.3749330000	-3.4122180000	0.2129580000
H	-3.0727250000	1.1872510000	0.5747260000
H	-3.7604140000	0.1169380000	1.8149990000
H	-5.3148350000	0.8798950000	-0.3767920000
H	-5.4453510000	-0.7399730000	0.3200390000
H	-4.8609390000	-1.4292540000	-1.9007470000

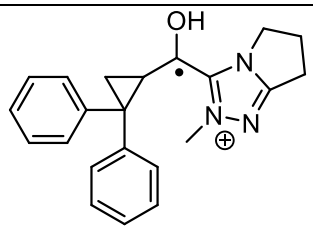
H -3.9645550000 0.0637420000 -2.2210070000

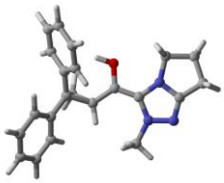
thermodynamic data

Zero-point correction= 0.400058 (Hartree/Particle)
Thermal correction to Energy= 0.421921
Thermal correction to Enthalpy= 0.422865
Thermal correction to Gibbs Free Energy= 0.347200
Sum of electronic and zero-point Energies= -1090.198350
Sum of electronic and thermal Energies= -1090.176487
Sum of electronic and thermal Enthalpies= -1090.175543
Sum of electronic and thermal Free Energies= -1090.251208

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.759	86.385	159.251

uB3LYP/6-31G*	**Job15radpr**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C -0.9611410000 -0.0523880000 0.6958160000

O -1.1432840000 1.2568410000 0.9858130000

H -0.2823820000 1.7271550000 0.9473450000

C 0.3264510000 -0.6991160000 0.9292450000

C 1.2152930000 -0.2655050000 2.0832990000

C 1.7173980000 0.0259750000 0.6994500000

H 0.3630160000 -1.7477000000 0.6731940000

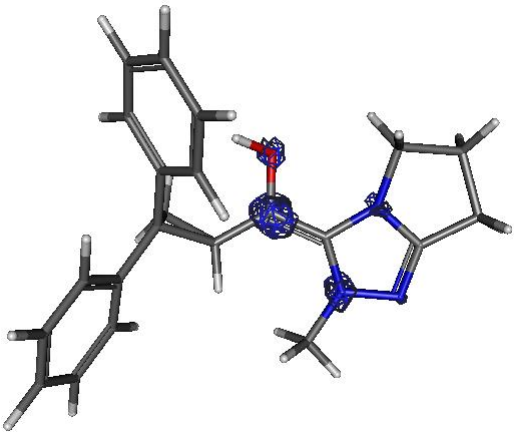
H	1.7001830000	-1.0459980000	2.6613830000
H	0.8496120000	0.5645370000	2.6817780000
C	-2.1337300000	-0.6746280000	0.2184960000
N	-2.4062020000	-1.9856610000	-0.0924620000
N	-3.6994770000	-2.1549060000	-0.5319220000
N	-3.3239380000	-0.0315240000	-0.0237680000
C	-4.2153640000	-0.9566210000	-0.4788490000
C	1.6880760000	1.4603400000	0.2276310000
C	2.1376660000	2.4982640000	1.0615350000
C	2.1575250000	3.8197730000	0.6073210000
C	1.7326780000	4.1220400000	-0.6866510000
C	1.2848870000	3.0991550000	-1.5279100000
C	1.2630860000	1.7807510000	-1.0757000000
H	2.4906410000	2.2669600000	2.0627790000
H	2.5136310000	4.6082300000	1.2636760000
H	1.7509720000	5.1486970000	-1.0400810000
H	0.9566960000	3.3286860000	-2.5375640000
H	0.9230590000	0.9863930000	-1.7354250000
C	2.8112310000	-0.8561290000	0.1315620000
C	3.7346420000	-0.3520630000	-0.7967500000
C	4.7525830000	-1.1591060000	-1.3080500000
C	4.8711560000	-2.4880330000	-0.9065190000
C	3.9638540000	-3.0030560000	0.0211770000
C	2.9502470000	-2.1969450000	0.5344740000
H	3.6735370000	0.6809040000	-1.1187110000
H	5.4559010000	-0.7392920000	-2.0214260000
H	5.6632500000	-3.1147950000	-1.3050000000
H	4.0480550000	-4.0337420000	0.3537190000

H	2.2756150000	-2.6312130000	1.2681000000
C	-1.5675070000	-3.1757970000	0.0019670000
C	-3.8666300000	1.3410720000	-0.0025420000
C	-5.3884970000	1.0752060000	-0.1638600000
C	-5.5259080000	-0.3282510000	-0.8256120000
H	-0.7193700000	-3.1113400000	-0.6851760000
H	-2.2003380000	-4.0148040000	-0.2842800000
H	-1.2166380000	-3.3186880000	1.0273520000
H	-3.4379020000	1.9077360000	-0.8347420000
H	-3.6072700000	1.8403850000	0.9295160000
H	-5.8685130000	1.8590480000	-0.7525510000
H	-5.8600790000	1.0635020000	0.8228400000
H	-6.3764090000	-0.9004200000	-0.4480150000
H	-5.6296560000	-0.2639530000	-1.9153190000

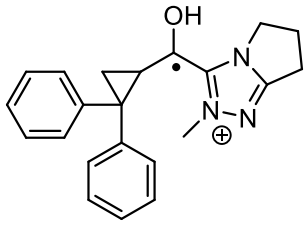
thermodynamic data

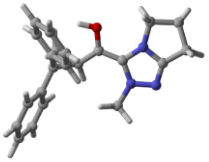
Zero-point correction= 0.411000 (Hartree/Particle)
Thermal correction to Energy= 0.433233
Thermal correction to Enthalpy= 0.434178
Thermal correction to Gibbs Free Energy= 0.357050
Sum of electronic and zero-point Energies= -1090.984017
Sum of electronic and thermal Energies= -1090.961784
Sum of electronic and thermal Enthalpies= -1090.960840
Sum of electronic and thermal Free Energies= -1091.037967

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	271.858	88.323	162.329



uM062X/6-31++G**	**Job15radpr**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9158020000	0.0403570000	0.9047900000
O	-1.2777810000	1.2882220000	1.2527740000
H	-0.5015810000	1.8670990000	1.3492630000
C	0.3914300000	-0.5211010000	1.2237700000
C	1.3046950000	0.1185430000	2.2385730000
C	1.7015350000	0.2075710000	0.7979700000
H	0.4396740000	-1.6002540000	1.1634310000
H	1.8620380000	-0.5540660000	2.8815970000
H	0.9531040000	1.0184640000	2.7354600000
C	-1.9375690000	-0.6611000000	0.2324210000
N	-1.9020170000	-1.8467290000	-0.4361490000
N	-3.1229510000	-2.1800360000	-0.9488080000

N	-3.2300220000	-0.2518080000	0.1176770000
C	-3.8992900000	-1.1955470000	-0.5989630000
C	1.4980280000	1.5289720000	0.1107050000
C	1.8421220000	2.7292730000	0.7390690000
C	1.6248390000	3.9517140000	0.0976800000
C	1.0653250000	3.9806720000	-1.1765650000
C	0.7284320000	2.7852330000	-1.8156050000
C	0.9423250000	1.5692510000	-1.1745310000
H	2.3003330000	2.7079590000	1.7247660000
H	1.9016790000	4.8762300000	0.5938890000
H	0.8977620000	4.9298130000	-1.6748730000
H	0.3025500000	2.8042570000	-2.8137710000
H	0.6880590000	0.6361730000	-1.6740660000
C	2.8076630000	-0.6791260000	0.2872910000
C	3.6567190000	-0.2477730000	-0.7371380000
C	4.6853820000	-1.0677500000	-1.2006570000
C	4.8827230000	-2.3310060000	-0.6520400000
C	4.0459660000	-2.7692740000	0.3739190000
C	3.0215820000	-1.9512920000	0.8385390000
H	3.5281370000	0.7377720000	-1.1721810000
H	5.3362120000	-0.7096750000	-1.9917460000
H	5.6841800000	-2.9670090000	-1.0125860000
H	4.1953670000	-3.7472520000	0.8200940000
H	2.4008290000	-2.3168850000	1.6534900000
C	-0.7671430000	-2.7133260000	-0.7357150000
C	-4.0719290000	0.8840820000	0.5250770000
C	-5.4870210000	0.3089640000	0.2757260000
C	-5.3270320000	-0.8047020000	-0.7927860000

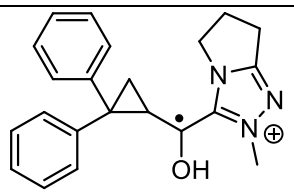
H	0.1013110000	-2.1111190000	-1.0104430000
H	-1.0701390000	-3.3324820000	-1.5781020000
H	-0.5309120000	-3.3520040000	0.1184250000
H	-3.8346560000	1.7442100000	-0.1059830000
H	-3.8824570000	1.1437100000	1.5657030000
H	-6.1833890000	1.0866730000	-0.0377530000
H	-5.8638420000	-0.1288470000	1.2031250000
H	-6.0107490000	-1.6414680000	-0.6486750000
H	-5.4642070000	-0.4228680000	-1.8094780000

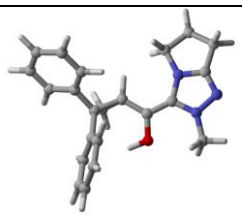
thermodynamic data

Zero-point correction= 0.413424 (Hartree/Particle)
Thermal correction to Energy= 0.435472
Thermal correction to Enthalpy= 0.436416
Thermal correction to Gibbs Free Energy= 0.360570
Sum of electronic and zero-point Energies= -1090.582760
Sum of electronic and thermal Energies= -1090.560711
Sum of electronic and thermal Enthalpies= -1090.559767
Sum of electronic and thermal Free Energies= -1090.635613

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	273.263	87.865	159.631

uB3LYP/6-31G*	**Job15radprko2**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9586190000	-0.7871950000	0.4581310000
O	-0.5763710000	-2.0737280000	0.5728090000
H	0.4048390000	-2.1366020000	0.5450030000
C	-0.0364000000	0.3137280000	0.7524440000
C	1.5103560000	0.1995540000	0.6402430000
C	0.8640990000	0.2717260000	1.9901600000
H	-0.4091670000	1.2946050000	0.4853270000
H	0.9521350000	1.1912630000	2.5610520000
H	0.8066880000	-0.6309800000	2.5919960000
C	-2.3088800000	-0.6034990000	0.1007610000
N	-3.2051810000	-1.5621230000	-0.3077020000
N	-4.4429190000	-1.0321670000	-0.5772810000
N	-3.0465850000	0.5577420000	0.0869430000
C	-4.3083340000	0.2419510000	-0.3329050000
C	2.1490850000	-1.0998950000	0.1891770000
C	2.1790330000	-1.4365680000	-1.1775140000
C	2.8178280000	-2.5958220000	-1.6112310000
C	3.4431720000	-3.4412380000	-0.6897520000
C	3.4252630000	-3.1195990000	0.6668350000
C	2.7851200000	-1.9565530000	1.1044170000
H	1.7120430000	-0.7756640000	-1.9024580000
H	2.8335010000	-2.8376940000	-2.6699350000
H	3.9439320000	-4.3426700000	-1.0300150000
H	3.9170440000	-3.7650620000	1.3885380000
H	2.7973960000	-1.7044290000	2.1610290000
C	2.2066430000	1.4452660000	0.1321830000

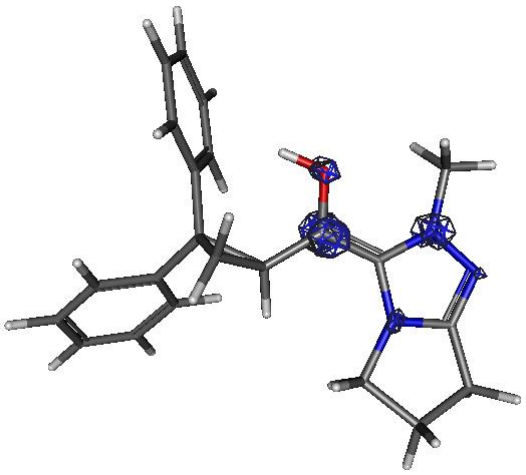
C	3.3100180000	1.9502030000	0.8331190000
C	3.9943340000	3.0709300000	0.3638260000
C	3.5853870000	3.7005500000	-0.8138820000
C	2.4888640000	3.2037290000	-1.5195250000
C	1.8041630000	2.0820470000	-1.0483630000
H	3.6353970000	1.4606760000	1.7475520000
H	4.8468650000	3.4525180000	0.9181730000
H	4.1183870000	4.5735620000	-1.1787300000
H	2.1658830000	3.6876820000	-2.4369340000
H	0.9510670000	1.7002200000	-1.6051240000
C	-2.8838680000	1.9879200000	0.4042210000
C	-4.3589650000	2.4766010000	0.4388300000
C	-5.1799500000	1.4531450000	-0.3981340000
C	-3.0178540000	-3.0026860000	-0.4886440000
H	-2.2112120000	-3.1925870000	-1.1984600000
H	-3.9617350000	-3.3804920000	-0.8788390000
H	-2.7822430000	-3.4788520000	0.4642330000
H	-2.2962460000	2.4739950000	-0.3817080000
H	-2.3744380000	2.1158940000	1.3611760000
H	-4.4480370000	3.4948060000	0.0560180000
H	-4.7144990000	2.4759240000	1.4729430000
H	-6.1777670000	1.2707230000	0.0068010000
H	-5.2990540000	1.7730460000	-1.4402220000

thermodynamic data

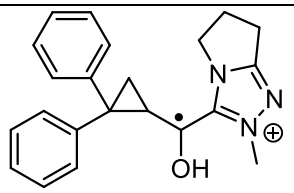
Zero-point correction= 0.410514 (Hartree/Particle)
Thermal correction to Energy= 0.433031
Thermal correction to Enthalpy= 0.433975
Thermal correction to Gibbs Free Energy= 0.355771
Sum of electronic and zero-point Energies= -1090.985940

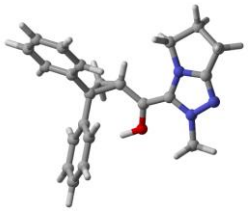
Sum of electronic and thermal Energies= -1090.963422
Sum of electronic and thermal Enthalpies= -1090.962478
Sum of electronic and thermal Free Energies= -1091.040683

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	271.731	88.401	164.595



uM062X/6-31++G**	**Job15radprko2**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8920220000	-0.8165730000	0.7022100000
O	-0.5685880000	-2.1025160000	0.8893850000
H	0.3979040000	-2.2333280000	0.9023110000
C	0.0313360000	0.2772810000	0.9977850000
C	1.5427660000	0.1785930000	0.7241430000
C	1.0419290000	0.1863340000	2.1302190000

H	-0.3703890000	1.2646430000	0.8100070000
H	1.1830070000	1.0841590000	2.7226380000
H	1.0552150000	-0.7435010000	2.6918270000
C	-2.2006710000	-0.6031160000	0.2268370000
N	-3.0710880000	-1.5394590000	-0.2456970000
N	-4.2529280000	-0.9879170000	-0.6408550000
N	-2.8926010000	0.5717370000	0.1307210000
C	-4.1128870000	0.2828850000	-0.4058040000
C	2.0898270000	-1.1013740000	0.1451070000
C	1.8936880000	-1.3885990000	-1.2128290000
C	2.3892870000	-2.5650160000	-1.7647950000
C	3.0918550000	-3.4715410000	-0.9676410000
C	3.3020770000	-3.1906360000	0.3792290000
C	2.8043880000	-2.0088700000	0.9344340000
H	1.3544660000	-0.6801090000	-1.8368690000
H	2.2322210000	-2.7750920000	-2.8178680000
H	3.4793810000	-4.3887010000	-1.3986020000
H	3.8608220000	-3.8827110000	1.0007610000
H	2.9894070000	-1.7856640000	1.9818590000
C	2.1676080000	1.4369090000	0.1787540000
C	3.3476840000	1.9291550000	0.7413350000
C	3.9529430000	3.0689660000	0.2165370000
C	3.3862420000	3.7230690000	-0.8767970000
C	2.2112320000	3.2348100000	-1.4447630000
C	1.6054660000	2.0968770000	-0.9162990000
H	3.7925450000	1.4158730000	1.5905390000
H	4.8680260000	3.4466480000	0.6610190000
H	3.8590600000	4.6105330000	-1.2842040000

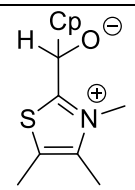
H	1.7674640000	3.7386340000	-2.2974790000
H	0.6884280000	1.7161490000	-1.3629380000
C	-2.7260190000	1.9985460000	0.4467050000
C	-4.1841080000	2.5095740000	0.3485650000
C	-4.9327610000	1.5173870000	-0.5759570000
C	-2.8830710000	-2.9804570000	-0.4061500000
H	-2.0056640000	-3.1736220000	-1.0237390000
H	-3.7835030000	-3.3431900000	-0.8975010000
H	-2.7589830000	-3.4543030000	0.5669300000
H	-2.0623780000	2.4604750000	-0.2912300000
H	-2.3054170000	2.1253310000	1.4452080000
H	-4.2213700000	3.5345530000	-0.0200700000
H	-4.6346450000	2.4905460000	1.3437120000
H	-5.9740710000	1.3658590000	-0.2911380000
H	-4.9072390000	1.8311870000	-1.6243900000

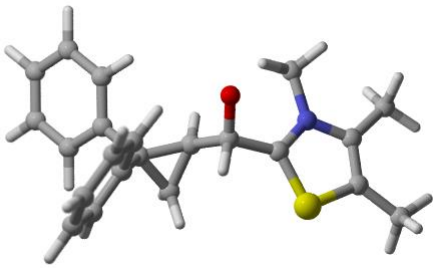
thermodynamic data

Zero-point correction= 0.413111 (Hartree/Particle)
Thermal correction to Energy= 0.435353
Thermal correction to Enthalpy= 0.436297
Thermal correction to Gibbs Free Energy= 0.359253
Sum of electronic and zero-point Energies= -1090.582270
Sum of electronic and thermal Energies= -1090.560027
Sum of electronic and thermal Enthalpies= -1090.559083
Sum of electronic and thermal Free Energies= -1090.636128

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	273.188	87.802	162.155

B3LYP/6-31G*	**Konformation 1 de**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	2.2461520000	0.1971840000	-0.1840020000
N	3.0540690000	-0.7830880000	-0.5994460000
C	4.3811610000	-0.7208480000	-0.1358920000
C	4.6041190000	0.3599050000	0.6603410000
S	3.1246960000	1.2932950000	0.8137950000
C	5.8645570000	0.8087240000	1.3356270000
C	5.3586360000	-1.7813470000	-0.5430050000
C	2.5646460000	-1.8444670000	-1.5030080000
C	0.7709690000	0.4313590000	-0.6498310000
H	3.3370540000	-2.0650180000	-2.2416180000
H	1.6636120000	-1.4187100000	-1.9775560000
H	2.3394100000	-2.7446760000	-0.9239990000
H	6.6757620000	0.0959520000	1.1666290000
H	5.7256630000	0.9051180000	2.4186370000
H	6.1938540000	1.7834700000	0.9566020000
H	6.3042850000	-1.6501030000	-0.0141330000
H	5.5713110000	-1.7467680000	-1.6182690000
H	4.9814010000	-2.7839460000	-0.3125650000

O	0.6561030000	0.1756010000	-1.9473820000
H	0.5944720000	1.4981170000	-0.3500940000
C	-0.1345960000	-0.4231340000	0.2604770000
C	-1.5828100000	-0.0478850000	0.5142160000
C	-0.5795850000	-0.0428530000	1.6543300000
H	0.0090350000	-1.4899130000	0.0931190000
H	-0.6371580000	-0.8202860000	2.4127460000
H	-0.2833500000	0.9328570000	2.0351470000
C	-2.1469280000	1.2822280000	0.0539390000
C	-2.0148630000	1.7205200000	-1.2724510000
C	-2.6122870000	2.9152130000	-1.6806980000
C	-3.3543870000	3.6829310000	-0.7818230000
C	-3.4869030000	3.2555860000	0.5410300000
C	-2.8854500000	2.0663330000	0.9523810000
H	-1.3960110000	1.1461350000	-1.9588660000
H	-2.4915020000	3.2477960000	-2.7089560000
H	-3.8201980000	4.6103850000	-1.1060870000
H	-4.0568580000	3.8482050000	1.2527670000
H	-2.9905610000	1.7377140000	1.9839410000
C	-2.5806810000	-1.1823160000	0.4266390000
C	-3.4055180000	-1.5252360000	1.5046070000
C	-4.3437240000	-2.5529450000	1.3870530000
C	-4.4710720000	-3.2510230000	0.1852770000
C	-3.6521090000	-2.9171080000	-0.8963490000
C	-2.7142060000	-1.8920040000	-0.7755260000
H	-3.3099450000	-0.9847940000	2.4432930000
H	-4.9745250000	-2.8080560000	2.2352340000
H	-5.2008710000	-4.0513820000	0.0926170000

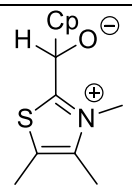
H	-3.7428170000	-3.4581620000	-1.8351350000
H	-2.0652360000	-1.6327510000	-1.6089800000

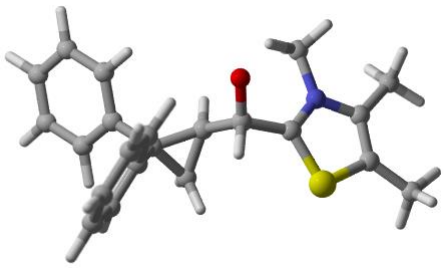
thermodynamic data

Zero-point correction= 0.396143 (Hartree/Particle)
Thermal correction to Energy= 0.419497
Thermal correction to Enthalpy= 0.420441
Thermal correction to Gibbs Free Energy= 0.341492
Sum of electronic and zero-point Energies= -1379.867188
Sum of electronic and thermal Energies= -1379.843834
Sum of electronic and thermal Enthalpies= -1379.842890
Sum of electronic and thermal Free Energies= -1379.921839

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	263.238	90.169	166.162

B3LYP/6-31G* PCM freq	**Konformation 1 de**





xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	2.2587410000	0.2358980000	-0.2707160000
N	3.0726470000	-0.7492030000	-0.6502550000
C	4.3729440000	-0.7101380000	-0.1112080000
C	4.5602020000	0.3607110000	0.7088500000
S	3.0865340000	1.3091490000	0.7848700000
C	5.7807430000	0.7858570000	1.4665980000
C	5.3578550000	-1.7790180000	-0.4725300000

C	2.6285230000	-1.8153440000	-1.5707340000
C	0.7918870000	0.4664110000	-0.7511090000
H	3.4139220000	-1.9983920000	-2.3052870000
H	1.7230340000	-1.4312220000	-2.0530480000
H	2.4361910000	-2.7298410000	-1.0039670000
H	6.5870550000	0.0596630000	1.3425910000
H	5.5708280000	0.8764220000	2.5378490000
H	6.1463170000	1.7574710000	1.1155310000
H	6.2804800000	-1.6504800000	0.0949660000
H	5.6140700000	-1.7477990000	-1.5378370000
H	4.9630250000	-2.7766860000	-0.2522010000
O	0.6627510000	0.2586720000	-2.0649440000
H	0.5962570000	1.5179920000	-0.4132150000
C	-0.1051380000	-0.4261100000	0.1366730000
C	-1.5471600000	-0.0685440000	0.4599360000
C	-0.4978560000	-0.0922340000	1.5566980000
H	0.0411640000	-1.4860180000	-0.0681380000
H	-0.5240430000	-0.8908600000	2.2940520000
H	-0.1872450000	0.8722770000	1.9538120000
C	-2.1454180000	1.2679200000	0.0655970000
C	-2.0215210000	1.7807680000	-1.2348430000
C	-2.6498880000	2.9790680000	-1.5859800000
C	-3.4164490000	3.6788300000	-0.6516010000
C	-3.5413700000	3.1783930000	0.6474260000
C	-2.9094430000	1.9849850000	0.9998370000
H	-1.3848670000	1.2559780000	-1.9445240000
H	-2.5362500000	3.3685470000	-2.5950360000
H	-3.9061910000	4.6087350000	-0.9292290000

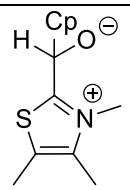
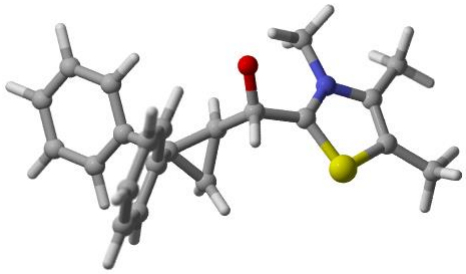
H	-4.1288370000	3.7176780000	1.3864230000
H	-3.0094090000	1.6017710000	2.0126960000
C	-2.5484800000	-1.2033440000	0.3974100000
C	-3.2662560000	-1.6135950000	1.5288680000
C	-4.2130160000	-2.6380890000	1.4436750000
C	-4.4574630000	-3.2679590000	0.2215640000
C	-3.7463900000	-2.8683080000	-0.9138180000
C	-2.8013300000	-1.8455410000	-0.8242560000
H	-3.0784200000	-1.1313610000	2.4849380000
H	-4.7572350000	-2.9447700000	2.3333930000
H	-5.1919120000	-4.0662100000	0.1544490000
H	-3.9253350000	-3.3563850000	-1.8685690000
H	-2.2399830000	-1.5415530000	-1.7042510000

thermodynamic data

Zero-point correction= 0.396350 (Hartree/Particle)
Thermal correction to Energy= 0.419777
Thermal correction to Enthalpy= 0.420721
Thermal correction to Gibbs Free Energy= 0.341269
Sum of electronic and zero-point Energies= -1379.888854
Sum of electronic and thermal Energies= -1379.865427
Sum of electronic and thermal Enthalpies= -1379.864483
Sum of electronic and thermal Free Energies= -1379.943936

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	263.414	90.189	167.221

M062X/6-31++G**	**Konformation 1 de**

xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	2.2158320000	0.2503330000	-0.2869500000
N	3.0196930000	-0.7310770000	-0.6720730000
C	4.3059920000	-0.7116330000	-0.1139020000
C	4.4839020000	0.3387160000	0.7270670000
S	3.0268230000	1.2904440000	0.7946840000
C	5.6993750000	0.7424920000	1.5021970000
C	5.2856270000	-1.7769430000	-0.4890690000
C	2.5759870000	-1.7887010000	-1.5988120000
C	0.7548230000	0.4636060000	-0.7699820000
H	3.3683900000	-1.9691940000	-2.3257970000
H	1.6740370000	-1.3980800000	-2.0909750000
H	2.3767000000	-2.6996360000	-1.0288220000
H	6.4871960000	-0.0054620000	1.4016850000
H	5.4697780000	0.8490590000	2.5657960000
H	6.0931010000	1.6973890000	1.1425340000
H	6.1918530000	-1.6832490000	0.1086590000
H	5.5674280000	-1.7032360000	-1.5439850000
H	4.8677330000	-2.7733520000	-0.3194090000
O	0.6257230000	0.2140080000	-2.0670620000
H	0.5433440000	1.5170970000	-0.4533910000

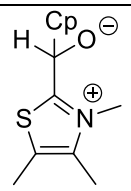
C	-0.0990340000	-0.4353930000	0.1391300000
C	-1.5190720000	-0.0688680000	0.4737750000
C	-0.4695800000	-0.0862220000	1.5588770000
H	0.0448550000	-1.4949310000	-0.0728380000
H	-0.4981160000	-0.8810060000	2.2984760000
H	-0.1513300000	0.8839440000	1.9354320000
C	-2.0936140000	1.2628640000	0.0576620000
C	-2.0295070000	1.7000410000	-1.2697190000
C	-2.6326320000	2.9032890000	-1.6351210000
C	-3.3078610000	3.6745240000	-0.6901360000
C	-3.3716190000	3.2432130000	0.6344410000
C	-2.7645510000	2.0447900000	1.0025950000
H	-1.4627720000	1.1150970000	-1.9935190000
H	-2.5675280000	3.2416150000	-2.6651270000
H	-3.7773410000	4.6093000000	-0.9822700000
H	-3.8915770000	3.8388460000	1.3790470000
H	-2.8105460000	1.7048290000	2.0351310000
C	-2.5227230000	-1.1909350000	0.4226210000
C	-3.2796000000	-1.5472630000	1.5404730000
C	-4.2287170000	-2.5660310000	1.4584300000
C	-4.4309750000	-3.2361650000	0.2534360000
C	-3.6794240000	-2.8837510000	-0.8684640000
C	-2.7311460000	-1.8675000000	-0.7832540000
H	-3.1207150000	-1.0235830000	2.4803610000
H	-4.8096120000	-2.8359530000	2.3354460000
H	-5.1692450000	-4.0296250000	0.1877020000
H	-3.8324160000	-3.4019740000	-1.8104680000
H	-2.1349290000	-1.5863160000	-1.6493550000

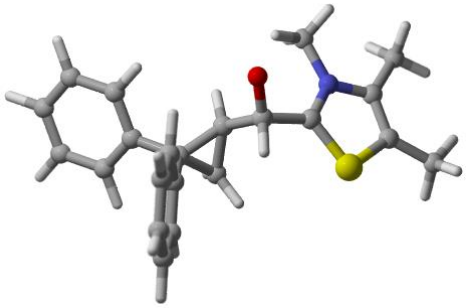
thermodynamic data

Zero-point correction= 0.398313 (Hartree/Particle)
Thermal correction to Energy= 0.421562
Thermal correction to Enthalpy= 0.422506
Thermal correction to Gibbs Free Energy= 0.343803
Sum of electronic and zero-point Energies= -1379.472205
Sum of electronic and thermal Energies= -1379.448956
Sum of electronic and thermal Enthalpies= -1379.448011
Sum of electronic and thermal Free Energies= -1379.526715

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.534	89.664	165.646

M062X/6-31++G** PCM freq	**Konformation 1 de**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	2.2095440000	0.1669530000	-0.3668700000
N	3.0072870000	-0.8608200000	-0.6145570000
C	4.2790320000	-0.7905240000	-0.0270250000
C	4.4463970000	0.3512370000	0.6900350000
S	3.0009520000	1.3152770000	0.6078150000
C	5.6393020000	0.8287370000	1.4569140000
C	5.2531490000	-1.9030020000	-0.2429620000
C	2.5851130000	-2.0200310000	-1.4168760000

C	0.7648590000	0.3518280000	-0.8888420000
H	3.3904400000	-2.2813670000	-2.1028850000
H	1.6991870000	-1.7156770000	-1.9746000000
H	2.3795930000	-2.8599640000	-0.7502010000
H	6.4435670000	0.0941460000	1.4087820000
H	5.3878470000	0.9920040000	2.5079120000
H	6.0142470000	1.7696820000	1.0460200000
H	6.1442410000	-1.7419710000	0.3620270000
H	5.5609200000	-1.9606310000	-1.2911530000
H	4.8186630000	-2.8653950000	0.0409010000
O	0.6714810000	0.1259770000	-2.2098790000
H	0.5255330000	1.3972820000	-0.5758060000
C	-0.1196120000	-0.5519780000	-0.0178350000
C	-1.4992920000	-0.1129780000	0.4058920000
C	-0.3999200000	-0.2343900000	1.4289460000
H	-0.0352230000	-1.6077030000	-0.2721310000
H	-0.4452640000	-1.0523540000	2.1410830000
H	0.0097930000	0.6939760000	1.8214260000
C	-1.9972230000	1.2640910000	0.0475060000
C	-2.1976160000	1.6155950000	-1.2922610000
C	-2.7119450000	2.8670230000	-1.6261010000
C	-3.0387450000	3.7823890000	-0.6235670000
C	-2.8429080000	3.4396030000	0.7136860000
C	-2.3238790000	2.1869800000	1.0447600000
H	-1.9144040000	0.9090730000	-2.0678520000
H	-2.8531510000	3.1312120000	-2.6700270000
H	-3.4384780000	4.7577310000	-0.8841930000
H	-3.0907190000	4.1466740000	1.4998400000

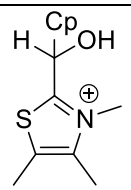
H	-2.1672580000	1.9222050000	2.0878840000
C	-2.5905320000	-1.1524930000	0.4065820000
C	-3.3542850000	-1.3763570000	1.5561190000
C	-4.3962770000	-2.3030470000	1.5486710000
C	-4.6882050000	-3.0161620000	0.3851790000
C	-3.9317100000	-2.7987620000	-0.7668750000
C	-2.8887630000	-1.8727110000	-0.7544740000
H	-3.1238450000	-0.8206460000	2.4622260000
H	-4.9779220000	-2.4706050000	2.4502890000
H	-5.4986760000	-3.7385770000	0.3773090000
H	-4.1521340000	-3.3523980000	-1.6746610000
H	-2.2939590000	-1.7052110000	-1.6499330000

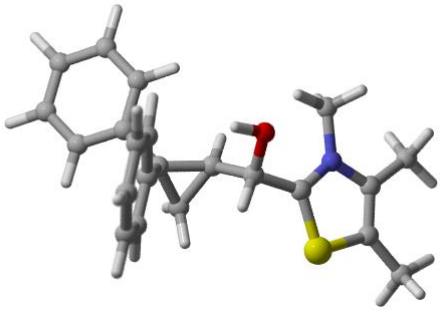
thermodynamic data

Zero-point correction= 0.398134 (Hartree/Particle)
Thermal correction to Energy= 0.420670
Thermal correction to Enthalpy= 0.421615
Thermal correction to Gibbs Free Energy= 0.344539
Sum of electronic and zero-point Energies= -1379.500737
Sum of electronic and thermal Energies= -1379.478201
Sum of electronic and thermal Enthalpies= -1379.477256
Sum of electronic and thermal Free Energies= -1379.554332

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	263.975	87.853	162.218

B3LYP/6-31G*	**Konformation 1 pr**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	2.2237540000	0.2586430000	-0.1978500000
N	2.9590630000	-0.7100120000	-0.7455840000
C	4.2818430000	-0.7900850000	-0.2702060000
C	4.5495610000	0.1562490000	0.6766710000
S	3.1338350000	1.1448310000	0.9437840000
C	5.8140870000	0.4286450000	1.4341610000
C	5.2102320000	-1.8306940000	-0.8165310000
C	2.4564830000	-1.6594900000	-1.7632390000
C	0.7574270000	0.5569080000	-0.4369760000
H	3.1505060000	-1.6708440000	-2.6049780000
H	1.4828030000	-1.3212760000	-2.1057920000
H	2.3966420000	-2.6574060000	-1.3221890000
H	6.5856970000	-0.2993800000	1.1759290000
H	5.6487230000	0.3714940000	2.5154050000
H	6.2053200000	1.4262510000	1.2060790000
H	6.1692670000	-1.7881750000	-0.2992700000
H	5.4044840000	-1.6780500000	-1.8844620000

H	4.8080800000	-2.8413920000	-0.6867800000
H	0.5751130000	1.5587630000	-0.0237000000
C	-0.1261170000	-0.4353080000	0.3051630000
C	-1.5892670000	-0.0703180000	0.5832900000
C	-0.5853160000	-0.1352540000	1.7121230000
H	0.0586700000	-1.4777390000	0.0564810000
H	-0.6598190000	-0.9658410000	2.4069880000
H	-0.2505950000	0.7934190000	2.1675910000
C	-2.0930090000	1.2753160000	0.0999720000
C	-2.5714700000	1.3950660000	-1.2189860000
C	-3.0287040000	2.6193640000	-1.7074330000
C	-3.0268130000	3.7479290000	-0.8835020000
C	-2.5756610000	3.6372080000	0.4309240000
C	-2.1120570000	2.4114390000	0.9182990000
H	-2.6343820000	0.5088750000	-1.8476430000
H	-3.3996390000	2.6883390000	-2.7261750000
H	-3.3876890000	4.7003250000	-1.2601240000
H	-2.5897470000	4.5034950000	1.0863160000
H	-1.7854860000	2.3410910000	1.9517600000
C	-2.5968240000	-1.1954210000	0.4824320000
C	-3.6028570000	-1.3086790000	1.4522480000
C	-4.5648960000	-2.3134710000	1.3622080000
C	-4.5375220000	-3.2187850000	0.2983620000
C	-3.5435180000	-3.1122130000	-0.6740930000
C	-2.5797120000	-2.1055260000	-0.5814350000
H	-3.6312730000	-0.6037460000	2.2793400000
H	-5.3365110000	-2.3902290000	2.1229500000
H	-5.2870690000	-4.0017180000	0.2292170000

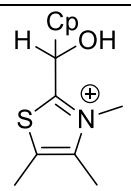
H	-3.5166410000	-3.8106820000	-1.5058360000
H	-1.8092530000	-2.0288270000	-1.3456100000
O	0.5427240000	0.5624430000	-1.8400260000
H	-0.3516480000	0.9273610000	-1.9803680000

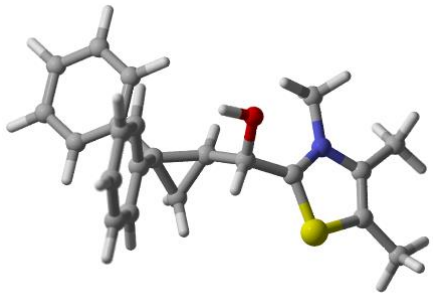
thermodynamic data

Zero-point correction= 0.410806 (Hartree/Particle)
Thermal correction to Energy= 0.434469
Thermal correction to Enthalpy= 0.435413
Thermal correction to Gibbs Free Energy= 0.355790
Sum of electronic and zero-point Energies= -1380.304606
Sum of electronic and thermal Energies= -1380.280943
Sum of electronic and thermal Enthalpies= -1380.279999
Sum of electronic and thermal Free Energies= -1380.359622

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.634	91.499	167.582

B3LYP/6-31G* PCM freq	**Konformation 1 pr**





xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	2.2401760000	0.2673390000	-0.2231950000
N	2.9585920000	-0.7536820000	-0.6901290000
C	4.2808830000	-0.8079090000	-0.2193840000
C	4.5667440000	0.2170460000	0.6368380000

S	3.1679420000	1.2411660000	0.8255970000
C	5.8426340000	0.5386380000	1.3527560000
C	5.1910340000	-1.9047010000	-0.6755360000
C	2.4390290000	-1.7810870000	-1.6176920000
C	0.7763160000	0.5571510000	-0.4827370000
H	3.1485250000	-1.9010440000	-2.4366110000
H	1.4853520000	-1.4464480000	-2.0141140000
H	2.3316000000	-2.7256440000	-1.0804140000
H	6.5794480000	-0.2522410000	1.2006680000
H	5.6749010000	0.6425070000	2.4294910000
H	6.2725420000	1.4771540000	0.9864420000
H	6.1457870000	-1.8404940000	-0.1533040000
H	5.3930010000	-1.8351380000	-1.7502640000
H	4.7625200000	-2.8919180000	-0.4736770000
H	0.5885940000	1.5663350000	-0.0926900000
C	-0.1152420000	-0.4263330000	0.2618500000
C	-1.5750260000	-0.0685530000	0.5577900000
C	-0.5551870000	-0.1300640000	1.6738140000
H	0.0675110000	-1.4690380000	0.0171160000
H	-0.6136080000	-0.9625050000	2.3680280000
H	-0.2202230000	0.7997160000	2.1249980000
C	-2.1088240000	1.2726670000	0.0957870000
C	-2.6072190000	1.4028250000	-1.2140970000
C	-3.1014170000	2.6228760000	-1.6766280000
C	-3.1183810000	3.7376400000	-0.8338450000
C	-2.6441570000	3.6171290000	0.4725120000
C	-2.1446580000	2.3952220000	0.9332530000
H	-2.6391500000	0.5319300000	-1.8656250000

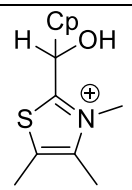
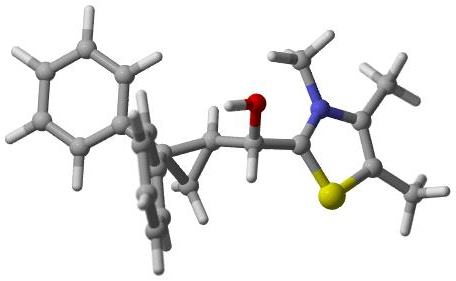
H	-3.4788610000	2.6998240000	-2.6924840000
H	-3.5047390000	4.6878870000	-1.1911400000
H	-2.6640500000	4.4734020000	1.1410860000
H	-1.7915150000	2.3180730000	1.9569730000
C	-2.5816090000	-1.1961570000	0.4717700000
C	-3.5749040000	-1.3131540000	1.4556840000
C	-4.5350420000	-2.3222500000	1.3821550000
C	-4.5190920000	-3.2306570000	0.3194770000
C	-3.5372910000	-3.1214100000	-0.6662680000
C	-2.5756680000	-2.1100830000	-0.5897370000
H	-3.5909310000	-0.6088750000	2.2837140000
H	-5.2945580000	-2.4012000000	2.1553480000
H	-5.2656960000	-4.0179700000	0.2628390000
H	-3.5161360000	-3.8226720000	-1.4961130000
H	-1.8134630000	-2.0340660000	-1.3609820000
O	0.5773080000	0.5353080000	-1.8921440000
H	-0.3311240000	0.8500410000	-2.0481710000

thermodynamic data

Zero-point correction= 0.411079 (Hartree/Particle)
Thermal correction to Energy= 0.434674
Thermal correction to Enthalpy= 0.435619
Thermal correction to Gibbs Free Energy= 0.356734
Sum of electronic and zero-point Energies= -1380.365686
Sum of electronic and thermal Energies= -1380.342091
Sum of electronic and thermal Enthalpies= -1380.341146
Sum of electronic and thermal Free Energies= -1380.420031

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.762	91.555	166.027

M062X/6-31++G**	**Konformation 1 pr**

xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	2.2000520000	0.2738990000	-0.1743890000
N	2.8800040000	-0.7320650000	-0.7085060000
C	4.2083370000	-0.8305950000	-0.2793900000
C	4.5293000000	0.1397480000	0.6204330000
S	3.1639510000	1.1676760000	0.8942480000
C	5.8424560000	0.3948760000	1.2959280000
C	5.0972740000	-1.9028030000	-0.8199760000
C	2.3160890000	-1.7129330000	-1.6541810000
C	0.7385330000	0.5881430000	-0.3914280000
H	2.9816660000	-1.7863130000	-2.5144500000
H	1.3415140000	-1.3668330000	-1.9852490000
H	2.2437580000	-2.6812360000	-1.1549000000
H	6.3614560000	-0.5463090000	1.4860710000
H	5.7009430000	0.8941480000	2.2561880000
H	6.4833960000	1.0258410000	0.6739070000
H	6.0640660000	-1.8655170000	-0.3187230000
H	5.2740360000	-1.7680490000	-1.8914180000
H	4.6706750000	-2.8971520000	-0.6621370000
H	0.5631780000	1.5812680000	0.0459220000
C	-0.1269790000	-0.4201470000	0.3347140000

C	-1.5753720000	-0.0608890000	0.6127150000
C	-0.5816550000	-0.1303100000	1.7406910000
H	0.0627890000	-1.4603980000	0.0796250000
H	-0.6620480000	-0.9672650000	2.4252540000
H	-0.2419030000	0.7963280000	2.1946930000
C	-2.0717220000	1.2800440000	0.1248130000
C	-2.6082280000	1.3696910000	-1.1690720000
C	-3.0427370000	2.5909020000	-1.6778980000
C	-2.9616360000	3.7433560000	-0.8947720000
C	-2.4566920000	3.6599940000	0.3993220000
C	-2.0151330000	2.4359500000	0.9062750000
H	-2.7151960000	0.4652890000	-1.7656180000
H	-3.4580090000	2.6411770000	-2.6795140000
H	-3.3063910000	4.6944650000	-1.2866080000
H	-2.4140700000	4.5463360000	1.0242630000
H	-1.6472150000	2.3860400000	1.9268070000
C	-2.5748280000	-1.1824540000	0.4937940000
C	-3.5925520000	-1.3036460000	1.4442240000
C	-4.5474410000	-2.3102860000	1.3285380000
C	-4.4971220000	-3.2038980000	0.2582980000
C	-3.4897360000	-3.0856100000	-0.6960030000
C	-2.5333700000	-2.0777690000	-0.5765590000
H	-3.6341350000	-0.6029610000	2.2748310000
H	-5.3314080000	-2.3987860000	2.0736730000
H	-5.2422250000	-3.9874860000	0.1684790000
H	-3.4486710000	-3.7744420000	-1.5337150000
H	-1.7516790000	-1.9838430000	-1.3283050000
O	0.5174370000	0.6195080000	-1.7847010000

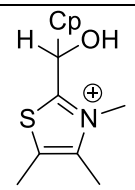
H -0.3582920000 1.0096920000 -1.9363540000

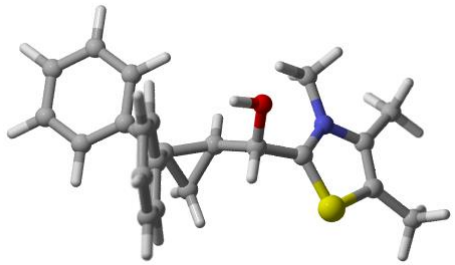
thermodynamic data

Zero-point correction= 0.413502 (Hartree/Particle)
Thermal correction to Energy= 0.436924
Thermal correction to Enthalpy= 0.437868
Thermal correction to Gibbs Free Energy= 0.359392
Sum of electronic and zero-point Energies= -1379.906392
Sum of electronic and thermal Energies= -1379.882970
Sum of electronic and thermal Enthalpies= -1379.882026
Sum of electronic and thermal Free Energies= -1379.960502

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	274.174	90.878	165.167

M062X/6-31++G** PCM freq	**Konformation 1 pr**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C 2.2143890000 0.2848770000 -0.1924640000

N 2.8858800000 -0.7523060000 -0.6737240000

C 4.2121570000 -0.8341840000 -0.2438980000

C 4.5403290000 0.1838360000 0.5998300000

S 3.1844560000 1.2311910000 0.8215410000

C 5.8583870000 0.4664010000 1.2518300000

C 5.0933690000 -1.9381340000 -0.7265960000

C 2.3175010000 -1.7805990000 -1.5634470000

C	0.7543130000	0.5918150000	-0.4234810000
H	2.9979930000	-1.9227490000	-2.4023320000
H	1.3560350000	-1.4395570000	-1.9339320000
H	2.2161740000	-2.7117810000	-1.0035650000
H	6.3698260000	-0.4677900000	1.4892810000
H	5.7245350000	1.0229940000	2.1806770000
H	6.4975800000	1.0543560000	0.5877630000
H	6.0563240000	-1.8841570000	-0.2201720000
H	5.2732480000	-1.8527390000	-1.8022150000
H	4.6520160000	-2.9177690000	-0.5254050000
H	0.5737270000	1.5892470000	-0.0002060000
C	-0.1159850000	-0.4129860000	0.3027130000
C	-1.5631170000	-0.0621680000	0.5920070000
C	-0.5582160000	-0.1253790000	1.7113270000
H	0.0765580000	-1.4531700000	0.0532140000
H	-0.6242880000	-0.9637510000	2.3956120000
H	-0.2218560000	0.8034390000	2.1621070000
C	-2.0856210000	1.2737730000	0.1198320000
C	-2.6130880000	1.3748040000	-1.1768640000
C	-3.0833040000	2.5919130000	-1.6642310000
C	-3.0469940000	3.7294060000	-0.8553360000
C	-2.5454390000	3.6350700000	0.4404740000
C	-2.0688170000	2.4149780000	0.9254640000
H	-2.6700020000	0.4853150000	-1.8020190000
H	-3.4824880000	2.6511040000	-2.6719130000
H	-3.4148480000	4.6784920000	-1.2316520000
H	-2.5260720000	4.5108200000	1.0815160000
H	-1.6927380000	2.3567090000	1.9422150000

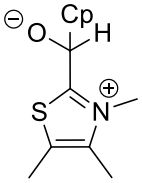
C	-2.5608580000	-1.1863440000	0.4832200000
C	-3.5687390000	-1.3132780000	1.4453010000
C	-4.5218150000	-2.3242140000	1.3411380000
C	-4.4793210000	-3.2190700000	0.2700300000
C	-3.4805220000	-3.0964330000	-0.6942660000
C	-2.5265620000	-2.0836660000	-0.5865350000
H	-3.5995280000	-0.6159020000	2.2793630000
H	-5.2960280000	-2.4167230000	2.0965050000
H	-5.2210940000	-4.0073520000	0.1891500000
H	-3.4416180000	-3.7872280000	-1.5307620000
H	-1.7496120000	-1.9905430000	-1.3422590000
O	0.5393690000	0.6089520000	-1.8220640000
H	-0.3535440000	0.9517070000	-1.9793210000

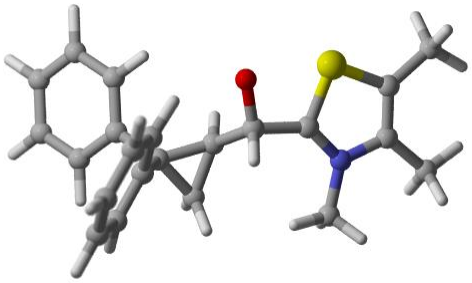
thermodynamic data

Zero-point correction= 0.413163 (Hartree/Particle)
Thermal correction to Energy= 0.435856
Thermal correction to Enthalpy= 0.436800
Thermal correction to Gibbs Free Energy= 0.360148
Sum of electronic and zero-point Energies= -1379.969528
Sum of electronic and thermal Energies= -1379.946835
Sum of electronic and thermal Enthalpies= -1379.945891
Sum of electronic and thermal Free Energies= -1380.022543

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	273.504	89.016	161.328

B3LYP/6-31G*	**Konformation 2 de**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.2553040000	0.2713690000	0.1195810000
N	-3.0823800000	0.3929730000	-0.9221600000
C	-4.4015570000	-0.0401520000	-0.6694410000
C	-4.5395970000	-0.4852570000	0.6111790000
S	-3.0166830000	-0.3503220000	1.5118870000
C	-5.7701820000	-1.0192500000	1.2808580000
C	-5.4255250000	0.0410360000	-1.7623650000
C	-2.6494830000	0.9255890000	-2.2162100000
C	-0.7784030000	0.5478180000	0.4340200000
H	-2.6022120000	0.1258040000	-2.9606140000
H	-1.6593900000	1.3606270000	-2.0992310000
H	-3.3496600000	1.6941390000	-2.5514970000
H	-6.6215780000	-1.0574890000	0.5956860000
H	-6.0583940000	-0.3944170000	2.1347420000
H	-5.6040040000	-2.0334870000	1.6626570000
H	-6.3698910000	-0.3895650000	-1.4245730000
H	-5.1137200000	-0.5094150000	-2.6584210000
H	-5.6266180000	1.0771370000	-2.0634690000

O	-0.6611780000	0.2651570000	1.7408930000
H	-0.5912320000	1.6141460000	0.1384100000
C	0.1271600000	-0.3435660000	-0.4383150000
C	1.6132590000	-0.0769030000	-0.5541120000
C	0.7303180000	-0.0205440000	-1.7900370000
H	-0.1045000000	-1.3952740000	-0.2808340000
H	0.7961300000	-0.8153100000	-2.5301390000
H	0.5767100000	0.9708580000	-2.2122410000
C	2.2224770000	1.2295070000	-0.0806320000
C	2.0398630000	1.6950860000	1.2303690000
C	2.6741320000	2.8651820000	1.6540090000
C	3.5036010000	3.5794360000	0.7878490000
C	3.6883150000	3.1234860000	-0.5189490000
C	3.0500730000	1.9592450000	-0.9467420000
H	1.3537940000	1.1623380000	1.8859980000
H	2.5141930000	3.2206070000	2.6692100000
H	3.9978740000	4.4873700000	1.1250240000
H	4.3279660000	3.6735700000	-1.2051830000
H	3.1967430000	1.6081310000	-1.9659150000
C	2.5104700000	-1.2747350000	-0.3323170000
C	3.4583110000	-1.6773010000	-1.2803770000
C	4.2966670000	-2.7658090000	-1.0310820000
C	4.1994470000	-3.4630130000	0.1742850000
C	3.2568310000	-3.0674690000	1.1266270000
C	2.4175370000	-1.9823080000	0.8748950000
H	3.5388990000	-1.1361210000	-2.2202590000
H	5.0253680000	-3.0690700000	-1.7790490000
H	4.8517380000	-4.3105800000	0.3691020000

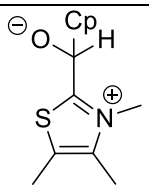
H	3.1728510000	-3.6075670000	2.0665260000
H	1.6714690000	-1.6720300000	1.6032990000

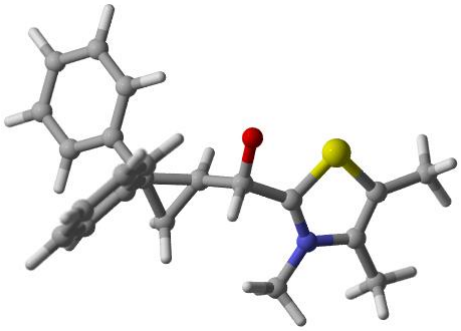
thermodynamic data

Zero-point correction= 0.396019 (Hartree/Particle)
Thermal correction to Energy= 0.419666
Thermal correction to Enthalpy= 0.420610
Thermal correction to Gibbs Free Energy= 0.340930
Sum of electronic and zero-point Energies= -1379.865712
Sum of electronic and thermal Energies= -1379.842064
Sum of electronic and thermal Enthalpies= -1379.841120
Sum of electronic and thermal Free Energies= -1379.920801

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	263.344	90.456	167.701

B3LYP/6-31G* PCM freq	**Konformation 2 de**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.2669030000	0.2765230000	0.2253590000
N	-3.0482640000	0.5060610000	-0.8293570000
C	-4.3700410000	0.0288860000	-0.7006880000
C	-4.5731690000	-0.5628250000	0.5102260000
S	-3.1113840000	-0.5030650000	1.4896930000
C	-5.8240970000	-1.1842370000	1.0543320000

C	-5.3405210000	0.2171000000	-1.8265460000
C	-2.5753300000	1.2022920000	-2.0343090000
C	-0.7930820000	0.5503190000	0.5695290000
H	-2.3361250000	0.4797600000	-2.8177770000
H	-1.6860860000	1.7753480000	-1.7807820000
H	-3.3523180000	1.8815650000	-2.3845610000
H	-6.6311720000	-1.1605340000	0.3183910000
H	-6.1706870000	-0.6546220000	1.9491890000
H	-5.6556890000	-2.2298670000	1.3352910000
H	-6.2841010000	-0.2781920000	-1.5933080000
H	-4.9616460000	-0.2089520000	-2.7622040000
H	-5.5579090000	1.2770710000	-2.0038290000
O	-0.6465600000	0.2740180000	1.8777300000
H	-0.6002450000	1.6135730000	0.2679570000
C	0.0961800000	-0.3430160000	-0.3248790000
C	1.5796320000	-0.0812700000	-0.5072800000
C	0.6408690000	-0.0197140000	-1.6988760000
H	-0.1337220000	-1.3950740000	-0.1635420000
H	0.6735500000	-0.8132300000	-2.4418760000
H	0.4607540000	0.9694060000	-2.1124230000
C	2.2216030000	1.2161970000	-0.0540070000
C	2.0804800000	1.6881860000	1.2602210000
C	2.7460630000	2.8465510000	1.6708490000
C	3.5683330000	3.5452400000	0.7837890000
C	3.7110430000	3.0852440000	-0.5280260000
C	3.0410890000	1.9321540000	-0.9406270000
H	1.3968930000	1.1658750000	1.9267260000
H	2.6183160000	3.2063130000	2.6892710000

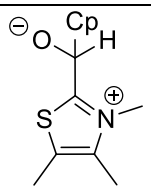
H	4.0871540000	4.4438720000	1.1078600000
H	4.3414770000	3.6247450000	-1.2305870000
H	3.1537680000	1.5819660000	-1.9640530000
C	2.4910410000	-1.2795030000	-0.3471670000
C	3.3777030000	-1.6717060000	-1.3588240000
C	4.2384620000	-2.7565560000	-1.1731250000
C	4.2261650000	-3.4641240000	0.0312680000
C	3.3440430000	-3.0826040000	1.0462430000
C	2.4839520000	-1.9998840000	0.8564920000
H	3.3903770000	-1.1278040000	-2.3002100000
H	4.9166690000	-3.0499890000	-1.9704950000
H	4.8943900000	-4.3089440000	0.1760270000
H	3.3229780000	-3.6315950000	1.9843600000
H	1.7847370000	-1.7057460000	1.6354310000

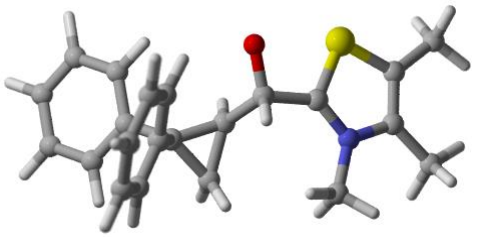
thermodynamic data

Zero-point correction= 0.396482 (Hartree/Particle)
Thermal correction to Energy= 0.420015
Thermal correction to Enthalpy= 0.420959
Thermal correction to Gibbs Free Energy= 0.341593
Sum of electronic and zero-point Energies= -1379.888932
Sum of electronic and thermal Energies= -1379.865400
Sum of electronic and thermal Enthalpies= -1379.864455
Sum of electronic and thermal Free Energies= -1379.943822

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	263.563	90.269	167.040

M062X/6-31++G**	**Konformation 2 de**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.2388390000	0.2582190000	0.2438650000
N	-2.9939870000	0.4675650000	-0.8279630000
C	-4.3120810000	-0.0010730000	-0.7150060000
C	-4.5302750000	-0.5629490000	0.5029330000
S	-3.0945020000	-0.4950230000	1.4982370000
C	-5.7923410000	-1.1720420000	1.0325700000
C	-5.2557090000	0.1673450000	-1.8637850000
C	-2.4783330000	1.1253180000	-2.0281590000
C	-0.7681330000	0.5264380000	0.5907040000
H	-2.1587070000	0.3791170000	-2.7591420000
H	-1.6248980000	1.7380380000	-1.7421830000
H	-3.2570280000	1.7586410000	-2.4531680000
H	-6.6034540000	-1.0954870000	0.3065120000
H	-6.1128170000	-0.6665830000	1.9478980000
H	-5.6459680000	-2.2300530000	1.2677720000
H	-6.1880520000	-0.3581060000	-1.6590330000
H	-4.8365100000	-0.2440370000	-2.7871280000
H	-5.4974460000	1.2209100000	-2.0386740000
O	-0.6357130000	0.2456990000	1.8866050000

H	-0.5680020000	1.5888890000	0.2858620000
C	0.0917650000	-0.3805570000	-0.3038400000
C	1.5553350000	-0.0979910000	-0.4975840000
C	0.6222610000	-0.0616330000	-1.6831930000
H	-0.1258130000	-1.4311950000	-0.1158020000
H	0.6710860000	-0.8649420000	-2.4134820000
H	0.4376090000	0.9260250000	-2.0983550000
C	2.1568460000	1.2138090000	-0.0527630000
C	2.0390280000	1.6570270000	1.2689700000
C	2.6655050000	2.8391350000	1.6633650000
C	3.4177050000	3.5822670000	0.7545850000
C	3.5370410000	3.1440080000	-0.5637480000
C	2.9067570000	1.9671320000	-0.9616450000
H	1.4142770000	1.0921070000	1.9598160000
H	2.5592350000	3.1830000000	2.6880910000
H	3.9051460000	4.5002680000	1.0697140000
H	4.1194430000	3.7166960000	-1.2796780000
H	2.9984980000	1.6211620000	-1.9892850000
C	2.4907320000	-1.2665850000	-0.3364280000
C	3.3630240000	-1.6444110000	-1.3584500000
C	4.2528480000	-2.7020930000	-1.1755010000
C	4.2782860000	-3.3886760000	0.0372350000
C	3.4090850000	-3.0154660000	1.0628750000
C	2.5188480000	-1.9601290000	0.8773530000
H	3.3423870000	-1.1043910000	-2.3024690000
H	4.9255070000	-2.9891120000	-1.9783760000
H	4.9715860000	-4.2116130000	0.1823180000
H	3.4241030000	-3.5492560000	2.0085040000

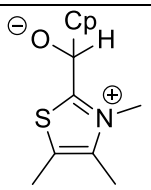
H 1.8293370000 -1.6608260000 1.6652740000

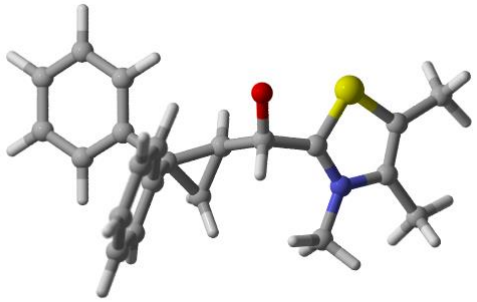
thermodynamic data

Zero-point correction= 0.398200 (Hartree/Particle)
Thermal correction to Energy= 0.420705
Thermal correction to Enthalpy= 0.421650
Thermal correction to Gibbs Free Energy= 0.344939
Sum of electronic and zero-point Energies= -1379.469591
Sum of electronic and thermal Energies= -1379.447086
Sum of electronic and thermal Enthalpies= -1379.446141
Sum of electronic and thermal Free Energies= -1379.522852

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	263.997	87.739	161.451

M062X/6-31++G** PCM freq	**Konformation 2 de**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C -2.2349690000 0.2046010000 0.3607940000

N -2.9608210000 0.6029460000 -0.6739000000

C -4.2696980000 0.0946680000 -0.7111270000

C -4.5230950000 -0.7074130000 0.3558340000

S -3.1319060000 -0.7982060000 1.3981960000

C -5.7849030000 -1.4302810000 0.7119010000

C -5.1785660000 0.4790580000 -1.8336920000

C	-2.4570140000	1.5082920000	-1.7120840000
C	-0.7685720000	0.4540880000	0.7462940000
H	-2.2030460000	0.9387960000	-2.6076220000
H	-1.5742670000	2.0177750000	-1.3330590000
H	-3.2267420000	2.2441150000	-1.9416030000
H	-6.5398610000	-1.2964970000	-0.0632160000
H	-6.1941620000	-1.0537710000	1.6531970000
H	-5.6003920000	-2.5013380000	0.8275070000
H	-6.0981040000	-0.1025240000	-1.7832170000
H	-4.7109090000	0.2886670000	-2.8036110000
H	-5.4463980000	1.5388920000	-1.7836700000
O	-0.6130320000	0.1421660000	2.0465170000
H	-0.5533100000	1.5179580000	0.4830270000
C	0.0829950000	-0.4274090000	-0.1801850000
C	1.5287750000	-0.1065260000	-0.4542300000
C	0.5251020000	-0.0743500000	-1.5796190000
H	-0.1144950000	-1.4849710000	-0.0077050000
H	0.5531410000	-0.8669290000	-2.3212970000
H	0.2827810000	0.9083680000	-1.9722840000
C	2.1110890000	1.2092160000	-0.0004930000
C	2.2082800000	1.5084400000	1.3636040000
C	2.8035160000	2.6966700000	1.7847700000
C	3.3135560000	3.5995080000	0.8495100000
C	3.2193990000	3.3092250000	-0.5110950000
C	2.6200840000	2.1207620000	-0.9309960000
H	1.7700830000	0.8186610000	2.0798820000
H	2.8636670000	2.9226000000	2.8454850000
H	3.7759270000	4.5248620000	1.1798030000

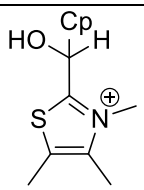
H	3.6102280000	4.0069850000	-1.2457300000
H	2.5459440000	1.8975460000	-1.9928920000
C	2.5141520000	-1.2453960000	-0.3937250000
C	3.4530380000	-1.4322650000	-1.4140130000
C	4.3876940000	-2.4642590000	-1.3385950000
C	4.3958200000	-3.3220180000	-0.2371630000
C	3.4653740000	-3.1406880000	0.7860780000
C	2.5314710000	-2.1074560000	0.7063430000
H	3.4443610000	-0.7663780000	-2.2740650000
H	5.1080620000	-2.6013340000	-2.1395180000
H	5.1216030000	-4.1273230000	-0.1786100000
H	3.4646280000	-3.8040490000	1.6457270000
H	1.8005980000	-1.9655660000	1.4988310000

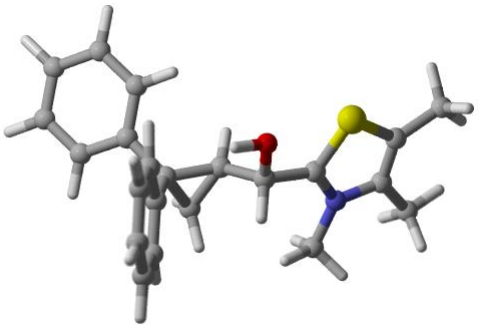
thermodynamic data

Zero-point correction= 0.399222 (Hartree/Particle)
Thermal correction to Energy= 0.422370
Thermal correction to Enthalpy= 0.423314
Thermal correction to Gibbs Free Energy= 0.345127
Sum of electronic and zero-point Energies= -1379.499436
Sum of electronic and thermal Energies= -1379.476287
Sum of electronic and thermal Enthalpies= -1379.475343
Sum of electronic and thermal Free Energies= -1379.553530

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	265.041	89.554	164.559

B3LYP/6-31G*	**Konformation 2 pr**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.2263160000	0.2886440000	0.1760160000
N	-3.0372860000	0.2690720000	-0.8826230000
C	-4.3373890000	-0.2057640000	-0.6206050000
C	-4.4982640000	-0.5430920000	0.6920660000
S	-3.0230810000	-0.2556760000	1.5844180000
C	-5.7137400000	-1.0628740000	1.4000860000
C	-5.3456900000	-0.2794280000	-1.7260710000
C	-2.6301910000	0.6981140000	-2.2319190000
C	-0.7649560000	0.6724610000	0.2301450000
H	-2.4303670000	-0.1760630000	-2.8559760000
H	-1.7316330000	1.3056590000	-2.1618400000
H	-3.4305390000	1.2927960000	-2.6723780000
H	-6.4957800000	-1.3330220000	0.6873440000
H	-6.1259800000	-0.3096990000	2.0811890000
H	-5.4777820000	-1.9542010000	1.9905290000
H	-6.2555120000	-0.7642890000	-1.3700620000
H	-4.9740000000	-0.8589760000	-2.5782550000

H	-5.6270690000	0.7164670000	-2.0888430000
H	-0.6248580000	1.6366380000	-0.2839620000
C	0.1187860000	-0.3911130000	-0.4165070000
C	1.6209300000	-0.1297390000	-0.5878150000
C	0.7142780000	-0.2153920000	-1.7940160000
H	-0.1390880000	-1.4042340000	-0.1177960000
H	0.7979050000	-1.0951090000	-2.4249570000
H	0.4974600000	0.6991680000	-2.3389390000
C	2.1757420000	1.2157240000	-0.1596020000
C	2.6279410000	1.3782410000	1.1646930000
C	3.1260290000	2.6038520000	1.6080800000
C	3.1954650000	3.6911430000	0.7337130000
C	2.7742810000	3.5366090000	-0.5861600000
C	2.2685450000	2.3106180000	-1.0285250000
H	2.6348280000	0.5227300000	1.8368100000
H	3.4733380000	2.7040640000	2.6324610000
H	3.5889940000	4.6437980000	1.0752380000
H	2.8458070000	4.3683270000	-1.2814040000
H	1.9727800000	2.2082540000	-2.0684960000
C	2.5392090000	-1.3045850000	-0.3251740000
C	3.6124410000	-1.5457530000	-1.1941650000
C	4.4927130000	-2.6003540000	-0.9575000000
C	4.3145630000	-3.4268260000	0.1548760000
C	3.2527820000	-3.1916700000	1.0282380000
C	2.3702790000	-2.1356470000	0.7888670000
H	3.7576470000	-0.9018180000	-2.0580170000
H	5.3180250000	-2.7775770000	-1.6412280000
H	5.0000900000	-4.2489860000	0.3385000000

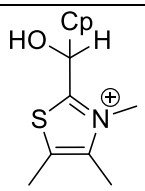
H	3.1088780000	-3.8285600000	1.8965070000
H	1.5451770000	-1.9571220000	1.4746720000
O	-0.5158930000	0.8039420000	1.6174020000
H	0.4044900000	1.1085330000	1.7250400000

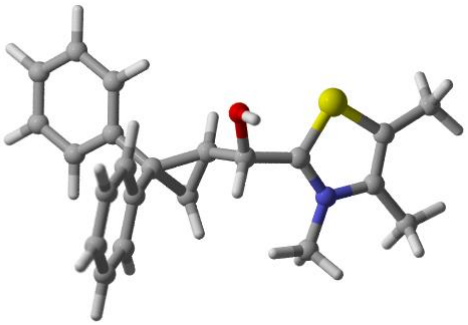
thermodynamic data

Zero-point correction= 0.410290 (Hartree/Particle)
Thermal correction to Energy= 0.434133
Thermal correction to Enthalpy= 0.435077
Thermal correction to Gibbs Free Energy= 0.354786
Sum of electronic and zero-point Energies= -1380.304745
Sum of electronic and thermal Energies= -1380.280903
Sum of electronic and thermal Enthalpies= -1380.279959
Sum of electronic and thermal Free Energies= -1380.360250

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.422	91.695	168.987

B3LYP/6-31G* PCM freq	**Konformation 2 pr**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.2429490000	0.1174460000	0.3520830000
N	-3.0130780000	0.6430970000	-0.5984880000
C	-4.3212490000	0.1273140000	-0.6502940000
C	-4.5362860000	-0.8140110000	0.3140740000

S	-3.0969640000	-1.0374710000	1.2779980000
C	-5.7752520000	-1.5988620000	0.6199880000
C	-5.2815020000	0.6293980000	-1.6829100000
C	-2.5728660000	1.6932990000	-1.5348730000
C	-0.7759620000	0.3873920000	0.6458050000
H	-2.4614340000	1.2692600000	-2.5342710000
H	-1.6247760000	2.1067390000	-1.2026620000
H	-3.3195810000	2.4868740000	-1.5499700000
H	-6.5899020000	-1.3118690000	-0.0474080000
H	-6.1057340000	-1.4252170000	1.6494210000
H	-5.5996810000	-2.6731520000	0.5003670000
H	-6.2149210000	0.0688230000	-1.6276400000
H	-4.8797810000	0.5103500000	-2.6948100000
H	-5.5189400000	1.6886680000	-1.5333060000
H	-0.5515820000	1.4463560000	0.4743720000
C	0.1197080000	-0.4862630000	-0.2119000000
C	1.5696200000	-0.1018250000	-0.4868460000
C	0.5515590000	-0.1079530000	-1.6071950000
H	-0.0566230000	-1.5457560000	-0.0412030000
H	0.5969220000	-0.9029570000	-2.3452770000
H	0.2451500000	0.8524580000	-2.0093790000
C	2.0987000000	1.2328750000	-0.0024170000
C	2.4115300000	1.4164180000	1.3549690000
C	2.9420200000	2.6241340000	1.8077910000
C	3.1775680000	3.6702070000	0.9106550000
C	2.8786350000	3.4970510000	-0.4412210000
C	2.3440750000	2.2871390000	-0.8928980000
H	2.2310000000	0.6089830000	2.0579150000

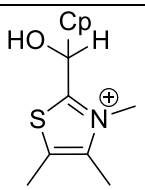
H	3.1729450000	2.7485830000	2.8624280000
H	3.5922880000	4.6104080000	1.2636460000
H	3.0628680000	4.3008990000	-1.1489090000
H	2.1247450000	2.1614690000	-1.9495500000
C	2.5889710000	-1.2200470000	-0.4399810000
C	3.5592590000	-1.3252930000	-1.4472110000
C	4.5285110000	-2.3277760000	-1.4003690000
C	4.5440210000	-3.2400790000	-0.3412750000
C	3.5844240000	-3.1418700000	0.6678930000
C	2.6141340000	-2.1376620000	0.6182250000
H	3.5508590000	-0.6175330000	-2.2724460000
H	5.2702690000	-2.3982800000	-2.1915190000
H	5.2974310000	-4.0221990000	-0.3052950000
H	3.5877960000	-3.8472150000	1.4946470000
H	1.8675830000	-2.0676700000	1.4050330000
O	-0.5278110000	0.0280030000	1.9995850000
H	-0.8514710000	0.7396210000	2.5780230000

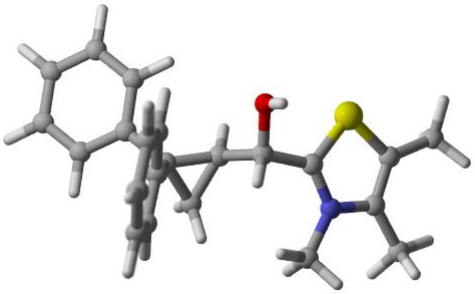
thermodynamic data

Zero-point correction= 0.410585 (Hartree/Particle)
Thermal correction to Energy= 0.434346
Thermal correction to Enthalpy= 0.435290
Thermal correction to Gibbs Free Energy= 0.355714
Sum of electronic and zero-point Energies= -1380.366829
Sum of electronic and thermal Energies= -1380.343067
Sum of electronic and thermal Enthalpies= -1380.342123
Sum of electronic and thermal Free Energies= -1380.421699

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.556	91.777	167.482

M062X/6-31++G** PCM freq	**Konformation 2 pr**





xyz-matrix

49

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.2081570000	0.1516170000	0.3500860000
N	-2.9611250000	0.5589050000	-0.6603630000
C	-4.2618400000	0.0458590000	-0.6591370000
C	-4.4836680000	-0.7686360000	0.4078430000
S	-3.0634610000	-0.8795390000	1.3903360000
C	-5.7368780000	-1.5093800000	0.7617840000
C	-5.2211770000	0.4097510000	-1.7436450000
C	-2.5019260000	1.4665580000	-1.7214120000
C	-0.7405670000	0.4438140000	0.5902690000
H	-2.2909500000	0.8906410000	-2.6236480000
H	-1.6061100000	1.9869020000	-1.3920000000
H	-3.2847830000	2.1978770000	-1.9151140000
H	-6.6141110000	-0.8950610000	0.5506290000
H	-5.7514500000	-1.7666870000	1.8219380000
H	-5.8112030000	-2.4349530000	0.1843320000
H	-6.1279250000	-0.1855050000	-1.6390660000
H	-4.7959200000	0.2077320000	-2.7303730000
H	-5.4980850000	1.4669810000	-1.6944980000

H	-0.5256600000	1.4954870000	0.3619160000
C	0.1165380000	-0.4688180000	-0.2555550000
C	1.5576870000	-0.1040870000	-0.5278440000
C	0.5566870000	-0.1206580000	-1.6523420000
H	-0.0767730000	-1.5215570000	-0.0603880000
H	0.6061670000	-0.9327650000	-2.3694650000
H	0.2622120000	0.8357740000	-2.0701200000
C	2.0714130000	1.2295510000	-0.0420660000
C	2.4289160000	1.3797550000	1.3046140000
C	2.9217460000	2.5930420000	1.7772790000
C	3.0715210000	3.6758430000	0.9076980000
C	2.7297520000	3.5325640000	-0.4348260000
C	2.2331480000	2.3148630000	-0.9062810000
H	2.3125570000	0.5388010000	1.9828500000
H	3.1899940000	2.6946120000	2.8244330000
H	3.4558040000	4.6218630000	1.2759530000
H	2.8508840000	4.3648430000	-1.1212760000
H	1.9809490000	2.2111660000	-1.9578630000
C	2.5657660000	-1.2198810000	-0.4415120000
C	3.5536300000	-1.3506730000	-1.4232020000
C	4.5124900000	-2.3578310000	-1.3302590000
C	4.4952950000	-3.2434010000	-0.2509290000
C	3.5160910000	-3.1158770000	0.7333310000
C	2.5567740000	-2.1075310000	0.6370520000
H	3.5643650000	-0.6605450000	-2.2638130000
H	5.2714600000	-2.4544170000	-2.1005470000
H	5.2410360000	-4.0289270000	-0.1791550000
H	3.4969350000	-3.8004220000	1.5756770000

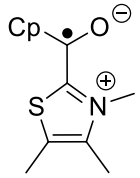
H	1.7920520000	-2.0081930000	1.4039720000
O	-0.4545860000	0.1462620000	1.9409450000
H	-0.6609440000	0.9078840000	2.4995580000

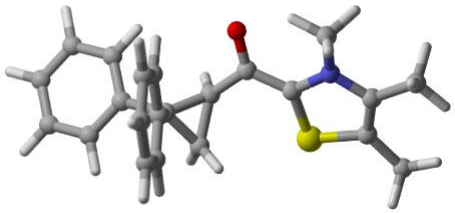
thermodynamic data

Zero-point correction= 0.412985 (Hartree/Particle)
Thermal correction to Energy= 0.436557
Thermal correction to Enthalpy= 0.437502
Thermal correction to Gibbs Free Energy= 0.358508
Sum of electronic and zero-point Energies= -1379.969770
Sum of electronic and thermal Energies= -1379.946198
Sum of electronic and thermal Enthalpies= -1379.945253
Sum of electronic and thermal Free Energies= -1380.024247

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	273.944	91.182	166.256

uB3LYP/6-31G*	**Konformation 1 radde**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0427780000	-0.4066390000	0.4334710000
N	-3.1781120000	0.2311230000	0.9196760000
C	-4.3634870000	-0.1127230000	0.2682150000
C	-4.2040710000	-1.0275630000	-0.7235620000
S	-2.5065640000	-1.4841180000	-0.8850980000

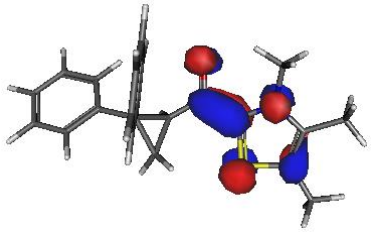
C	-5.2178220000	-1.6502910000	-1.6323580000
C	-5.6493260000	0.5259680000	0.7030750000
C	-3.1261640000	1.3197620000	1.9005700000
C	-0.7234920000	-0.3383940000	0.9767610000
H	-3.2853060000	2.2870940000	1.4079730000
H	-2.1433830000	1.2966520000	2.3670450000
H	-3.9010160000	1.1727870000	2.6578480000
H	-6.2178820000	-1.2498790000	-1.4458050000
H	-5.2659530000	-2.7385300000	-1.4971860000
H	-4.9770820000	-1.4641230000	-2.6868740000
H	-6.4778870000	0.1807180000	0.0826820000
H	-5.6056130000	1.6186400000	0.6248140000
H	-5.8891210000	0.2812420000	1.7451340000
O	-0.4524540000	0.2519350000	2.0536100000
C	0.3974920000	-1.0778110000	0.2829440000
C	1.5934700000	-0.3495160000	-0.3216970000
C	0.6619640000	-1.1542610000	-1.2040690000
H	0.6829640000	-1.9699580000	0.8403470000
H	1.0098290000	-2.1016300000	-1.6078630000
H	0.0164560000	-0.5929640000	-1.8727570000
C	1.5830650000	1.1576360000	-0.4796600000
C	1.6864510000	1.9974860000	0.6396190000
C	1.7450080000	3.3818850000	0.4856040000
C	1.7086030000	3.9541850000	-0.7883610000
C	1.6095070000	3.1292070000	-1.9085280000
C	1.5484760000	1.7428230000	-1.7520910000
H	1.6904110000	1.5592130000	1.6312350000
H	1.8170280000	4.0167690000	1.3652390000

H	1.7557950000	5.0339200000	-0.9055770000
H	1.5817830000	3.5613760000	-2.9058200000
H	1.4767330000	1.1066030000	-2.6306150000
C	2.9607610000	-0.9143490000	-0.0020080000
C	3.9049360000	-1.1192230000	-1.0171140000
C	5.1775900000	-1.6069400000	-0.7202470000
C	5.5280780000	-1.8934650000	0.6010800000
C	4.5971860000	-1.6885360000	1.6205040000
C	3.3233390000	-1.2027150000	1.3201540000
H	3.6375580000	-0.8939510000	-2.0467730000
H	5.8959150000	-1.7644280000	-1.5209830000
H	6.5192000000	-2.2744180000	0.8333410000
H	4.8610010000	-1.9080380000	2.6520550000
H	2.5973010000	-1.0436920000	2.1136760000

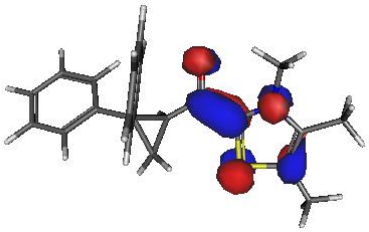
thermodynamic data

Zero-point correction= 0.385048 (Hartree/Particle)
Thermal correction to Energy= 0.408562
Thermal correction to Enthalpy= 0.409506
Thermal correction to Gibbs Free Energy= 0.328945
Sum of electronic and zero-point Energies= -1379.309602
Sum of electronic and thermal Energies= -1379.286088
Sum of electronic and thermal Enthalpies= -1379.285143
Sum of electronic and thermal Free Energies= -1379.365704

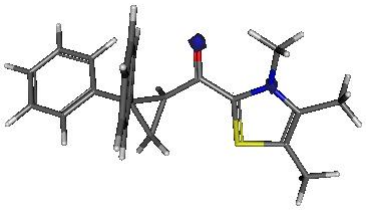
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	256.377	89.942	169.554



Alpha-SOMO

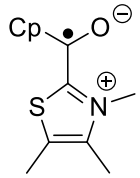
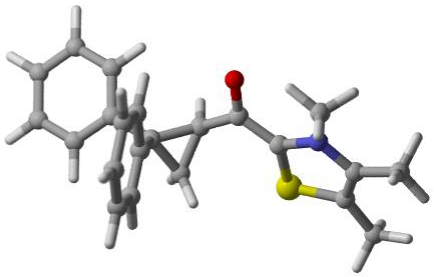


Beta-SOMO



Spin-Dichte

uB3LYP/6-31G* PCM freq	**Konformation 1 radde**

xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0573120000	-0.3746140000	0.4429390000
N	-3.1980300000	0.2723380000	0.8948770000
C	-4.3801280000	-0.1046780000	0.2532070000
C	-4.2093130000	-1.0580480000	-0.7010530000
S	-2.5078060000	-1.5063010000	-0.8340850000
C	-5.2130870000	-1.7221180000	-1.5919030000
C	-5.6708610000	0.5446180000	0.6548380000

C	-3.1705070000	1.3929350000	1.8424440000
C	-0.7392330000	-0.2804860000	0.9803550000
H	-3.3593400000	2.3368600000	1.3186460000
H	-2.1876040000	1.4117100000	2.3055040000
H	-3.9389120000	1.2492430000	2.6057780000
H	-6.2152400000	-1.3199980000	-1.4249220000
H	-5.2538510000	-2.8040040000	-1.4141780000
H	-4.9657670000	-1.5745210000	-2.6504330000
H	-6.4938000000	0.1673750000	0.0466290000
H	-5.6305440000	1.6324050000	0.5281220000
H	-5.9112260000	0.3433520000	1.7054990000
O	-0.4614360000	0.3506930000	2.0389790000
C	0.3781310000	-1.0487140000	0.3101830000
C	1.5880190000	-0.3491660000	-0.3057880000
C	0.6413350000	-1.1493100000	-1.1750600000
H	0.6459330000	-1.9393160000	0.8795370000
H	0.9760610000	-2.1057400000	-1.5678500000
H	0.0017150000	-0.5896460000	-1.8503030000
C	1.6066790000	1.1564990000	-0.4761100000
C	1.8169890000	1.9961790000	0.6295810000
C	1.8968610000	3.3795150000	0.4714980000
C	1.7745750000	3.9529890000	-0.7979160000
C	1.5721450000	3.1293020000	-1.9058220000
C	1.4914670000	1.7431740000	-1.7436760000
H	1.8967520000	1.5583270000	1.6184540000
H	2.0528950000	4.0123420000	1.3415490000
H	1.8368500000	5.0311160000	-0.9201770000
H	1.4793690000	3.5614150000	-2.8989270000

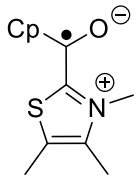
H	1.3423490000	1.1112290000	-2.6148800000
C	2.9494680000	-0.9340540000	0.0050490000
C	3.8905440000	-1.1202900000	-1.0184300000
C	5.1617820000	-1.6229840000	-0.7378480000
C	5.5153070000	-1.9444610000	0.5758690000
C	4.5880200000	-1.7600020000	1.6033390000
C	3.3153610000	-1.2585580000	1.3183400000
H	3.6211730000	-0.8705940000	-2.0418970000
H	5.8759640000	-1.7657980000	-1.5447500000
H	6.5045510000	-2.3371040000	0.7953490000
H	4.8527750000	-2.0075040000	2.6281110000
H	2.5950450000	-1.1186110000	2.1203080000

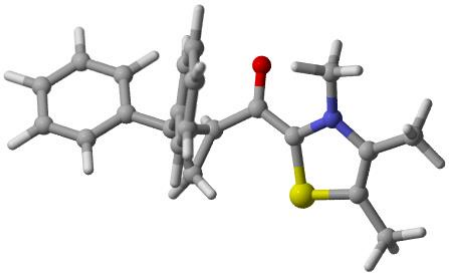
thermodynamic data

Zero-point correction= 0.384757 (Hartree/Particle)
Thermal correction to Energy= 0.408356
Thermal correction to Enthalpy= 0.409301
Thermal correction to Gibbs Free Energy= 0.328364
Sum of electronic and zero-point Energies= -1379.321353
Sum of electronic and thermal Energies= -1379.297754
Sum of electronic and thermal Enthalpies= -1379.296810
Sum of electronic and thermal Free Energies= -1379.377747

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	256.248	90.052	170.346

uM062X/6-31++G**	**Konformation 1 radde**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.8229380000	-0.6147360000	0.5033310000
N	-2.8499800000	0.2141890000	0.9008720000
C	-4.0766960000	-0.0717760000	0.3114720000
C	-4.0311960000	-1.1070860000	-0.5620650000
S	-2.4068520000	-1.7594920000	-0.6822050000
C	-5.1199580000	-1.7129360000	-1.3891850000
C	-5.2796330000	0.7447870000	0.6700660000
C	-2.5853150000	1.4279740000	1.6741600000
C	-0.5448560000	-0.6440230000	1.1336070000
H	-3.4070070000	2.1267470000	1.5233660000
H	-1.6562060000	1.8762140000	1.3151960000
H	-2.4659090000	1.1968690000	2.7329970000
H	-6.0675540000	-1.1956670000	-1.2299730000
H	-5.2657650000	-2.7692470000	-1.1410810000
H	-4.8808730000	-1.6507000000	-2.4559830000
H	-6.1813260000	0.2849380000	0.2669430000
H	-5.2122670000	1.7603160000	0.2667670000
H	-5.3929890000	0.8165170000	1.7557710000

O	-0.3453630000	-0.0836600000	2.2326610000
C	0.6176270000	-1.3299050000	0.4735160000
C	1.6016320000	-0.4628330000	-0.2925020000
C	0.8075980000	-1.5193900000	-1.0091150000
H	1.0822780000	-2.0729200000	1.1176610000
H	1.3299320000	-2.4163080000	-1.3265030000
H	0.0269900000	-1.1822280000	-1.6829790000
C	1.2369370000	0.9820420000	-0.5261910000
C	1.3342840000	1.8971300000	0.5292660000
C	1.0171570000	3.2381480000	0.3339480000
C	0.6001140000	3.6864140000	-0.9209260000
C	0.5070900000	2.7844560000	-1.9775280000
C	0.8248820000	1.4400210000	-1.7788180000
H	1.6367330000	1.5420220000	1.5103070000
H	1.0927230000	3.9353180000	1.1632130000
H	0.3534760000	4.7328450000	-1.0731830000
H	0.1891050000	3.1242900000	-2.9586040000
H	0.7537850000	0.7407680000	-2.6077370000
C	3.0698150000	-0.6938060000	-0.0550080000
C	3.9490490000	-0.7461660000	-1.1406470000
C	5.3150810000	-0.9242530000	-0.9393620000
C	5.8189780000	-1.0480580000	0.3557900000
C	4.9500490000	-0.9909950000	1.4435210000
C	3.5818060000	-0.8136860000	1.2388370000
H	3.5515510000	-0.6461410000	-2.1481830000
H	5.9867150000	-0.9671250000	-1.7914730000
H	6.8835950000	-1.1887680000	0.5153620000
H	5.3366050000	-1.0854800000	2.4538090000

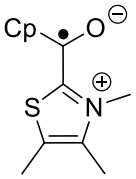
H 2.8997770000 -0.7683610000 2.0851850000

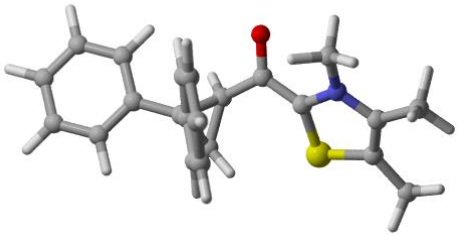
thermodynamic data

Zero-point correction= 0.387240 (Hartree/Particle)
Thermal correction to Energy= 0.410470
Thermal correction to Enthalpy= 0.411414
Thermal correction to Gibbs Free Energy= 0.332063
Sum of electronic and zero-point Energies= -1378.911599
Sum of electronic and thermal Energies= -1378.888369
Sum of electronic and thermal Enthalpies= -1378.887425
Sum of electronic and thermal Free Energies= -1378.966777

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.574	89.331	167.010

uM062X/6-31++G** PCM freq	**Konformation 1 radde**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C -1.8031430000 -0.6286760000 0.5219690000

N -2.8300890000 0.1970310000 0.9176720000

C -4.0547120000 -0.0744590000 0.3120360000

C -4.0013150000 -1.0931310000 -0.5816140000

S -2.3768570000 -1.7437440000 -0.6958660000

C -5.0807840000 -1.6767530000 -1.4367630000

C -5.2573940000 0.7398040000 0.6749450000

C -2.5819500000 1.4033570000 1.7094170000

C	-0.5376520000	-0.6869630000	1.1701490000
H	-3.3694450000	2.1261280000	1.5044300000
H	-1.6191180000	1.8227480000	1.4124980000
H	-2.5501870000	1.1733730000	2.7747660000
H	-6.0238700000	-1.1503770000	-1.2846540000
H	-5.2400860000	-2.7345630000	-1.2064130000
H	-4.8208330000	-1.6008050000	-2.4972250000
H	-6.1589010000	0.2790980000	0.2733030000
H	-5.1904640000	1.7553390000	0.2726310000
H	-5.3666420000	0.8091590000	1.7608070000
O	-0.3568560000	-0.1713310000	2.3031050000
C	0.6383130000	-1.3498750000	0.5123730000
C	1.6037180000	-0.4726020000	-0.2722030000
C	0.8307130000	-1.5562820000	-0.9677450000
H	1.1209980000	-2.0761920000	1.1627240000
H	1.3726500000	-2.4467930000	-1.2693760000
H	0.0461640000	-1.2503270000	-1.6505450000
C	1.2051940000	0.9612090000	-0.5201320000
C	1.3363100000	1.8995720000	0.5119400000
C	0.9828400000	3.2313630000	0.3110210000
C	0.4949930000	3.6476190000	-0.9301530000
C	0.3705180000	2.7237900000	-1.9656620000
C	0.7250710000	1.3885320000	-1.7603790000
H	1.7025710000	1.5719880000	1.4812410000
H	1.0835320000	3.9453620000	1.1229900000
H	0.2174580000	4.6853350000	-1.0878370000
H	-0.0006870000	3.0395790000	-2.9359880000
H	0.6286930000	0.6757210000	-2.5747610000

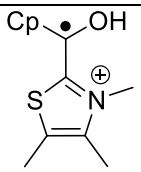
C	3.0805570000	-0.6682030000	-0.0542720000
C	3.9403120000	-0.6871510000	-1.1585520000
C	5.3152110000	-0.8300430000	-0.9868220000
C	5.8494200000	-0.9534260000	0.2975760000
C	5.0007000000	-0.9322500000	1.4034010000
C	3.6231690000	-0.7892460000	1.2274060000
H	3.5209490000	-0.5922720000	-2.1578050000
H	5.9694560000	-0.8476680000	-1.8531260000
H	6.9204010000	-1.0671450000	0.4342960000
H	5.4094010000	-1.0285770000	2.4047320000
H	2.9626120000	-0.7748890000	2.0909990000

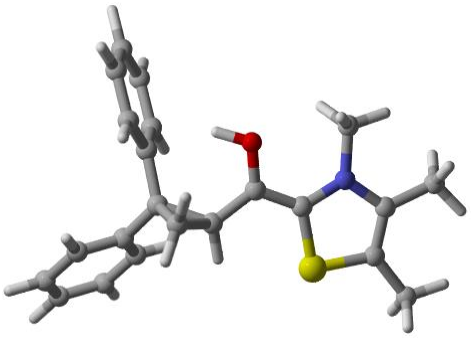
thermodynamic data

Zero-point correction= 0.386999 (Hartree/Particle)
Thermal correction to Energy= 0.410328
Thermal correction to Enthalpy= 0.411272
Thermal correction to Gibbs Free Energy= 0.330067
Sum of electronic and zero-point Energies= -1378.925563
Sum of electronic and thermal Energies= -1378.902234
Sum of electronic and thermal Enthalpies= -1378.901290
Sum of electronic and thermal Free Energies= -1378.982496

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.485	89.403	170.911

uB3LYP/6-31G*	**Konformation 1 radpr**





xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	-2.1678840000	0.0761060000	-0.2643010000
N	-3.2679910000	0.8500670000	0.0446620000
C	-4.4411020000	0.1237980000	0.2494340000
C	-4.2762180000	-1.2275330000	0.1080850000
S	-2.6212220000	-1.6141410000	-0.2994890000
C	-5.2697190000	-2.3398640000	0.2487710000
C	-5.7238850000	0.8225370000	0.5889430000
C	-3.2126950000	2.3182000000	0.1724860000
C	-0.8652850000	0.5010330000	-0.5506640000
H	-4.1836300000	2.6764350000	0.5028330000
H	-2.9633550000	2.7705160000	-0.7881510000
H	-2.4552910000	2.5984390000	0.9045940000
H	-6.2652440000	-1.9549660000	0.4775280000
H	-4.9834790000	-3.0257650000	1.0545420000
H	-5.3421390000	-2.9247730000	-0.6753020000
H	-6.5326870000	0.0977520000	0.6824700000
H	-6.0132450000	1.5383450000	-0.1885930000

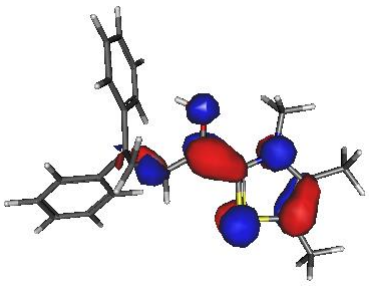
H	-5.6548500000	1.3604650000	1.5414450000
C	0.2156190000	-0.4525450000	-0.8334960000
C	1.7257010000	-0.1332470000	-0.6510120000
C	1.1462890000	-0.2329160000	-2.0281640000
H	-0.0326400000	-1.4887170000	-0.6303430000
H	1.3734430000	-1.1093610000	-2.6271920000
H	0.9897220000	0.6773760000	-2.6006770000
C	2.1563390000	1.2209550000	-0.1209520000
C	2.0875760000	1.4936220000	1.2584250000
C	2.5368900000	2.7098570000	1.7662570000
C	3.0676420000	3.6781750000	0.9079280000
C	3.1458370000	3.4216680000	-0.4600290000
C	2.6957790000	2.2008810000	-0.9722950000
H	1.6953450000	0.7382440000	1.9337070000
H	2.4800980000	2.9013710000	2.8338460000
H	3.4215950000	4.6242480000	1.3064820000
H	3.5669240000	4.1630280000	-1.1326710000
H	2.7846010000	2.0014950000	-2.0365100000
C	2.5714170000	-1.2903270000	-0.1610490000
C	3.7740250000	-1.5842950000	-0.8179740000
C	4.5938170000	-2.6168350000	-0.3645460000
C	4.2223470000	-3.3682840000	0.7525940000
C	3.0274790000	-3.0816920000	1.4133960000
C	2.2071450000	-2.0474210000	0.9590070000
H	4.0696310000	-1.0009560000	-1.6864150000
H	5.5218130000	-2.8356150000	-0.8848280000
H	4.8601750000	-4.1738200000	1.1042870000
H	2.7310660000	-3.6629960000	2.2818570000

H	1.2759430000	-1.8340510000	1.4790530000
O	-0.6441610000	1.8226010000	-0.6241960000
H	0.3222870000	2.0070420000	-0.5842610000

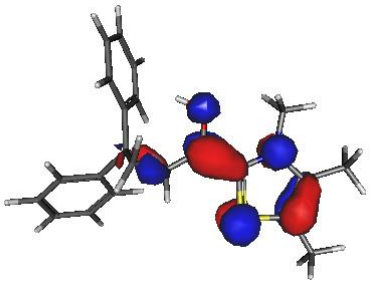
thermodynamic data

Zero-point correction= 0.397860 (Hartree/Particle)
Thermal correction to Energy= 0.421572
Thermal correction to Enthalpy= 0.422516
Thermal correction to Gibbs Free Energy= 0.341384
Sum of electronic and zero-point Energies= -1379.702033
Sum of electronic and thermal Energies= -1379.678321
Sum of electronic and thermal Enthalpies= -1379.677377
Sum of electronic and thermal Free Energies= -1379.758509

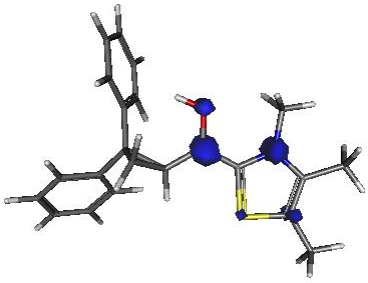
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.540	91.193	170.758



Alpha-SOMO

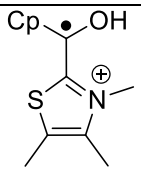
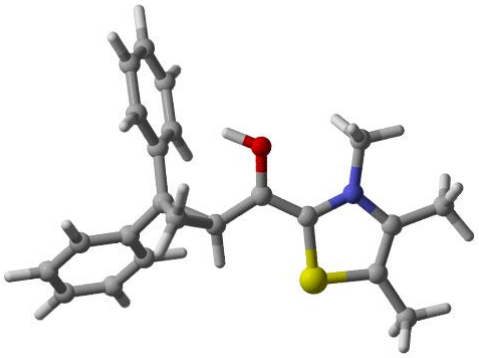


Beta-SOMO



Spin-Dichte

uB3LYP/6-31G* PCM freq	**Konformation 1 radpr**

xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	-2.1520610000	0.0799210000	-0.3155460000
N	-3.2549350000	0.8438930000	-0.0018040000
C	-4.4095520000	0.1083140000	0.2520510000
C	-4.2270520000	-1.2445960000	0.1444250000
S	-2.5779830000	-1.6173210000	-0.2900080000
C	-5.2004950000	-2.3644760000	0.3436330000
C	-5.6923440000	0.7975260000	0.6055650000
C	-3.2208430000	2.3152980000	0.0869750000
C	-0.8642560000	0.5169910000	-0.6404250000
H	-4.1860790000	2.6654560000	0.4395230000

H	-3.0128030000	2.7435550000	-0.8937990000
H	-2.4460540000	2.6230830000	0.7881940000
H	-6.1982960000	-1.9826600000	0.5659890000
H	-4.8926520000	-3.0094290000	1.1747160000
H	-5.2700860000	-2.9891570000	-0.5537960000
H	-6.4889060000	0.0645420000	0.7320800000
H	-6.0033770000	1.4942490000	-0.1800970000
H	-5.6038310000	1.3560250000	1.5439800000
C	0.2276260000	-0.4290560000	-0.9193480000
C	1.7248460000	-0.1169510000	-0.6714230000
C	1.1956310000	-0.1852220000	-2.0735950000
H	-0.0284050000	-1.4690270000	-0.7506440000
H	1.4456910000	-1.0478820000	-2.6830450000
H	1.0699070000	0.7390250000	-2.6304670000
C	2.1387100000	1.2225890000	-0.0958340000
C	1.9620740000	1.4879560000	1.2749780000
C	2.3913970000	2.6927860000	1.8270530000
C	3.0089050000	3.6553950000	1.0215900000
C	3.1928140000	3.4047800000	-0.3378090000
C	2.7633370000	2.1956100000	-0.8939040000
H	1.4884670000	0.7428590000	1.9081880000
H	2.2439410000	2.8818300000	2.8864510000
H	3.3425920000	4.5943980000	1.4535390000
H	3.6755730000	4.1440360000	-0.9703190000
H	2.9248020000	2.0032130000	-1.9506440000
C	2.5604500000	-1.2782870000	-0.1742760000
C	3.7878290000	-1.5560520000	-0.7928590000
C	4.5977250000	-2.5930650000	-0.3293200000

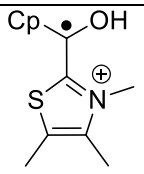
C	4.1915250000	-3.3668180000	0.7612980000
C	2.9714310000	-3.0967960000	1.3836190000
C	2.1614000000	-2.0579250000	0.9187640000
H	4.1074670000	-0.9575920000	-1.6421010000
H	5.5443060000	-2.7984920000	-0.8216200000
H	4.8206970000	-4.1761710000	1.1209580000
H	2.6457230000	-3.6950200000	2.2301090000
H	1.2107010000	-1.8588100000	1.4065080000
O	-0.6633410000	1.8410280000	-0.7562390000
H	0.2950290000	2.0460880000	-0.7246980000

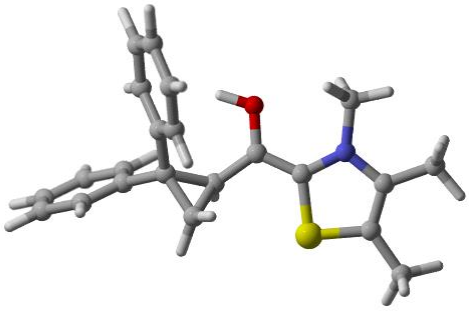
thermodynamic data

Zero-point correction= 0.397761 (Hartree/Particle)
Thermal correction to Energy= 0.421478
Thermal correction to Enthalpy= 0.422422
Thermal correction to Gibbs Free Energy= 0.341052
Sum of electronic and zero-point Energies= -1379.757964
Sum of electronic and thermal Energies= -1379.734247
Sum of electronic and thermal Enthalpies= -1379.733303
Sum of electronic and thermal Free Energies= -1379.814673

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.481	91.331	171.258

uM062X/6-31++G**	**Konformation 1 radpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.1227810000	-0.1670510000	0.2815050000
N	-3.2458460000	0.5316070000	0.6309070000
C	-4.4309310000	-0.0802470000	0.2467380000
C	-4.2348610000	-1.2638400000	-0.4069610000
S	-2.5463420000	-1.6205470000	-0.5601760000
C	-5.2497850000	-2.1970000000	-0.9914890000
C	-5.7522350000	0.5543490000	0.5425660000
C	-3.1996980000	1.8247040000	1.3290210000
C	-0.7890990000	0.1377700000	0.5560590000
H	-4.2103590000	2.2156640000	1.4000010000
H	-2.5768800000	2.5199390000	0.7670400000
H	-2.7831760000	1.6942440000	2.3277990000
H	-6.2013300000	-2.1153700000	-0.4643610000
H	-4.9163840000	-3.2340300000	-0.9108430000
H	-5.4211240000	-1.9772430000	-2.0496340000
H	-6.5563050000	-0.0871940000	0.1850700000
H	-5.8522200000	1.5201350000	0.0383530000
H	-5.8927800000	0.7048030000	1.6168010000
C	0.2877840000	-0.7970330000	0.1431180000
C	1.6172440000	-0.3033050000	-0.4075530000
C	0.6308880000	-0.9735100000	-1.3206330000
H	0.3330400000	-1.6987080000	0.7544090000
H	0.8677120000	-1.9787630000	-1.6517240000
H	0.0766290000	-0.3717900000	-2.0329500000
C	1.8413140000	1.1900820000	-0.4942500000
C	2.5684350000	1.8151130000	0.5320660000

C	2.7409440000	3.1980890000	0.5425270000
C	2.2029190000	3.9779940000	-0.4805860000
C	1.5020970000	3.3636610000	-1.5155360000
C	1.3206360000	1.9800750000	-1.5221930000
H	3.0224560000	1.2077600000	1.3117860000
H	3.3078200000	3.6630480000	1.3427350000
H	2.3435870000	5.0536980000	-0.4791340000
H	1.1014500000	3.9596650000	-2.3294290000
H	0.7860820000	1.5236150000	-2.3488260000
C	2.8370080000	-1.1002130000	-0.0210470000
C	3.8378350000	-1.2991740000	-0.9771310000
C	4.9941910000	-2.0002390000	-0.6496540000
C	5.1634450000	-2.5063990000	0.6400040000
C	4.1740840000	-2.3055840000	1.5987240000
C	3.0145370000	-1.6031290000	1.2683290000
H	3.7060220000	-0.8984940000	-1.9794810000
H	5.7633420000	-2.1528130000	-1.3996840000
H	6.0640660000	-3.0549580000	0.8951610000
H	4.3019320000	-2.6942030000	2.6038560000
H	2.2494120000	-1.4440110000	2.0250410000
O	-0.5251760000	1.2188010000	1.2880230000
H	0.4269870000	1.4314250000	1.2585440000

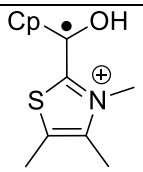
thermodynamic data

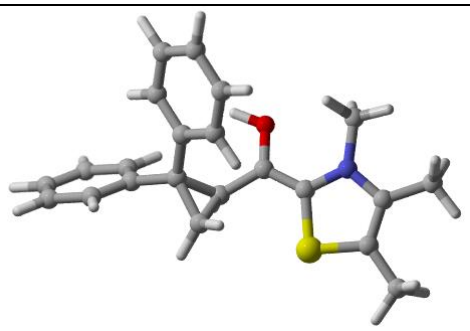
Zero-point correction= 0.400154 (Hartree/Particle)
Thermal correction to Energy= 0.422821
Thermal correction to Enthalpy= 0.423765
Thermal correction to Gibbs Free Energy= 0.345522
Sum of electronic and zero-point Energies= -1379.295243
Sum of electronic and thermal Energies= -1379.272576
Sum of electronic and thermal Enthalpies= -1379.271632

Sum of electronic and thermal Free Energies= -1379.349875

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	265.324	88.552	164.678

uM062X/6-31++G** PCM freq	**Konformation 1 radpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0028160000	-0.3801680000	0.4298680000
N	-3.0967240000	0.3783710000	0.7421200000
C	-4.2862760000	-0.1226980000	0.2479830000
C	-4.1271000000	-1.2745910000	-0.4707630000
S	-2.4661310000	-1.7468620000	-0.5317080000
C	-5.1890510000	-2.0809590000	-1.1531340000
C	-5.5871710000	0.5671870000	0.4973410000
C	-3.0065310000	1.6600890000	1.4556150000
C	-0.6868770000	-0.1873790000	0.8365330000
H	-3.9614080000	2.1694130000	1.3656710000
H	-2.2252710000	2.2674480000	0.9997150000
H	-2.7731830000	1.4876440000	2.5059760000
H	-5.9062480000	-2.4679870000	-0.4240720000
H	-4.7540630000	-2.9298010000	-1.6825820000

H	-5.7296480000	-1.4683150000	-1.8794500000
H	-6.3991320000	-0.0427980000	0.1018400000
H	-5.6232390000	1.5419670000	0.0022070000
H	-5.7585220000	0.7121080000	1.5673040000
C	0.4304510000	-1.0303490000	0.3526890000
C	1.6173620000	-0.3602410000	-0.3451340000
C	0.6821750000	-1.2538420000	-1.1133890000
H	0.6807170000	-1.8524590000	1.0229210000
H	1.0588680000	-2.2310600000	-1.3943360000
H	0.0071740000	-0.8053960000	-1.8332860000
C	1.5551740000	1.1385010000	-0.5416510000
C	2.5223170000	1.9537650000	0.0619760000
C	2.4528700000	3.3435240000	-0.0364440000
C	1.4136090000	3.9470030000	-0.7408800000
C	0.4482220000	3.1466230000	-1.3505110000
C	0.5185930000	1.7583070000	-1.2539840000
H	3.3422520000	1.4996090000	0.6101990000
H	3.2161900000	3.9511070000	0.4395030000
H	1.3574500000	5.0279720000	-0.8185280000
H	-0.3640880000	3.6019080000	-1.9085330000
H	-0.2506460000	1.1698810000	-1.7440730000
C	2.9818300000	-0.9182260000	-0.0399010000
C	3.8936360000	-1.0838880000	-1.0880550000
C	5.1784190000	-1.5594370000	-0.8387650000
C	5.5669530000	-1.8744920000	0.4650990000
C	4.6648580000	-1.7102420000	1.5142030000
C	3.3776910000	-1.2328340000	1.2610930000
H	3.5889360000	-0.8365620000	-2.1022230000

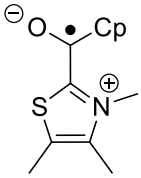
H	5.8764300000	-1.6874360000	-1.6601970000
H	6.5674850000	-2.2477990000	0.6595140000
H	4.9592050000	-1.9521570000	2.5306400000
H	2.6814460000	-1.1015320000	2.0859830000
O	-0.4357310000	0.7409180000	1.7661580000
H	0.5202940000	0.8941830000	1.8403030000

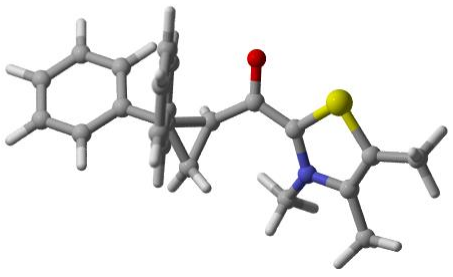
thermodynamic data

Zero-point correction= 0.399752 (Hartree/Particle)
Thermal correction to Energy= 0.423206
Thermal correction to Enthalpy= 0.424150
Thermal correction to Gibbs Free Energy= 0.344170
Sum of electronic and zero-point Energies= -1379.354493
Sum of electronic and thermal Energies= -1379.331039
Sum of electronic and thermal Enthalpies= -1379.330094
Sum of electronic and thermal Free Energies= -1379.410074

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	265.566	90.957	168.332

uB3LYP/6-31G* PCM freq	**Konformation 2 radde**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0269040000	-0.5122980000	0.6225860000
N	-2.6782720000	-1.2582770000	-0.3426740000
C	-4.0068740000	-0.8643880000	-0.5686860000

C	-4.4269420000	0.1371710000	0.2480990000
S	-3.1440280000	0.6305590000	1.3593240000
C	-5.7569420000	0.8223650000	0.3135160000
C	-4.7996460000	-1.5571040000	-1.6372690000
C	-2.1898850000	-2.5482340000	-0.8424160000
C	-0.6807330000	-0.4837130000	1.0877130000
H	-1.2710600000	-2.8092760000	-0.3261030000
H	-1.9948250000	-2.5048530000	-1.9174310000
H	-2.9337720000	-3.3252260000	-0.6456060000
H	-6.4654220000	0.3833950000	-0.3930310000
H	-5.6703010000	1.8913340000	0.0825430000
H	-6.1931900000	0.7410830000	1.3168550000
H	-5.7649240000	-1.0676420000	-1.7736760000
H	-4.9931330000	-2.6075120000	-1.3888890000
H	-4.2736180000	-1.5366550000	-2.5985530000
O	-0.4344740000	0.1627270000	2.1453630000
C	0.4673430000	-1.1556930000	0.3762930000
C	1.5739190000	-0.3263890000	-0.2828790000
C	0.6644060000	-1.1977920000	-1.1194010000
H	0.8487880000	-2.0194650000	0.9206060000
H	1.0710110000	-2.1058270000	-1.5566420000
H	-0.0712980000	-0.6936880000	-1.7396610000
C	1.4455710000	1.1773090000	-0.4128200000
C	1.6591290000	2.0079340000	0.6991290000
C	1.6057390000	3.3958630000	0.5749080000
C	1.3434030000	3.9834150000	-0.6665370000
C	1.1351530000	3.1694640000	-1.7803860000
C	1.1884720000	1.7784320000	-1.6524290000

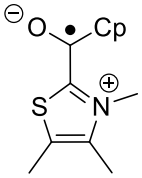
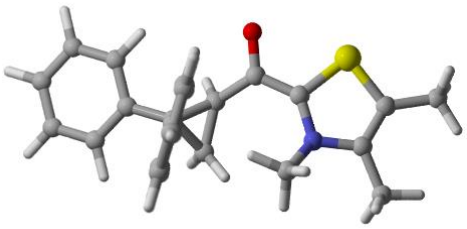
H	1.8491570000	1.5579190000	1.6674980000
H	1.7672520000	4.0209380000	1.4494680000
H	1.3021830000	5.0651740000	-0.7626090000
H	0.9340820000	3.6133010000	-2.7520620000
H	1.0333740000	1.1556290000	-2.5291800000
C	2.9969170000	-0.7904480000	-0.0535150000
C	3.9000320000	-0.8543800000	-1.1252200000
C	5.2233900000	-1.2477140000	-0.9222240000
C	5.6682060000	-1.5799330000	0.3607290000
C	4.7796230000	-1.5155690000	1.4356820000
C	3.4545520000	-1.1235450000	1.2283530000
H	3.5599340000	-0.5960050000	-2.1251640000
H	5.9071670000	-1.2971000000	-1.7657510000
H	6.6981840000	-1.8878340000	0.5195820000
H	5.1152750000	-1.7717980000	2.4372260000
H	2.7656940000	-1.0772480000	2.0678360000

thermodynamic data

Zero-point correction= 0.384881 (Hartree/Particle)
Thermal correction to Energy= 0.408476
Thermal correction to Enthalpy= 0.409421
Thermal correction to Gibbs Free Energy= 0.328746
Sum of electronic and zero-point Energies= -1379.317556
Sum of electronic and thermal Energies= -1379.293961
Sum of electronic and thermal Enthalpies= -1379.293017
Sum of electronic and thermal Free Energies= -1379.373692

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	256.323	90.045	169.795

uM062X/6-31++G**	**Konformation 2 radde**

xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0002410000	-0.6926830000	0.2448520000
N	-2.4709750000	0.1649920000	-0.7314840000
C	-3.8684030000	0.0961080000	-0.8815370000
C	-4.4751890000	-0.7167230000	0.0106410000
S	-3.3177140000	-1.4530780000	1.1066870000
C	-5.9278550000	-1.0445430000	0.1570280000
C	-4.5030560000	0.9096950000	-1.9662020000
C	-1.8385610000	1.4679320000	-0.9668390000
C	-0.6856750000	-1.1597160000	0.5607350000
H	-1.7673610000	1.6782750000	-2.0374210000
H	-0.8449820000	1.4737110000	-0.5268440000
H	-2.4231640000	2.2574570000	-0.4803690000
H	-6.5406650000	-0.4359050000	-0.5101010000
H	-6.2602450000	-0.8563120000	1.1828470000
H	-6.1211890000	-2.0982580000	-0.0666830000
H	-5.5640670000	0.6749960000	-2.0494370000
H	-4.0315010000	0.6984250000	-2.9312620000
H	-4.4110700000	1.9840500000	-1.7755260000
O	-0.5340460000	-1.7626900000	1.6432960000
C	0.4909990000	-1.1990370000	-0.3851060000
C	1.6054870000	-0.1813320000	-0.4711470000

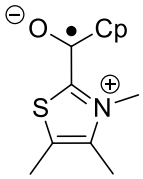
C	0.7573590000	-0.4850500000	-1.6824010000
H	0.8689640000	-2.2189490000	-0.3593360000
H	1.2035750000	-1.0777350000	-2.4750920000
H	0.0732080000	0.2800320000	-2.0274040000
C	1.4410590000	1.1595800000	0.1944520000
C	1.0786170000	1.2530650000	1.5414880000
C	0.9349830000	2.5021860000	2.1459910000
C	1.1593320000	3.6673010000	1.4146840000
C	1.5360570000	3.5804010000	0.0739410000
C	1.6768320000	2.3329630000	-0.5291920000
H	0.8879460000	0.3445130000	2.1073490000
H	0.6418070000	2.5621470000	3.1896900000
H	1.0436750000	4.6384030000	1.8861450000
H	1.7191750000	4.4838240000	-0.5001410000
H	1.9595650000	2.2621060000	-1.5772090000
C	3.0135220000	-0.7131960000	-0.4162620000
C	3.9325730000	-0.4217880000	-1.4261450000
C	5.2435440000	-0.8889250000	-1.3460010000
C	5.6466450000	-1.6516670000	-0.2510510000
C	4.7332390000	-1.9473820000	0.7605140000
C	3.4234800000	-1.4806120000	0.6775910000
H	3.6153620000	0.1690210000	-2.2824580000
H	5.9488300000	-0.6606660000	-2.1395300000
H	6.6664420000	-2.0186470000	-0.1889380000
H	5.0392190000	-2.5463580000	1.6127930000
H	2.7006170000	-1.7177730000	1.4557590000

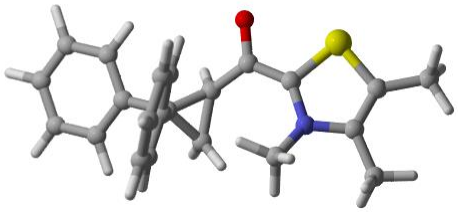
thermodynamic data

Zero-point correction= 0.387167 (Hartree/Particle)
Thermal correction to Energy= 0.410414
Thermal correction to Enthalpy= 0.411358
Thermal correction to Gibbs Free Energy= 0.332777
Sum of electronic and zero-point Energies= -1378.896781
Sum of electronic and thermal Energies= -1378.873534
Sum of electronic and thermal Enthalpies= -1378.872590
Sum of electronic and thermal Free Energies= -1378.951171

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.539	89.369	165.388

uM062X/6-31++G** PCM freq	**Konformation 2 radde**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0147080000	-0.6975660000	0.2441430000
N	-2.4876820000	0.1852960000	-0.6978460000
C	-3.8829940000	0.1353590000	-0.8554690000
C	-4.4993210000	-0.7019700000	0.0099970000
S	-3.3424420000	-1.4804650000	1.0732870000
C	-5.9549850000	-1.0153630000	0.1556770000
C	-4.5118280000	0.9896640000	-1.9111280000
C	-1.8069560000	1.4453730000	-1.0164040000
C	-0.7084230000	-1.1749470000	0.5660460000
H	-1.6992630000	1.5706730000	-2.0961160000
H	-0.8296310000	1.4541640000	-0.5420630000
H	-2.3856560000	2.2810910000	-0.6116060000

H	-6.5579050000	-0.3908480000	-0.5047020000
H	-6.2843960000	-0.8355450000	1.1836410000
H	-6.1599540000	-2.0634780000	-0.0818040000
H	-5.5712450000	0.7551700000	-2.0073210000
H	-4.0347440000	0.8171020000	-2.8803710000
H	-4.4223300000	2.0545940000	-1.6758140000
O	-0.5853050000	-1.8157520000	1.6445250000
C	0.4845950000	-1.2178290000	-0.3557070000
C	1.6026670000	-0.1998660000	-0.4550970000
C	0.7587160000	-0.5218570000	-1.6617860000
H	0.8653960000	-2.2367100000	-0.3170220000
H	1.2073240000	-1.1284940000	-2.4421690000
H	0.0804310000	0.2382390000	-2.0255200000
C	1.4466600000	1.1495880000	0.1948150000
C	1.0815820000	1.2624520000	1.5399500000
C	0.9567910000	2.5190240000	2.1346520000
C	1.2017140000	3.6735550000	1.3917670000
C	1.5785330000	3.5674860000	0.0515110000
C	1.7014730000	2.3121240000	-0.5406530000
H	0.8764530000	0.3624830000	2.1143500000
H	0.6624480000	2.5944680000	3.1770610000
H	1.0989980000	4.6508220000	1.8531420000
H	1.7728760000	4.4623040000	-0.5319570000
H	1.9817040000	2.2282400000	-1.5882640000
C	3.0147890000	-0.7238700000	-0.4039440000
C	3.8904290000	-0.5259020000	-1.4745210000
C	5.2097660000	-0.9745940000	-1.4028550000
C	5.6654560000	-1.6258870000	-0.2571180000

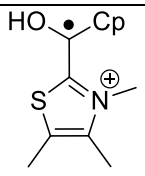
C	4.7957450000	-1.8286570000	0.8159480000
C	3.4788360000	-1.3792320000	0.7411370000
H	3.5341960000	-0.0219850000	-2.3700000000
H	5.8802010000	-0.8174490000	-2.2424560000
H	6.6908830000	-1.9778360000	-0.2015190000
H	5.1421710000	-2.3404830000	1.7087490000
H	2.7961030000	-1.5426510000	1.5721390000

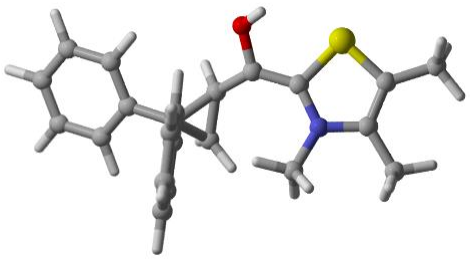
thermodynamic data

Zero-point correction= 0.386934 (Hartree/Particle)
Thermal correction to Energy= 0.410141
Thermal correction to Enthalpy= 0.411086
Thermal correction to Gibbs Free Energy= 0.332522
Sum of electronic and zero-point Energies= -1378.913041
Sum of electronic and thermal Energies= -1378.889833
Sum of electronic and thermal Enthalpies= -1378.888889
Sum of electronic and thermal Free Energies= -1378.967453

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.368	89.462	165.351

uB3LYP/6-31G*	**Konformation 2 radpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	-2.0476820000	-0.7360160000	0.1159640000

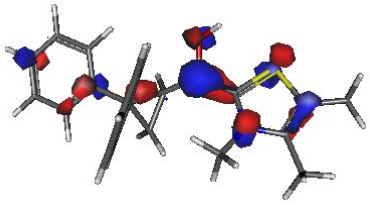
N	-2.5877210000	0.2952610000	-0.6018000000
C	-3.9839760000	0.2844390000	-0.6830550000
C	-4.5626340000	-0.7289150000	0.0285850000
S	-3.3415240000	-1.7243080000	0.7817580000
C	-6.0097670000	-1.0677560000	0.2150740000
C	-4.6901520000	1.3401380000	-1.4789000000
C	-1.8271180000	1.4689890000	-1.0559370000
C	-0.7110460000	-1.1309450000	0.3475400000
H	-1.7060320000	1.4534030000	-2.1417980000
H	-0.8566200000	1.4822620000	-0.5662970000
H	-2.3678310000	2.3722260000	-0.7686650000
H	-6.6493450000	-0.3598890000	-0.3156240000
H	-6.2862140000	-1.0378990000	1.2751900000
H	-6.2351670000	-2.0723730000	-0.1600640000
H	-5.7465820000	1.0913720000	-1.5841530000
H	-4.2681970000	1.4306560000	-2.4852890000
H	-4.6300820000	2.3237380000	-0.9977110000
C	0.5007890000	-1.1532440000	-0.4968340000
C	1.6620310000	-0.1284140000	-0.5109470000
C	0.8567510000	-0.4116600000	-1.7576410000
H	0.8859400000	-2.1721410000	-0.4579620000
H	1.3180900000	-1.0114780000	-2.5370900000
H	0.2093440000	0.3688560000	-2.1351790000
C	1.4823480000	1.2066030000	0.1765520000
C	1.1784810000	1.2845310000	1.5440020000
C	1.0785050000	2.5226250000	2.1818940000
C	1.2866860000	3.7010690000	1.4630160000
C	1.5978260000	3.6352900000	0.1031440000

C	1.6970170000	2.3974360000	-0.5339830000
H	1.0392800000	0.3710320000	2.1159720000
H	0.8479080000	2.5655790000	3.2427480000
H	1.2149750000	4.6638490000	1.9604950000
H	1.7715080000	4.5471520000	-0.4612660000
H	1.9514090000	2.3531100000	-1.5900200000
C	3.0557030000	-0.7074970000	-0.4088570000
C	4.0076320000	-0.4257580000	-1.3969030000
C	5.3078210000	-0.9203160000	-1.2886560000
C	5.6700220000	-1.7034240000	-0.1914440000
C	4.7264190000	-1.9904870000	0.7967450000
C	3.4274920000	-1.4934960000	0.6893500000
H	3.7319430000	0.1822550000	-2.2551160000
H	6.0357690000	-0.6961940000	-2.0631350000
H	6.6811370000	-2.0911550000	-0.1086940000
H	5.0003380000	-2.6036900000	1.6505380000
H	2.6946010000	-1.7268760000	1.4579790000
O	-0.5122310000	-1.9448920000	1.4200380000
H	-1.1787830000	-1.8117140000	2.1170730000

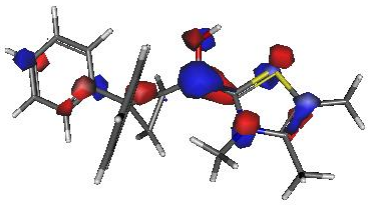
thermodynamic data

Zero-point correction= 0.397639 (Hartree/Particle)
Thermal correction to Energy= 0.421331
Thermal correction to Enthalpy= 0.422276
Thermal correction to Gibbs Free Energy= 0.342211
Sum of electronic and zero-point Energies= -1379.673633
Sum of electronic and thermal Energies= -1379.649941
Sum of electronic and thermal Enthalpies= -1379.648997
Sum of electronic and thermal Free Energies= -1379.729061

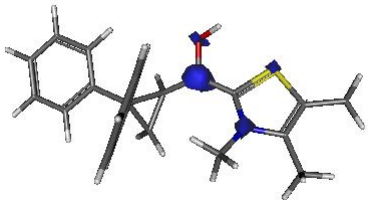
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.389	91.523	168.510



Alpha-SOMO

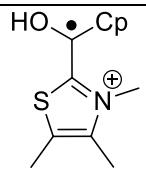
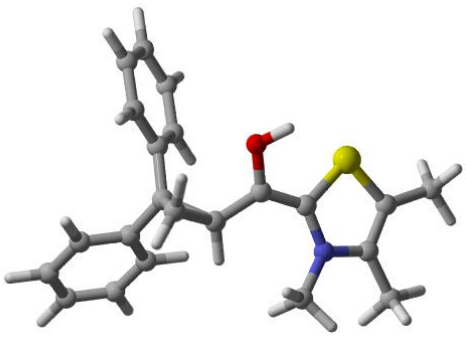


Beta-SOMO



Spin-Dichte

uB3LYP/6-31G* PCM freq	**Konformation 2 radpr**

xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C -2.0964780000 0.1520950000 -0.5661340000

N	-2.7314010000	-1.0578830000	-0.4376910000
C	-3.9635020000	-0.9977070000	0.2124410000
C	-4.3356400000	0.2734750000	0.5550790000
S	-3.1036610000	1.4238830000	0.0966790000
C	-5.5787540000	0.7593710000	1.2326250000
C	-4.7444940000	-2.2512460000	0.4626550000
C	-2.2512120000	-2.2977150000	-1.0668300000
C	-0.8296380000	0.4512190000	-1.0946170000
H	-1.5575230000	-2.8255720000	-0.4072790000
H	-1.7663060000	-2.0549700000	-2.0117630000
H	-3.1034400000	-2.9406700000	-1.2742880000
H	-6.2343290000	-0.0744300000	1.4898410000
H	-6.1379940000	1.4392440000	0.5800190000
H	-5.3414320000	1.3019180000	2.1544140000
H	-5.5892290000	-2.0424940000	1.1192550000
H	-4.1253650000	-3.0143380000	0.9448820000
H	-5.1446180000	-2.6721800000	-0.4669850000
C	0.3090520000	-0.4586370000	-1.2117930000
C	1.7455410000	-0.0749260000	-0.7197720000
C	1.4442240000	-0.1770250000	-2.1837110000
H	0.0863830000	-1.4989740000	-1.0307050000
H	1.8310320000	-1.0275460000	-2.7371630000
H	1.3649450000	0.7455980000	-2.7493380000
C	2.0249630000	1.2701260000	-0.0919080000
C	1.6023660000	1.5427450000	1.2180060000
C	1.9085030000	2.7594390000	1.8267550000
C	2.6525760000	3.7217650000	1.1380310000
C	3.0862680000	3.4562510000	-0.1618870000

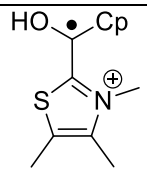
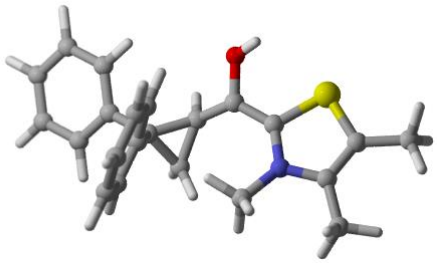
C	2.7741130000	2.2390140000	-0.7717430000
H	1.0296090000	0.7979870000	1.7641830000
H	1.5671070000	2.9559050000	2.8395120000
H	2.8934100000	4.6690850000	1.6123980000
H	3.6694900000	4.1953750000	-0.7044720000
H	3.1189600000	2.0408250000	-1.7827140000
C	2.5139090000	-1.2159230000	-0.0834830000
C	3.8264590000	-1.4763750000	-0.5036910000
C	4.5762480000	-2.4910390000	0.0921530000
C	4.0242660000	-3.2613980000	1.1191550000
C	2.7186900000	-3.0097070000	1.5445660000
C	1.9694930000	-1.9929650000	0.9473810000
H	4.2601980000	-0.8801000000	-1.3023730000
H	5.5905990000	-2.6814950000	-0.2478290000
H	4.6068220000	-4.0532680000	1.5816250000
H	2.2794140000	-3.6047980000	2.3405370000
H	0.9527230000	-1.8084460000	1.2844550000
O	-0.5481530000	1.7337850000	-1.4074700000
H	-1.3485830000	2.2610910000	-1.5791450000

thermodynamic data

Zero-point correction= 0.397635 (Hartree/Particle)
Thermal correction to Energy= 0.421378
Thermal correction to Enthalpy= 0.422322
Thermal correction to Gibbs Free Energy= 0.341253
Sum of electronic and zero-point Energies= -1379.749015
Sum of electronic and thermal Energies= -1379.725271
Sum of electronic and thermal Enthalpies= -1379.724327
Sum of electronic and thermal Free Energies= -1379.805396

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.419	91.708	170.624

uM062X/6-31++G**	**Konformation 2 radpr**

xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	-1.9991000000	-0.7627860000	0.1226820000
N	-2.5167980000	0.2683640000	-0.5934380000
C	-3.9067060000	0.2544820000	-0.7010700000
C	-4.4903960000	-0.7623300000	-0.0095070000
S	-3.2880900000	-1.7540230000	0.7484980000
C	-5.9404260000	-1.1026730000	0.1354750000
C	-4.5989700000	1.3157660000	-1.4958090000
C	-1.7647270000	1.4663990000	-0.9844790000
C	-0.6639040000	-1.1525700000	0.3672280000
H	-1.6277720000	1.4992020000	-2.0670970000
H	-0.8030210000	1.4666130000	-0.4764860000
H	-2.3238840000	2.3457990000	-0.6624340000
H	-6.5636480000	-0.2680060000	-0.1866960000
H	-6.1849220000	-1.3169740000	1.1788380000
H	-6.2004960000	-1.9808490000	-0.4624150000
H	-5.6334350000	1.0282720000	-1.6793500000
H	-4.1155470000	1.4570390000	-2.4657640000
H	-4.6033220000	2.2754820000	-0.9694190000
C	0.5425070000	-1.1685330000	-0.4828420000

C	1.6612640000	-0.1282200000	-0.5015100000
C	0.8622820000	-0.4156130000	-1.7429080000
H	0.9383110000	-2.1836260000	-0.4514520000
H	1.3339200000	-1.0002100000	-2.5260500000
H	0.1896650000	0.3525090000	-2.1000550000
C	1.4377010000	1.1893510000	0.1907110000
C	1.0514090000	1.2418570000	1.5329910000
C	0.8403790000	2.4698820000	2.1604950000
C	1.0252860000	3.6563020000	1.4520580000
C	1.4352750000	3.6113440000	0.1190370000
C	1.6422440000	2.3837720000	-0.5067620000
H	0.9267680000	0.3162670000	2.0903080000
H	0.5416960000	2.4999470000	3.2036530000
H	0.8655570000	4.6124580000	1.9396330000
H	1.5985610000	4.5328690000	-0.4307520000
H	1.9591310000	2.3477310000	-1.5464860000
C	3.0659130000	-0.6620180000	-0.4042360000
C	3.9950090000	-0.3885050000	-1.4092570000
C	5.3057420000	-0.8491610000	-1.2976620000
C	5.6936290000	-1.5859740000	-0.1801280000
C	4.7687010000	-1.8620540000	0.8262340000
C	3.4599700000	-1.4001250000	0.7144970000
H	3.6924440000	0.1842440000	-2.2828150000
H	6.0222240000	-0.6362810000	-2.0844900000
H	6.7128880000	-1.9481690000	-0.0952560000
H	5.0656980000	-2.4398410000	1.6954770000
H	2.7347170000	-1.6201710000	1.4952870000
O	-0.4616000000	-1.9463610000	1.4387760000

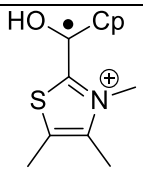
H -1.1442040000 -1.8591440000 2.1202730000

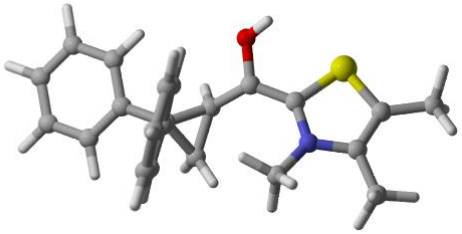
thermodynamic data

Zero-point correction= 0.400435 (Hartree/Particle)
Thermal correction to Energy= 0.423747
Thermal correction to Enthalpy= 0.424691
Thermal correction to Gibbs Free Energy= 0.345864
Sum of electronic and zero-point Energies= -1379.270948
Sum of electronic and thermal Energies= -1379.247636
Sum of electronic and thermal Enthalpies= -1379.246691
Sum of electronic and thermal Free Energies= -1379.325518

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	265.905	90.671	165.905

uM062X/6-31++G** PCM freq	**Konformation 2 radpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C -2.0443730000 -0.7092980000 0.1619360000

N -2.5727380000 0.2855130000 -0.5847180000

C -3.9586510000 0.2449790000 -0.7039370000

C -4.5243530000 -0.7678170000 0.0098710000

S -3.3089960000 -1.7075540000 0.8064690000

C -5.9687480000 -1.1312360000 0.1465200000

C -4.6622150000 1.2753840000 -1.5261200000

C -1.8283230000 1.4695990000 -1.0251770000

C	-0.6932900000	-1.0367930000	0.4297720000
H	-1.6875550000	1.4543350000	-2.1067770000
H	-0.8711770000	1.4922460000	-0.5092080000
H	-2.3958040000	2.3564750000	-0.7436570000
H	-6.6005550000	-0.2983440000	-0.1627390000
H	-6.2087280000	-1.3703250000	1.1848310000
H	-6.2114430000	-2.0016800000	-0.4691810000
H	-5.6923180000	0.9689410000	-1.7019650000
H	-4.1751340000	1.3977900000	-2.4964230000
H	-4.6763370000	2.2460350000	-1.0207950000
C	0.4846260000	-1.1220290000	-0.4616490000
C	1.6429840000	-0.1364330000	-0.5077690000
C	0.8105510000	-0.3955760000	-1.7345860000
H	0.8259080000	-2.1577760000	-0.4447310000
H	1.2422520000	-1.0056290000	-2.5209930000
H	0.1748900000	0.4043690000	-2.0867990000
C	1.4950300000	1.1985380000	0.1739400000
C	1.2173820000	1.2757290000	1.5426580000
C	1.0998340000	2.5157240000	2.1703250000
C	1.2662350000	3.6898840000	1.4356280000
C	1.5558160000	3.6196210000	0.0724170000
C	1.6707950000	2.3794620000	-0.5538030000
H	1.0903220000	0.3605140000	2.1161690000
H	0.8765410000	2.5637420000	3.2315750000
H	1.1709420000	4.6550720000	1.9229050000
H	1.6886530000	4.5302030000	-0.5034680000
H	1.8859200000	2.3242890000	-1.6182820000
C	3.0293870000	-0.7184480000	-0.4274240000

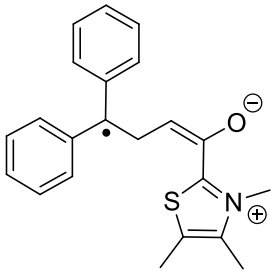
C	3.9740940000	-0.4339820000	-1.4165500000
C	5.2705580000	-0.9387510000	-1.3191920000
C	5.6320670000	-1.7319440000	-0.2297690000
C	4.6924390000	-2.0199030000	0.7605270000
C	3.3971480000	-1.5144770000	0.6611830000
H	3.6903980000	0.1802120000	-2.2677510000
H	5.9964360000	-0.7165620000	-2.0953500000
H	6.6400240000	-2.1277070000	-0.1550800000
H	4.9666090000	-2.6402510000	1.6081080000
H	2.6597230000	-1.7442030000	1.4274500000
O	-0.4598550000	-1.7539960000	1.5499640000
H	-1.1115920000	-1.5909000000	2.2491730000

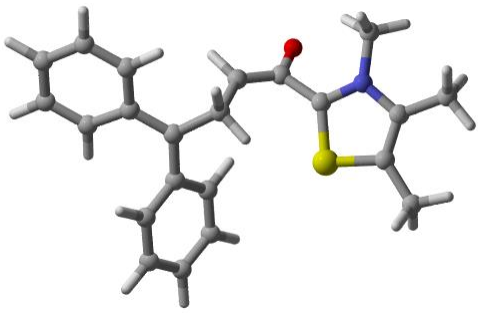
thermodynamic data

Zero-point correction= 0.399950 (Hartree/Particle)
Thermal correction to Energy= 0.423356
Thermal correction to Enthalpy= 0.424300
Thermal correction to Gibbs Free Energy= 0.345143
Sum of electronic and zero-point Energies= -1379.335128
Sum of electronic and thermal Energies= -1379.311722
Sum of electronic and thermal Enthalpies= -1379.310778
Sum of electronic and thermal Free Energies= -1379.389934

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	265.660	90.786	166.600

uB3LYP/6-31G*	**Konformation 1offende**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	4.0387460000	0.8612490000	-0.6304210000
C	4.4887940000	-0.4081610000	-0.4408270000
N	3.5182750000	-1.2445800000	0.1337460000
C	2.3201860000	-0.6765460000	0.3733830000
S	2.3778890000	0.9914070000	-0.0806180000
C	3.7578350000	-2.6679100000	0.4283190000
H	3.1444320000	-2.9027600000	1.3046440000
H	4.8163310000	-2.8192630000	0.6360710000
H	3.4572710000	-3.2776490000	-0.4291520000
C	4.7418630000	2.0561850000	-1.1997220000
H	5.7526550000	1.7998430000	-1.5271180000
H	4.8264910000	2.8594500000	-0.4581510000
H	4.2031950000	2.4612050000	-2.0642730000
C	5.8445400000	-0.9538460000	-0.7743720000
H	5.7776740000	-1.8304080000	-1.4286080000
H	6.3960350000	-1.2505650000	0.1258940000
H	6.4394330000	-0.1983190000	-1.2903120000

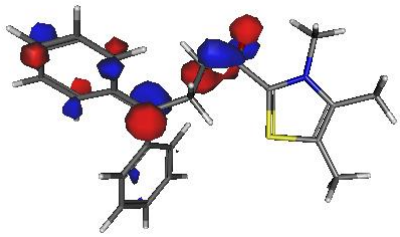
C	1.2194710000	-1.3689100000	1.1533440000
O	1.6617430000	-1.9407500000	2.2035450000
C	-0.0634390000	-1.3927170000	0.6445230000
C	-0.6409440000	-0.7288130000	-0.5856500000
H	-0.7682300000	-1.4644480000	-1.3952540000
H	0.0420240000	0.0219050000	-0.9925060000
C	-1.9834930000	-0.0639070000	-0.3126080000
C	-3.2039350000	-0.8283240000	-0.3520030000
C	-4.4272680000	-0.3191020000	0.1757510000
C	-5.6006640000	-1.0590930000	0.1457400000
C	-5.6201500000	-2.3480060000	-0.3996340000
C	-4.4306910000	-2.8864530000	-0.9008550000
C	-3.2512680000	-2.1535930000	-0.8738670000
H	-4.4343770000	0.6616360000	0.6374430000
H	-6.5090430000	-0.6331810000	0.5650960000
H	-6.5401310000	-2.9255530000	-0.4207170000
H	-4.4224420000	-3.8916500000	-1.3154610000
H	-2.3506140000	-2.6119840000	-1.2657930000
C	-1.9699920000	1.3698980000	0.0132790000
C	-2.8644610000	2.2765260000	-0.5984280000
C	-2.8023390000	3.6431180000	-0.3354440000
C	-1.8490410000	4.1511180000	0.5506210000
C	-0.9563800000	3.2722090000	1.1686430000
C	-1.0122660000	1.9054580000	0.9034240000
H	-3.5945350000	1.8998710000	-1.3086840000
H	-3.4975400000	4.3158730000	-0.8318710000
H	-1.8050740000	5.2169170000	0.7587090000
H	-0.2197470000	3.6505680000	1.8734290000

H	-0.3403170000	1.2250070000	1.4177300000
H	-0.7522130000	-2.0132220000	1.2150220000

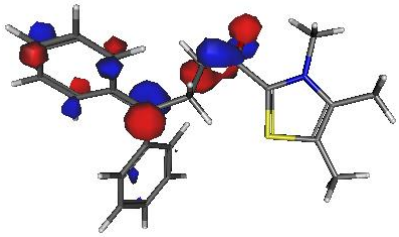
thermodynamic data

Zero-point correction= 0.383314 (Hartree/Particle)
Thermal correction to Energy= 0.407173
Thermal correction to Enthalpy= 0.408117
Thermal correction to Gibbs Free Energy= 0.326466
Sum of electronic and zero-point Energies= -1379.273917
Sum of electronic and thermal Energies= -1379.250059
Sum of electronic and thermal Enthalpies= -1379.249115
Sum of electronic and thermal Free Energies= -1379.330766

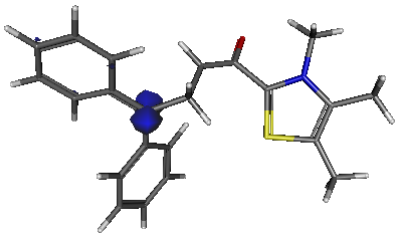
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	255.505	90.941	171.849



Alpha-SOMO

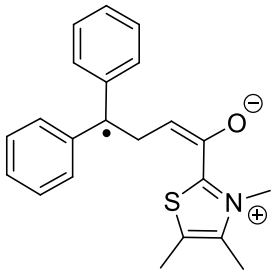


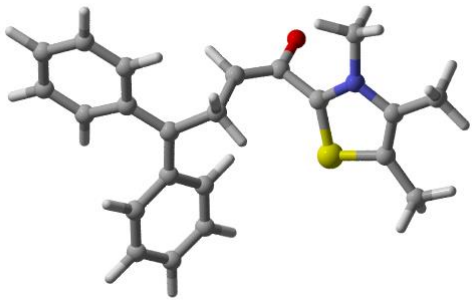
Beta-SOMO



Spin-Dichte

uB3LYP/6-31G*/PCM	**Konformation 1offende**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	4.1892670000	0.8315950000	-0.4291070000
C	4.4278640000	-0.5052810000	-0.5349080000
N	3.3625760000	-1.2753230000	-0.0361220000
C	2.3247870000	-0.5863400000	0.4506350000
S	2.6193310000	1.0989050000	0.3075080000
C	3.3872460000	-2.7451340000	0.0281170000
H	3.7430040000	-3.0554260000	1.0120320000
H	4.0341540000	-3.1296080000	-0.7573820000
H	2.3719120000	-3.1119240000	-0.1189370000
C	5.0350430000	1.9949650000	-0.8487670000
H	6.0112490000	1.6576240000	-1.2039170000
H	5.2005000000	2.6849200000	-0.0143180000
H	4.5587470000	2.5591870000	-1.6586120000
C	5.6392100000	-1.1773540000	-1.1043300000
H	5.3948350000	-1.7511190000	-2.0058040000
H	6.0961020000	-1.8610150000	-0.3808300000

H	6.3874030000	-0.4328700000	-1.3792090000
C	1.2262610000	-1.2411930000	1.2729380000
O	1.7248540000	-1.7553480000	2.3348140000
C	-0.0630880000	-1.2593580000	0.8027700000
C	-0.5927540000	-0.6532650000	-0.4831790000
H	-0.6455200000	-1.4048640000	-1.2866440000
H	0.0957750000	0.1102440000	-0.8605910000
C	-1.9702100000	-0.0291670000	-0.3116340000
C	-3.1478190000	-0.8666120000	-0.3167570000
C	-4.3973810000	-0.4166520000	0.2023120000
C	-5.5218370000	-1.2320190000	0.2146700000
C	-5.4619910000	-2.5401960000	-0.2809700000
C	-4.2440240000	-3.0195270000	-0.7758990000
C	-3.1134060000	-2.2107820000	-0.7883750000
H	-4.4665140000	0.5788610000	0.6258890000
H	-6.4522260000	-0.8493370000	0.6269610000
H	-6.3427840000	-3.1759120000	-0.2707980000
H	-4.1747840000	-4.0358540000	-1.1557590000
H	-2.1899440000	-2.6219750000	-1.1795440000
C	-2.0408150000	1.4203950000	-0.1039750000
C	-3.0335130000	2.2211560000	-0.7171270000
C	-3.0472630000	3.6054430000	-0.5591400000
C	-2.0757850000	4.2405220000	0.2205220000
C	-1.0844040000	3.4698710000	0.8357240000
C	-1.0633450000	2.0869200000	0.6726060000
H	-3.7785570000	1.7503310000	-1.3510910000
H	-3.8156120000	4.1925220000	-1.0559070000
H	-2.0904600000	5.3197290000	0.3453900000

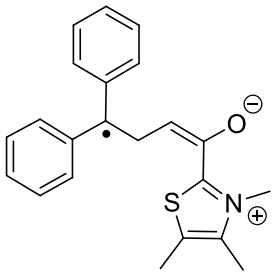
H	-0.3275500000	3.9481320000	1.4524700000
H	-0.3085680000	1.4945090000	1.1801940000
H	-0.7795890000	-1.8065200000	1.4138630000

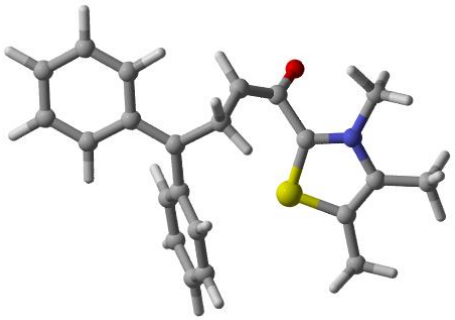
thermodynamic data

Zero-point correction= 0.383349 (Hartree/Particle)
Thermal correction to Energy= 0.406500
Thermal correction to Enthalpy= 0.407445
Thermal correction to Gibbs Free Energy= 0.328153
Sum of electronic and zero-point Energies= -1379.295471
Sum of electronic and thermal Energies= -1379.272320
Sum of electronic and thermal Enthalpies= -1379.271375
Sum of electronic and thermal Free Energies= -1379.350667

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	255.083	89.018	166.882

uM062X/6-31++G**	**Konformation 1offende**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	3.5677080000	0.7713000000	-0.0070870000
C	4.0549340000	-0.4720140000	-0.2597120000
N	3.0743860000	-1.4549910000	-0.1060000000
C	1.8742810000	-1.0112820000	0.2584670000
S	1.8867690000	0.6794150000	0.4343770000

C	3.3354080000	-2.8923830000	-0.2443490000
H	3.6343580000	-3.2930740000	0.7254040000
H	4.1068340000	-3.0398730000	-0.9988160000
H	2.4095770000	-3.3808600000	-0.5456590000
C	4.2606520000	2.0973230000	-0.0641230000
H	5.2606960000	1.9958830000	-0.4887680000
H	4.3557970000	2.5345190000	0.9339880000
H	3.6997510000	2.7995380000	-0.6874420000
C	5.4436960000	-0.8604580000	-0.6557280000
H	5.4698790000	-1.2873630000	-1.6632880000
H	5.8565960000	-1.5979830000	0.0387310000
H	6.0942080000	0.0136060000	-0.6432720000
C	0.7907020000	-1.9639370000	0.7448460000
O	1.2490140000	-2.6731900000	1.6918480000
C	-0.4311050000	-1.9618890000	0.1266780000
C	-0.8775420000	-1.1009740000	-1.0341860000
H	-1.3125730000	-1.7254250000	-1.8264230000
H	-0.0147470000	-0.5968960000	-1.4858710000
C	-1.8757650000	-0.0566520000	-0.5847480000
C	-3.2482850000	-0.3879930000	-0.3392480000
C	-4.2028640000	0.6007930000	0.0169490000
C	-5.5352810000	0.2753760000	0.2207070000
C	-5.9766500000	-1.0427920000	0.0785500000
C	-5.0579890000	-2.0320870000	-0.2792650000
C	-3.7230240000	-1.7172030000	-0.4859280000
H	-3.8852140000	1.6342300000	0.1129240000
H	-6.2402380000	1.0573760000	0.4875880000
H	-7.0197360000	-1.2936060000	0.2418840000

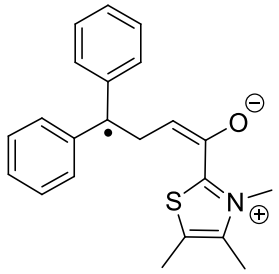
H	-5.3866260000	-3.0608730000	-0.3930370000
H	-3.0315000000	-2.5090590000	-0.7527690000
C	-1.3336770000	1.2796660000	-0.2743280000
C	-0.6856320000	2.0294180000	-1.2690980000
C	-0.0945740000	3.2546280000	-0.9734570000
C	-0.1285350000	3.7525930000	0.3302640000
C	-0.7732380000	3.0215400000	1.3286470000
C	-1.3753070000	1.8014470000	1.0288230000
H	-0.6492820000	1.6399370000	-2.2835840000
H	0.3914400000	3.8230200000	-1.7615160000
H	0.3357400000	4.7060010000	0.5639780000
H	-0.8017150000	3.3987650000	2.3465540000
H	-1.8616760000	1.2231340000	1.8099290000
H	-1.1601640000	-2.6477150000	0.5505910000

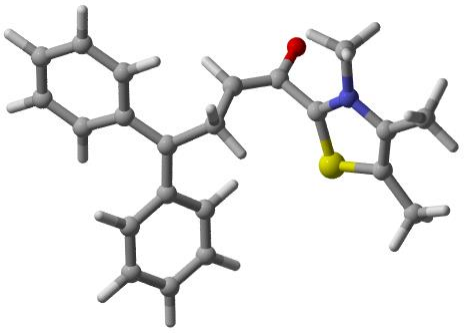
thermodynamic data

Zero-point correction= 0.385452 (Hartree/Particle)
Thermal correction to Energy= 0.409149
Thermal correction to Enthalpy= 0.410093
Thermal correction to Gibbs Free Energy= 0.329815
Sum of electronic and zero-point Energies= -1378.868389
Sum of electronic and thermal Energies= -1378.844693
Sum of electronic and thermal Enthalpies= -1378.843749
Sum of electronic and thermal Free Energies= -1378.924027

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	256.745	90.478	168.959

uM062X/6-31++G**/PCM	**Konformation 1offende**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	4.1034300000	0.8203010000	-0.1946710000
C	4.2428990000	-0.4576760000	-0.6356340000
N	3.1960130000	-1.2781590000	-0.1960720000
C	2.2796340000	-0.6799970000	0.5502940000
S	2.6627630000	0.9604970000	0.7717690000
C	3.1387180000	-2.7094350000	-0.5161200000
H	3.9453080000	-3.2250830000	0.0069400000
H	3.2463960000	-2.8373780000	-1.5929280000
H	2.1773070000	-3.0956500000	-0.1847150000
C	4.9756590000	2.0118660000	-0.4338550000
H	5.8389460000	1.7363890000	-1.0399390000
H	5.3391670000	2.4234570000	0.5108950000
H	4.4258830000	2.7963970000	-0.9598820000
C	5.3202880000	-1.0382670000	-1.4920930000
H	4.9193180000	-1.3811180000	-2.4503020000
H	5.7994240000	-1.8872470000	-0.9967540000
H	6.0841210000	-0.2885660000	-1.6925990000

C	1.1760870000	-1.4292260000	1.2775550000
O	1.6404980000	-2.0826620000	2.2813380000
C	-0.0907530000	-1.3551970000	0.7799500000
C	-0.5218240000	-0.6114040000	-0.4675470000
H	-0.5486310000	-1.2861040000	-1.3375380000
H	0.2064790000	0.1623760000	-0.7315720000
C	-1.8837070000	0.0281970000	-0.3204340000
C	-3.0589110000	-0.8115640000	-0.2807330000
C	-4.3000150000	-0.3493050000	0.2289090000
C	-5.4139590000	-1.1760520000	0.2847640000
C	-5.3420090000	-2.4998930000	-0.1574020000
C	-4.1247150000	-2.9880970000	-0.6380110000
C	-3.0046190000	-2.1679870000	-0.6918970000
H	-4.3757260000	0.6617960000	0.6137460000
H	-6.3449220000	-0.7881210000	0.6875210000
H	-6.2152240000	-3.1427670000	-0.1154240000
H	-4.0465270000	-4.0184900000	-0.9718520000
H	-2.0741240000	-2.5826800000	-1.0636360000
C	-1.9534050000	1.4817560000	-0.1813650000
C	-2.9675740000	2.2497440000	-0.7897280000
C	-2.9766210000	3.6374960000	-0.6871960000
C	-1.9795630000	4.3012020000	0.0305730000
C	-0.9656670000	3.5585340000	0.6388710000
C	-0.9502390000	2.1722290000	0.5294930000
H	-3.7348830000	1.7508410000	-1.3744090000
H	-3.7614790000	4.2041540000	-1.1791990000
H	-1.9902770000	5.3835150000	0.1108040000
H	-0.1861870000	4.0610140000	1.2040730000

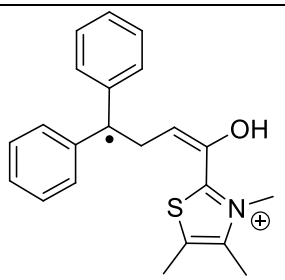
H	-0.1706070000	1.6019370000	1.0260880000
H	-0.8528420000	-1.9315600000	1.3018250000

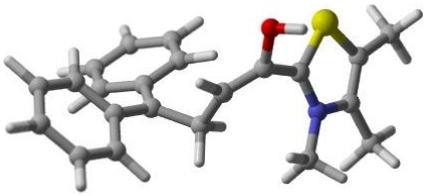
thermodynamic data

Zero-point correction= 0.386012 (Hartree/Particle)
Thermal correction to Energy= 0.409727
Thermal correction to Enthalpy= 0.410671
Thermal correction to Gibbs Free Energy= 0.329215
Sum of electronic and zero-point Energies= -1378.893073
Sum of electronic and thermal Energies= -1378.869358
Sum of electronic and thermal Enthalpies= -1378.868414
Sum of electronic and thermal Free Energies= -1378.949870

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.108	90.259	171.440

uB3LYP/6-31G*	**Konformation 1offenpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	4.3823650000	0.2172060000	0.2941620000
C	3.9463450000	-0.2974380000	-0.8925990000
N	2.7323230000	-0.9943710000	-0.7602220000
C	2.2086770000	-0.9869220000	0.4816320000
S	3.2550740000	-0.1593410000	1.5771440000
C	2.1841580000	-1.7926590000	-1.8709060000
H	2.9950610000	-2.3600780000	-2.3300540000

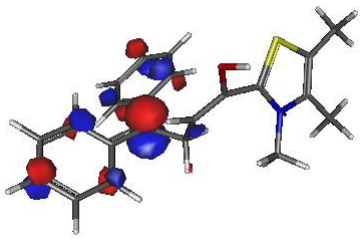
H	1.7223980000	-1.1447740000	-2.6187690000
H	1.4394260000	-2.4777300000	-1.4704520000
C	5.6275200000	0.9940930000	0.5989620000
H	6.1975030000	1.1916030000	-0.3110660000
H	6.2774750000	0.4419680000	1.2872330000
H	5.3914390000	1.9575080000	1.0635130000
C	4.6110450000	-0.2060410000	-2.2325190000
H	3.9203830000	0.1615370000	-2.9991250000
H	5.0004020000	-1.1759020000	-2.5644390000
H	5.4529680000	0.4856770000	-2.1885030000
C	0.9707170000	-1.5861980000	0.9578920000
C	-0.2417360000	-1.5459560000	0.3566100000
C	-0.6781340000	-0.7450990000	-0.8444780000
H	-0.9372190000	-1.4150440000	-1.6762830000
H	0.1196170000	-0.0933210000	-1.2062820000
C	-1.8850740000	0.0925710000	-0.4480390000
C	-3.1563350000	-0.5789290000	-0.2451880000
C	-4.1296480000	-0.0547110000	0.6479910000
C	-5.3348460000	-0.7078850000	0.8693760000
C	-5.6203080000	-1.9106420000	0.2149820000
C	-4.6755030000	-2.4570310000	-0.6578590000
C	-3.4637960000	-1.8120870000	-0.8781580000
H	-3.9107670000	0.8563300000	1.1937590000
H	-6.0520380000	-0.2846240000	1.5667890000
H	-6.5639780000	-2.4190270000	0.3884950000
H	-4.8874270000	-3.3891770000	-1.1739050000
H	-2.7654130000	-2.2559630000	-1.5805220000
C	-1.7061140000	1.5231870000	-0.2577880000

C	-2.7525500000	2.4360370000	-0.5478020000
C	-2.5710830000	3.8079280000	-0.4152000000
C	-1.3462060000	4.3234130000	0.0179260000
C	-0.2981580000	3.4448040000	0.3082900000
C	-0.4697380000	2.0730870000	0.1646420000
H	-3.6983220000	2.0566720000	-0.9190100000
H	-3.3877360000	4.4806000000	-0.6611900000
H	-1.2088190000	5.3951860000	0.1250140000
H	0.6544210000	3.8340750000	0.6575330000
H	0.3486340000	1.4109170000	0.4318540000
H	-1.0344890000	-2.0592960000	0.8954390000
O	1.0443800000	-2.0459220000	2.2615240000
H	1.7544020000	-2.7040660000	2.3534440000

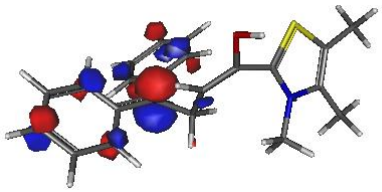
thermodynamic data

Zero-point correction= 0.396943 (Hartree/Particle)
Thermal correction to Energy= 0.420992
Thermal correction to Enthalpy= 0.421936
Thermal correction to Gibbs Free Energy= 0.340232
Sum of electronic and zero-point Energies= -1379.687043
Sum of electronic and thermal Energies= -1379.662994
Sum of electronic and thermal Enthalpies= -1379.662050
Sum of electronic and thermal Free Energies= -1379.743754

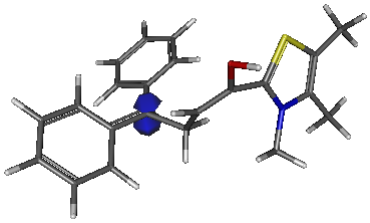
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.176	92.308	171.961



Alpha-SOMO

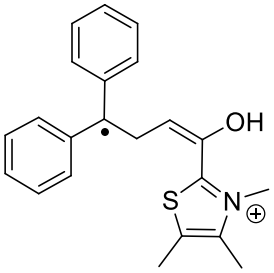


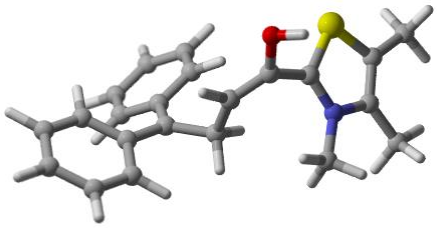
Beta-SOMO



Spin-Dichte

uB3LYP/6-31G*/PCM	**Konformation 1offenpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	4.3923120000	0.3287090000	0.1521290000
C	3.9518070000	-0.3571510000	-0.9453840000
N	2.7716890000	-1.0686780000	-0.6869760000
C	2.2848740000	-0.9211500000	0.5523500000
S	3.3101750000	0.0832010000	1.4958160000
C	2.1975000000	-1.9843180000	-1.6907540000
H	2.9938800000	-2.6212550000	-2.0765400000

H	1.7552100000	-1.4105380000	-2.5067980000
H	1.4395840000	-2.5978070000	-1.2108360000
C	5.6100420000	1.1852550000	0.3150450000
H	6.1305910000	1.3019880000	-0.6371110000
H	6.3085150000	0.7382670000	1.0307020000
H	5.3439370000	2.1816410000	0.6819800000
C	4.5804320000	-0.4243570000	-2.3017620000
H	3.8636330000	-0.1577710000	-3.0852820000
H	4.9638210000	-1.4276800000	-2.5185980000
H	5.4175140000	0.2714810000	-2.3623420000
C	1.0715380000	-1.5210940000	1.1222000000
C	-0.1641000000	-1.4619080000	0.5908130000
C	-0.6135120000	-0.7039840000	-0.6352710000
H	-0.7922930000	-1.4124770000	-1.4560740000
H	0.1704690000	-0.0305040000	-0.9892050000
C	-1.8870750000	0.0858440000	-0.3675170000
C	-3.1407740000	-0.6348720000	-0.2304440000
C	-4.2213400000	-0.1070620000	0.5287460000
C	-5.4108150000	-0.8077640000	0.6874010000
C	-5.5781290000	-2.0676880000	0.1018240000
C	-4.5266310000	-2.6190970000	-0.6364600000
C	-3.3311630000	-1.9252250000	-0.7942630000
H	-4.1032940000	0.8506870000	1.0232500000
H	-6.2094660000	-0.3743010000	1.2834350000
H	-6.5088480000	-2.6135990000	0.2260110000
H	-4.6391050000	-3.5972660000	-1.0963530000
H	-2.5459080000	-2.3828040000	-1.3863180000
C	-1.7872510000	1.5322940000	-0.2313560000

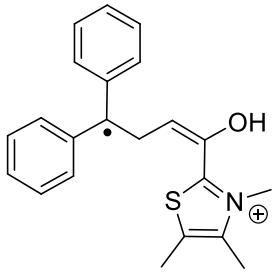
C	-2.8374810000	2.3930240000	-0.6427060000
C	-2.7190450000	3.7760290000	-0.5507650000
C	-1.5528640000	4.3572110000	-0.0419540000
C	-0.5007800000	3.5310150000	0.3657770000
C	-0.6106600000	2.1475600000	0.2668730000
H	-3.7368700000	1.9645260000	-1.0720490000
H	-3.5378120000	4.4054130000	-0.8891480000
H	-1.4635240000	5.4372380000	0.0310600000
H	0.4091830000	3.9674090000	0.7688750000
H	0.2111930000	1.5306990000	0.6162650000
H	-0.9413930000	-1.9588010000	1.1664400000
O	1.2310160000	-2.0167400000	2.4003020000
H	2.0169180000	-2.5887400000	2.4448900000

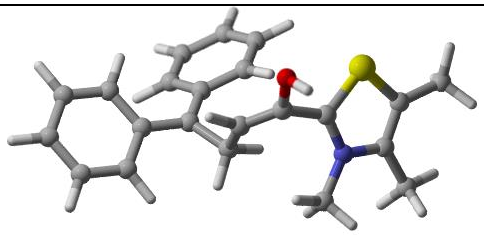
thermodynamic data

Zero-point correction= 0.397074 (Hartree/Particle)
Thermal correction to Energy= 0.421076
Thermal correction to Enthalpy= 0.422020
Thermal correction to Gibbs Free Energy= 0.340820
Sum of electronic and zero-point Energies= -1379.753251
Sum of electronic and thermal Energies= -1379.729249
Sum of electronic and thermal Enthalpies= -1379.728304
Sum of electronic and thermal Free Energies= -1379.809505

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.229	92.238	170.901

uM062X/6-31++G**	**Konformation 1offenpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	4.2090720000	0.2450260000	0.1889570000
C	3.7852120000	-0.4278040000	-0.9169820000
N	2.6200000000	-1.1581020000	-0.6719640000
C	2.1354950000	-1.0329640000	0.5651170000
S	3.1369540000	-0.0324320000	1.5169260000
C	2.0718890000	-2.0706780000	-1.6867240000
H	2.8880530000	-2.6775700000	-2.0796930000
H	1.6126880000	-1.4972850000	-2.4940260000
H	1.3266460000	-2.7084940000	-1.2165250000
C	5.4139300000	1.1269380000	0.3245100000
H	6.2891480000	0.6513560000	-0.1236650000
H	5.6421980000	1.3247570000	1.3730490000
H	5.2460050000	2.0874300000	-0.1711060000
C	4.4313380000	-0.4554970000	-2.2638900000
H	3.7127260000	-0.2225170000	-3.0545590000
H	4.8782860000	-1.4314100000	-2.4783440000
H	5.2235570000	0.2924520000	-2.3032700000
C	0.9135640000	-1.6307240000	1.1204590000

C	-0.2932070000	-1.5837330000	0.5344640000
C	-0.6652860000	-0.8562160000	-0.7295840000
H	-0.9455680000	-1.5804450000	-1.5054530000
H	0.1754220000	-0.2774060000	-1.1211410000
C	-1.8219170000	0.0740900000	-0.4378550000
C	-3.1463980000	-0.4954650000	-0.2654500000
C	-4.0990220000	0.1192670000	0.5809110000
C	-5.3548640000	-0.4391390000	0.7742830000
C	-5.7066820000	-1.6291400000	0.1348700000
C	-4.7788670000	-2.2616410000	-0.6917360000
C	-3.5173790000	-1.7113730000	-0.8825340000
H	-3.8299020000	1.0252740000	1.1139300000
H	-6.0606390000	0.0498600000	1.4381240000
H	-6.6899970000	-2.0621410000	0.2848830000
H	-5.0409730000	-3.1861920000	-1.1961440000
H	-2.8304620000	-2.2202740000	-1.5510000000
C	-1.5374750000	1.4881410000	-0.2671680000
C	-2.4925940000	2.4726580000	-0.6038020000
C	-2.2017430000	3.8249980000	-0.4817420000
C	-0.9545830000	4.2431270000	-0.0145420000
C	0.0045730000	3.2880640000	0.3224290000
C	-0.2780630000	1.9346310000	0.1907570000
H	-3.4561890000	2.1626240000	-0.9955770000
H	-2.9501570000	4.5594360000	-0.7620130000
H	-0.7333130000	5.3005250000	0.0844290000
H	0.9727780000	3.6029820000	0.7002370000
H	0.4719510000	1.2085320000	0.4937120000
H	-1.1116690000	-2.0284250000	1.0990900000

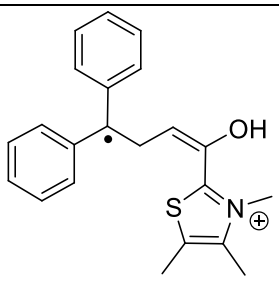
O	1.0416970000	-2.0366810000	2.4272890000
H	1.6426160000	-2.7893900000	2.5111970000

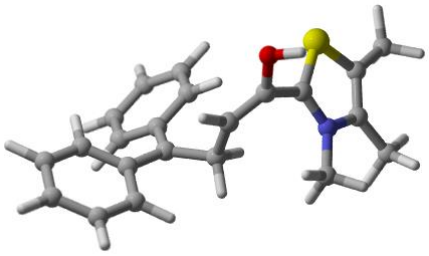
thermodynamic data

Zero-point correction= 0.398761 (Hartree/Particle)
Thermal correction to Energy= 0.422775
Thermal correction to Enthalpy= 0.423719
Thermal correction to Gibbs Free Energy= 0.340887
Sum of electronic and zero-point Energies= -1379.273975
Sum of electronic and thermal Energies= -1379.249961
Sum of electronic and thermal Enthalpies= -1379.249017
Sum of electronic and thermal Free Energies= -1379.331849

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	265.295	91.855	174.335

uM062X/6-31++G**/PCM	**Konformation 1offenpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	4.2185030000	0.3031220000	0.1464270000
C	3.8049010000	-0.4249530000	-0.9297910000
N	2.6565350000	-1.1616170000	-0.6532280000
C	2.1763050000	-0.9966940000	0.5777860000
S	3.1534600000	0.0634260000	1.4817930000
C	2.1006420000	-2.0967090000	-1.6434790000
H	2.9146060000	-2.7100080000	-2.0283810000

H	1.6396420000	-1.5339770000	-2.4567790000
H	1.3618520000	-2.7268180000	-1.1550010000
C	5.4095500000	1.2074470000	0.2360860000
H	6.3105000000	0.6782950000	-0.0827060000
H	5.5634900000	1.5562100000	1.2578350000
H	5.2715580000	2.0813900000	-0.4061020000
C	4.4509280000	-0.4994970000	-2.2730300000
H	3.7268760000	-0.3052310000	-3.0684630000
H	4.8990630000	-1.4827750000	-2.4435400000
H	5.2394980000	0.2500410000	-2.3390300000
C	0.9674720000	-1.6200430000	1.1469460000
C	-0.2472990000	-1.5593550000	0.5876480000
C	-0.6239430000	-0.7968770000	-0.6559790000
H	-0.8463190000	-1.5039630000	-1.4655650000
H	0.2078770000	-0.1814050000	-1.0081210000
C	-1.8264080000	0.0836220000	-0.3960090000
C	-3.1310740000	-0.5312530000	-0.2540230000
C	-4.1724050000	0.0990540000	0.4715500000
C	-5.4109940000	-0.5075300000	0.6315930000
C	-5.6620880000	-1.7671240000	0.0813350000
C	-4.6454700000	-2.4177020000	-0.6195870000
C	-3.4016220000	-1.8178440000	-0.7788360000
H	-3.9902150000	1.0600280000	0.9404450000
H	-6.1837410000	0.0006650000	1.2001800000
H	-6.6317170000	-2.2377270000	0.2069040000
H	-4.8210980000	-3.3997960000	-1.0477490000
H	-2.6405060000	-2.3520600000	-1.3368020000
C	-1.6034050000	1.5145960000	-0.2364760000

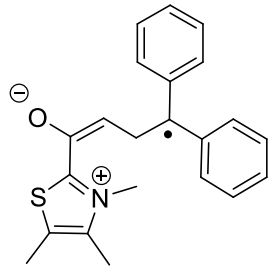
C	-2.5559390000	2.4673080000	-0.6591870000
C	-2.3075970000	3.8302800000	-0.5442110000
C	-1.1059540000	4.2884740000	0.0004820000
C	-0.1488650000	3.3634910000	0.4211310000
C	-0.3900530000	2.0000260000	0.2982180000
H	-3.4827930000	2.1285020000	-1.1118760000
H	-3.0518170000	4.5397740000	-0.8926330000
H	-0.9158640000	5.3530510000	0.0907900000
H	0.7879200000	3.7055510000	0.8506470000
H	0.3588620000	1.2979280000	0.6535090000
H	-1.0517380000	-2.0517260000	1.1309050000
O	1.1266010000	-2.1332140000	2.4085150000
H	1.8990390000	-2.7147640000	2.4557310000

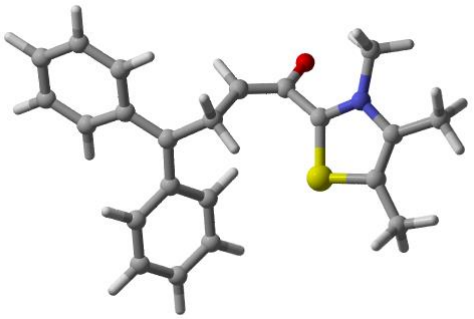
thermodynamic data

Zero-point correction= 0.399310 (Hartree/Particle)
Thermal correction to Energy= 0.423185
Thermal correction to Enthalpy= 0.424129
Thermal correction to Gibbs Free Energy= 0.343335
Sum of electronic and zero-point Energies= -1379.342852
Sum of electronic and thermal Energies= -1379.318977
Sum of electronic and thermal Enthalpies= -1379.318033
Sum of electronic and thermal Free Energies= -1379.398827

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	265.553	91.718	170.046

uB3LYP/6-31G*	**Konformation 2offende**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	4.0390490000	0.8612670000	-0.6304670000
C	4.4890790000	-0.4080770000	-0.4405100000
N	3.5184980000	-1.2444100000	0.1340680000
C	2.3203270000	-0.6763600000	0.3734100000
S	2.3781260000	0.9915200000	-0.0808860000
C	3.7579460000	-2.6677470000	0.4288110000
H	3.1445510000	-2.9024180000	1.3051920000
H	4.8164570000	-2.8191710000	0.6364540000
H	3.4573120000	-3.2775300000	-0.4286070000
C	4.7421800000	2.0560890000	-1.1999930000
H	5.7533080000	1.7998790000	-1.5264850000
H	4.8260120000	2.8598270000	-0.4588520000
H	4.2040120000	2.4604020000	-2.0651900000
C	5.8448580000	-0.9538060000	-0.7738790000
H	5.7780450000	-1.8302970000	-1.4282220000
H	6.3961580000	-1.2506590000	0.1264550000
H	6.4398760000	-0.1982510000	-1.2896410000

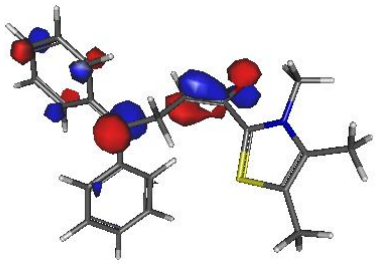
C	1.2195410000	-1.3685290000	1.1533440000
C	-0.0633600000	-1.3922330000	0.6444370000
C	-0.6408430000	-0.7282950000	-0.5857330000
H	-0.7679090000	-1.4638330000	-1.3954790000
H	0.0419770000	0.0226290000	-0.9924340000
C	-1.9835590000	-0.0637090000	-0.3127280000
C	-3.2037720000	-0.8285400000	-0.3520690000
C	-4.4271530000	-0.3199160000	0.1761050000
C	-5.6002920000	-1.0603320000	0.1461410000
C	-5.6194210000	-2.3490940000	-0.3995980000
C	-4.4298710000	-2.8869770000	-0.9012120000
C	-3.2507100000	-2.1536860000	-0.8742640000
H	-4.4345090000	0.6606680000	0.6381200000
H	-6.5087340000	-0.6348820000	0.5658270000
H	-6.5391950000	-2.9269720000	-0.4206490000
H	-4.4213510000	-3.8920580000	-1.3160900000
H	-2.3499580000	-2.6116140000	-1.2664950000
C	-1.9704630000	1.3700640000	0.0131130000
C	-2.8657260000	2.2763830000	-0.5979230000
C	-2.8039750000	3.6429790000	-0.3349050000
C	-1.8502950000	4.1513330000	0.5505560000
C	-0.9568520000	3.2727480000	1.1679200000
C	-1.0123510000	1.9059980000	0.9026410000
H	-3.5960970000	1.8994940000	-1.3077470000
H	-3.4997760000	4.3154820000	-0.8308320000
H	-1.8066420000	5.2171360000	0.7586820000
H	-0.2199040000	3.6513600000	1.8722380000
H	-0.3398090000	1.2258120000	1.4165190000

H	-0.7521960000	-2.0127120000	1.2148930000
O	1.6616050000	-1.9403880000	2.2036080000

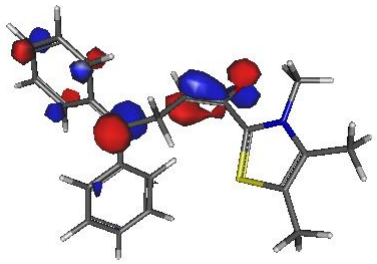
thermodynamic data

Zero-point correction= 0.383316 (Hartree/Particle)
Thermal correction to Energy= 0.407173
Thermal correction to Enthalpy= 0.408117
Thermal correction to Gibbs Free Energy= 0.326474
Sum of electronic and zero-point Energies= -1379.273916
Sum of electronic and thermal Energies= -1379.250058
Sum of electronic and thermal Enthalpies= -1379.249114
Sum of electronic and thermal Free Energies= -1379.330758

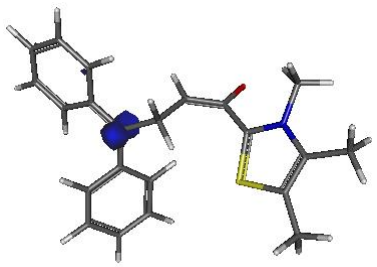
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	255.505	90.940	171.834



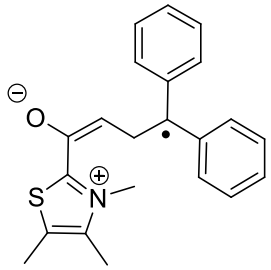
Alpha-SOMO

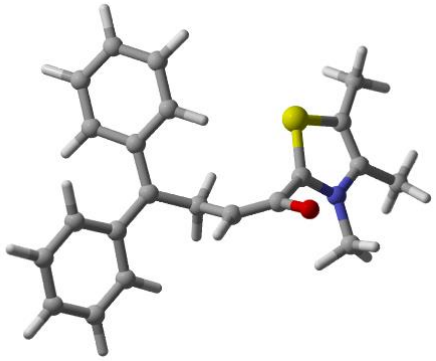


Beta-SOMO



uB3LYP/6-31G*/PCM	**Konformation 2offende**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	4.1909300000	0.8301940000	-0.4312440000
C	4.4271260000	-0.5071820000	-0.5361170000
N	3.3612450000	-1.2749560000	-0.0350980000
C	2.3253300000	-0.5837720000	0.4524690000
S	2.6224240000	1.1008300000	0.3073080000
C	3.3838600000	-2.7447320000	0.0306700000
H	3.7458600000	-3.0547350000	1.0124350000
H	4.0248880000	-3.1311630000	-0.7587230000
H	2.3669560000	-3.1098620000	-0.1092440000
C	5.0381520000	1.9917260000	-0.8530550000
H	6.0123010000	1.6521750000	-1.2117190000
H	5.2081400000	2.6808070000	-0.0187810000
H	4.5605350000	2.5575900000	-1.6609660000
C	5.6364150000	-1.1820350000	-1.1066120000
H	5.3897050000	-1.7559910000	-2.0073320000
H	6.0928510000	-1.8661020000	-0.3832110000
H	6.3857520000	-0.4392570000	-1.3829770000

C	1.2269000000	-1.2358370000	1.2771550000
C	-0.0625400000	-1.2550740000	0.8073740000
C	-0.5918540000	-0.6524130000	-0.4804100000
H	-0.6432310000	-1.4058190000	-1.2822260000
H	0.0962600000	0.1109310000	-0.8589760000
C	-1.9699810000	-0.0292450000	-0.3111470000
C	-3.1469320000	-0.8678400000	-0.3168850000
C	-4.3966540000	-0.4195950000	0.2031940000
C	-5.5204410000	-1.2359250000	0.2149740000
C	-5.4596910000	-2.5433990000	-0.2823670000
C	-4.2415150000	-3.0210690000	-0.7783590000
C	-3.1115710000	-2.2113550000	-0.7901760000
H	-4.4664230000	0.5752890000	0.6281450000
H	-6.4509730000	-0.8545550000	0.6281540000
H	-6.3399500000	-3.1798630000	-0.2727020000
H	-4.1715720000	-4.0368220000	-1.1596190000
H	-2.1879740000	-2.6212450000	-1.1823980000
C	-2.0420570000	1.4202410000	-0.1044060000
C	-3.0368600000	2.2194880000	-0.7162580000
C	-3.0520840000	3.6038230000	-0.5589800000
C	-2.0800280000	4.2405970000	0.2185970000
C	-1.0864790000	3.4715420000	0.8323240000
C	-1.0639270000	2.0885590000	0.6699040000
H	-3.7824040000	1.7474570000	-1.3487200000
H	-3.8220670000	4.1896460000	-1.0546990000
H	-2.0958940000	5.3198460000	0.3429490000
H	-0.3290690000	3.9511080000	1.4473750000
H	-0.3074290000	1.4974000000	1.1763620000

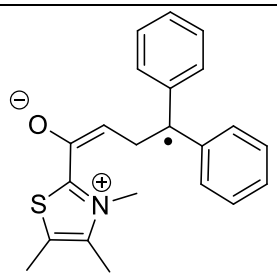
H	-0.7792010000	-1.8002650000	1.4200360000
O	1.7261040000	-1.7469170000	2.3402160000

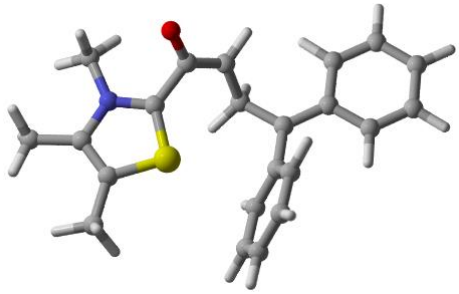
thermodynamic data

Zero-point correction= 0.383367 (Hartree/Particle)
Thermal correction to Energy= 0.407447
Thermal correction to Enthalpy= 0.408391
Thermal correction to Gibbs Free Energy= 0.324256
Sum of electronic and zero-point Energies= -1379.295453
Sum of electronic and thermal Energies= -1379.271373
Sum of electronic and thermal Enthalpies= -1379.270429
Sum of electronic and thermal Free Energies= -1379.354564

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	255.677	91.002	177.076

uM062X/6-31++G**	**Konformation 2offende**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

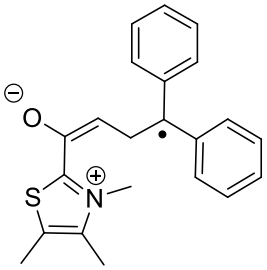
C	3.5675600000	0.7711230000	-0.0074160000
C	4.0548280000	-0.4722710000	-0.2595710000
N	3.0742690000	-1.4551930000	-0.1056400000
C	1.8741170000	-1.0113520000	0.2584900000
S	1.8865870000	0.6793960000	0.4339560000
C	3.3349360000	-2.8927250000	-0.2435520000
H	3.6310180000	-3.2937020000	0.7269620000

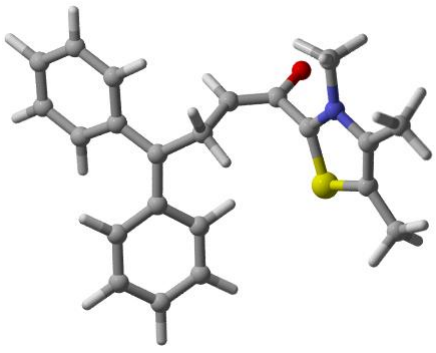
H	4.1080860000	-3.0405400000	-0.9961600000
H	2.4095650000	-3.3806110000	-0.5473190000
C	4.2604960000	2.0971450000	-0.0649100000
H	5.2605450000	1.9956050000	-0.4895270000
H	4.3556240000	2.5346490000	0.9330740000
H	3.6995760000	2.7991680000	-0.6884270000
C	5.4435820000	-0.8606550000	-0.6557310000
H	5.4696680000	-1.2878330000	-1.6631760000
H	5.8567220000	-1.5979080000	0.0388720000
H	6.0939620000	0.0135130000	-0.6435940000
C	0.7904410000	-1.9639510000	0.7448050000
C	-0.4313060000	-1.9617800000	0.1265180000
C	-0.8775310000	-1.1007220000	-1.0343450000
H	-1.3124630000	-1.7250620000	-1.8267110000
H	-0.0146560000	-0.5966310000	-1.4858550000
C	-1.8757490000	-0.0564700000	-0.5847420000
C	-3.2482570000	-0.3877660000	-0.3393130000
C	-4.2027050000	0.6009030000	0.0176200000
C	-5.5351150000	0.2755070000	0.2213660000
C	-5.9766780000	-1.0425220000	0.0784480000
C	-5.0581600000	-2.0317040000	-0.2800200000
C	-3.7231850000	-1.7168480000	-0.4866510000
H	-3.8849400000	1.6342420000	0.1142490000
H	-6.2399310000	1.0574370000	0.4888330000
H	-7.0197810000	-1.2932960000	0.2417350000
H	-5.3868940000	-3.0603970000	-0.3943730000
H	-3.0318010000	-2.5086410000	-0.7540380000
C	-1.3334750000	1.2797610000	-0.2742480000

C	-0.6857070000	2.0297590000	-1.2690370000
C	-0.0944400000	3.2548130000	-0.9732370000
C	-0.1278530000	3.7524020000	0.3306620000
C	-0.7721970000	3.0210900000	1.3290560000
C	-1.3744730000	1.8011230000	1.0290710000
H	-0.6497280000	1.6405790000	-2.2836500000
H	0.3913720000	3.8233700000	-1.7613020000
H	0.3365900000	4.7057050000	0.5644660000
H	-0.8002840000	3.3979600000	2.3471080000
H	-1.8604570000	1.2225610000	1.8102390000
H	-1.1605100000	-2.6475380000	0.5502830000
O	1.2485830000	-2.6732230000	1.6918640000

thermodynamic data

uM062X/6-31++G**/PCM	**Konformation 2offende**





xyz-matrix

47

XYZ file generated by gabedit : coordinates in Angstrom

C	4.1032940000	0.8205680000	-0.1948400000
C	4.2429590000	-0.4574540000	-0.6356600000

N	3.1962540000	-1.2780590000	-0.1958930000
C	2.2798180000	-0.6799420000	0.5504500000
S	2.6627420000	0.9606230000	0.7717740000
C	3.1390480000	-2.7093460000	-0.5158230000
H	3.9455480000	-3.2249410000	0.0074300000
H	3.2469310000	-2.8373940000	-1.5926010000
H	2.1776160000	-3.0955640000	-0.1844840000
C	4.9752320000	2.0123260000	-0.4341570000
H	5.8387510000	1.7369680000	-1.0399600000
H	5.3383400000	2.4243520000	0.5105580000
H	4.4253110000	2.7965100000	-0.9605640000
C	5.3204130000	-1.0379000000	-1.4921360000
H	4.9195370000	-1.3805560000	-2.4504580000
H	5.7995060000	-1.8869810000	-0.9969360000
H	6.0842880000	-0.2881620000	-1.6923600000
C	1.1763140000	-1.4291580000	1.2776890000
C	-0.0905650000	-1.3549590000	0.7801950000
C	-0.5216120000	-0.6110880000	-0.4672580000
H	-0.5482200000	-1.2856860000	-1.3373460000
H	0.2066110000	0.1628130000	-0.7311420000
C	-1.8836090000	0.0282860000	-0.3203060000
C	-3.0586400000	-0.8118090000	-0.2807480000
C	-4.2997220000	-0.3500220000	0.2293260000
C	-5.4134890000	-1.1770240000	0.2850570000
C	-5.3413300000	-2.5006680000	-0.1576700000
C	-4.1240230000	-2.9884170000	-0.6386890000
C	-3.0041040000	-2.1680320000	-0.6924440000
H	-4.3755540000	0.6609030000	0.6146060000

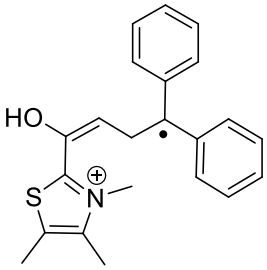
H	-6.3444580000	-0.7894560000	0.6881470000
H	-6.2144010000	-3.1437460000	-0.1157870000
H	-4.0456650000	-4.0186540000	-0.9729670000
H	-2.0735920000	-2.5823820000	-1.0645240000
C	-1.9536920000	1.4817790000	-0.1813070000
C	-2.9684130000	2.2494420000	-0.7892190000
C	-2.9778750000	3.6371880000	-0.6867410000
C	-1.9806840000	4.3012790000	0.0305010000
C	-0.9662200000	3.5589720000	0.6383010000
C	-0.9503790000	2.1726680000	0.5289840000
H	-3.7358390000	1.7502680000	-1.3735100000
H	-3.7631700000	4.2035510000	-1.1783860000
H	-1.9917250000	5.3835910000	0.1106840000
H	-0.1866160000	4.0617270000	1.2030850000
H	-0.1702690000	1.6027040000	1.0252010000
H	-0.8526490000	-1.9313190000	1.3020810000
O	1.6407190000	-2.0827820000	2.2813850000

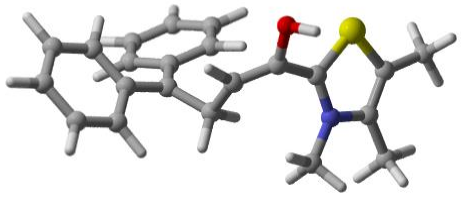
thermodynamic data

Zero-point correction= 0.386007 (Hartree/Particle)
Thermal correction to Energy= 0.409731
Thermal correction to Enthalpy= 0.410675
Thermal correction to Gibbs Free Energy= 0.328992
Sum of electronic and zero-point Energies= -1378.893078
Sum of electronic and thermal Energies= -1378.869354
Sum of electronic and thermal Enthalpies= -1378.868410
Sum of electronic and thermal Free Energies= -1378.950093

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.110	90.259	171.917

uB3LYP/6-31G*	**Konformation 2offenpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	4.3823900000	0.2171920000	0.2942130000
C	3.9463830000	-0.2973650000	-0.8925680000
N	2.7323450000	-0.9943030000	-0.7602510000
C	2.2086760000	-0.9868920000	0.4815870000
S	3.2550530000	-0.1594250000	1.5771680000
C	2.1841710000	-1.7924800000	-1.8709900000
H	2.9950790000	-2.3597720000	-2.3302840000
H	1.7222950000	-1.1445280000	-2.6187270000
H	1.4395200000	-2.4776660000	-1.4705810000
C	5.6275400000	0.9940300000	0.5991290000
H	6.1977180000	1.1913370000	-0.3108220000
H	6.2773180000	0.4419650000	1.2876160000
H	5.3914340000	1.9575390000	1.0634720000
C	4.6111240000	-0.2059010000	-2.2324650000
H	3.9204950000	0.1617560000	-2.9990610000
H	5.0004640000	-1.1757520000	-2.5644270000
H	5.4530680000	0.4857920000	-2.1883680000
C	0.9707160000	-1.5862400000	0.9577850000

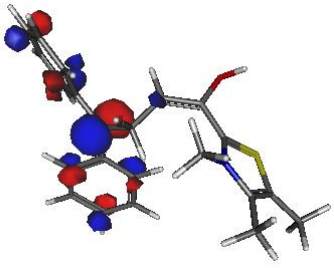
C	-0.2417180000	-1.5459460000	0.3564760000
C	-0.6781120000	-0.7449820000	-0.8445350000
H	-0.9371530000	-1.4148810000	-1.6763900000
H	0.1196330000	-0.0931530000	-1.2062620000
C	-1.8850910000	0.0926270000	-0.4480800000
C	-3.1563160000	-0.5789450000	-0.2452050000
C	-4.1295790000	-0.0548450000	0.6480960000
C	-5.3347380000	-0.7080800000	0.8695070000
C	-5.6202020000	-1.9107890000	0.2150280000
C	-4.6754340000	-2.4570730000	-0.6579200000
C	-3.4637690000	-1.8120650000	-0.8782490000
H	-3.9106900000	0.8561570000	1.1939250000
H	-6.0518980000	-0.2849040000	1.5670050000
H	-6.5638420000	-2.4192230000	0.3885600000
H	-4.8873620000	-3.3891810000	-1.1740330000
H	-2.7654170000	-2.2558540000	-1.5806990000
C	-1.7061790000	1.5232400000	-0.2577890000
C	-2.7526480000	2.4360710000	-0.5477550000
C	-2.5712160000	3.8079610000	-0.4151110000
C	-1.3463430000	4.3234680000	0.0179980000
C	-0.2982590000	3.4448820000	0.3083030000
C	-0.4698070000	2.0731650000	0.1646250000
H	-3.6984180000	2.0566910000	-0.9189490000
H	-3.3878960000	4.4806180000	-0.6610530000
H	-1.2089880000	5.3952420000	0.1251160000
H	0.6543150000	3.8341700000	0.6575370000
H	0.3485860000	1.4110060000	0.4318040000
H	-1.0344690000	-2.0594110000	0.8951890000

O	1.0443710000	-2.0461230000	2.2613520000
H	1.7544430000	-2.7042240000	2.3532040000

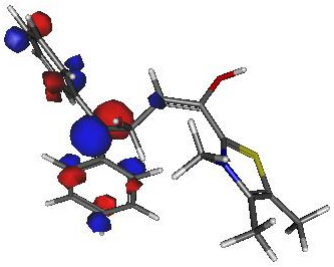
thermodynamic data

Zero-point correction= 0.396943 (Hartree/Particle)
Thermal correction to Energy= 0.420992
Thermal correction to Enthalpy= 0.421936
Thermal correction to Gibbs Free Energy= 0.340231
Sum of electronic and zero-point Energies= -1379.687043
Sum of electronic and thermal Energies= -1379.662994
Sum of electronic and thermal Enthalpies= -1379.662050
Sum of electronic and thermal Free Energies= -1379.743755

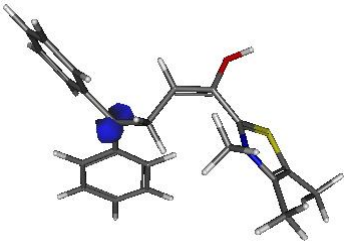
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	264.176	92.308	171.963



Alpha-SOMO

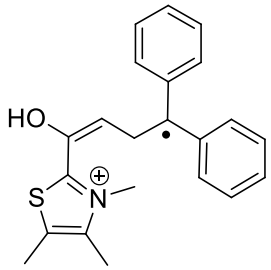


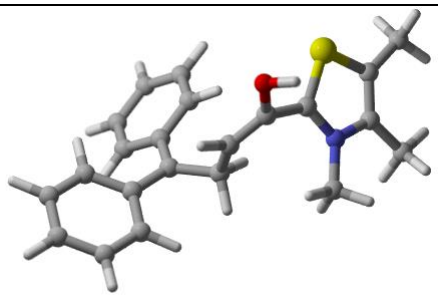
Beta-SOMO



Spin-Dichte

uB3LYP/6-31G*/PCM	**Konformation 2offenpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	4.4122540000	0.3334800000	0.1506160000
C	3.9740880000	-0.3586910000	-0.9431780000
N	2.7924040000	-1.0675350000	-0.6833710000
C	2.3015050000	-0.9109080000	0.5546080000
S	3.3258200000	0.0992000000	1.4929440000
C	2.2219110000	-1.9897720000	-1.6835790000
H	3.0188110000	-2.6322260000	-2.0590750000
H	1.7868080000	-1.4211780000	-2.5069860000
H	1.4592280000	-2.5971220000	-1.2040620000
C	5.6243540000	1.1989270000	0.3081690000
H	6.2254610000	1.1923550000	-0.6027060000
H	6.2533590000	0.8444510000	1.1312700000
H	5.3418160000	2.2349690000	0.5228900000
C	4.6042540000	-0.4330250000	-2.2985060000
H	3.8934540000	-0.1503440000	-3.0820630000
H	4.9693040000	-1.4423460000	-2.5187150000
H	5.4535780000	0.2480050000	-2.3556550000

C	1.0861890000	-1.5087220000	1.1288400000
C	-0.1663200000	-1.4532360000	0.5924960000
C	-0.6227650000	-0.7033900000	-0.6373610000
H	-0.8011410000	-1.4173890000	-1.4533090000
H	0.1573120000	-0.0289300000	-0.9974850000
C	-1.8992890000	0.0824890000	-0.3705970000
C	-3.1496370000	-0.6434950000	-0.2311310000
C	-4.2297640000	-0.1209800000	0.5320050000
C	-5.4160970000	-0.8264840000	0.6932220000
C	-5.5803530000	-2.0860820000	0.1061260000
C	-4.5290010000	-2.6322000000	-0.6363060000
C	-3.3366610000	-1.9334510000	-0.7964910000
H	-4.1138030000	0.8365230000	1.0275750000
H	-6.2145670000	-0.3970320000	1.2923980000
H	-6.5085900000	-2.6357750000	0.2322420000
H	-4.6391320000	-3.6099830000	-1.0975970000
H	-2.5514710000	-2.3868670000	-1.3918480000
C	-1.8071400000	1.5296830000	-0.2356590000
C	-2.8641650000	2.3836440000	-0.6440050000
C	-2.7543250000	3.7674250000	-0.5532820000
C	-1.5902690000	4.3564810000	-0.0487680000
C	-0.5315500000	3.5373900000	0.3558500000
C	-0.6327740000	2.1531760000	0.2582090000
H	-3.7623010000	1.9491630000	-1.0699960000
H	-3.5782960000	4.3913030000	-0.8892260000
H	-1.5077050000	5.4371020000	0.0233690000
H	0.3769070000	3.9799380000	0.7556310000
H	0.1941300000	1.5422450000	0.6053300000

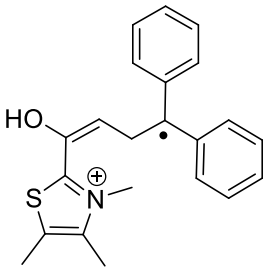
H	-0.9419440000	-1.9484430000	1.1722100000
O	1.2505760000	-1.9984460000	2.4120360000
H	2.0375690000	-2.5688450000	2.4583520000

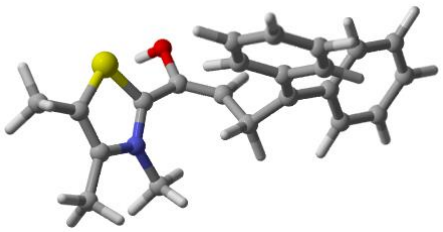
thermodynamic data

Zero-point correction= 0.396662 (Hartree/Particle)
Thermal correction to Energy= 0.419865
Thermal correction to Enthalpy= 0.420809
Thermal correction to Gibbs Free Energy= 0.341673
Sum of electronic and zero-point Energies= -1379.753300
Sum of electronic and thermal Energies= -1379.730097
Sum of electronic and thermal Enthalpies= -1379.729153
Sum of electronic and thermal Free Energies= -1379.808289

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	263.469	90.322	166.555

uM062X/6-31++G**	**Konformation 2offenpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	4.2090520000	0.2450870000	0.1888570000
C	3.7852070000	-0.4279030000	-0.9169900000
N	2.6200280000	-1.1581970000	-0.6718690000
C	2.1355270000	-1.0329110000	0.5651990000
S	3.1369700000	-0.0322080000	1.5168700000
C	2.0719050000	-2.0708680000	-1.6865470000

H	2.8880780000	-2.6777570000	-2.0794970000
H	1.6126590000	-1.4975430000	-2.4938710000
H	1.3266960000	-2.7086750000	-1.2162820000
C	5.4139280000	1.1270110000	0.3241930000
H	6.2892300000	0.6511200000	-0.1234960000
H	5.6419610000	1.3254300000	1.3726710000
H	5.2461580000	2.0872270000	-0.1720130000
C	4.4313480000	-0.4557350000	-2.2638870000
H	3.7127600000	-0.2228100000	-3.0545960000
H	4.8782860000	-1.4316730000	-2.4782540000
H	5.2235750000	0.2922020000	-2.3033110000
C	0.9136120000	-1.6306230000	1.1206280000
C	-0.2931710000	-1.5836760000	0.5346490000
C	-0.6652650000	-0.8562760000	-0.7294590000
H	-0.9455160000	-1.5805740000	-1.5052770000
H	0.1754260000	-0.2774750000	-1.1210710000
C	-1.8219180000	0.0740360000	-0.4378440000
C	-3.1464060000	-0.4955050000	-0.2654640000
C	-4.0990680000	0.1193000000	0.5808080000
C	-5.3549270000	-0.4390670000	0.7741450000
C	-5.7067280000	-1.6291170000	0.1348050000
C	-4.7788810000	-2.2616880000	-0.6917050000
C	-3.5173750000	-1.7114470000	-0.8824850000
H	-3.8299590000	1.0253300000	1.1137910000
H	-6.0607280000	0.0499720000	1.4379300000
H	-6.6900570000	-2.0620910000	0.2848120000
H	-5.0409600000	-3.1862760000	-1.1960580000
H	-2.8304370000	-2.2204250000	-1.5508690000

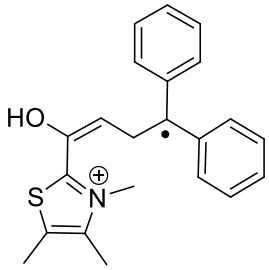
C	-1.5374900000	1.4880950000	-0.2671860000
C	-2.4925950000	2.4726000000	-0.6038850000
C	-2.2017500000	3.8249440000	-0.4818570000
C	-0.9546140000	4.2430840000	-0.0146060000
C	0.0045280000	3.2880320000	0.3224320000
C	-0.2780930000	1.9345960000	0.1907640000
H	-3.4561760000	2.1625500000	-0.9956830000
H	-2.9501540000	4.5593760000	-0.7621710000
H	-0.7333530000	5.3004860000	0.0843540000
H	0.9727120000	3.6029700000	0.7002790000
H	0.4719070000	1.2085100000	0.4937780000
H	-1.1116240000	-2.0283110000	1.0993330000
O	1.0417570000	-2.0364520000	2.4274730000
H	1.6427830000	-2.7890630000	2.5114850000

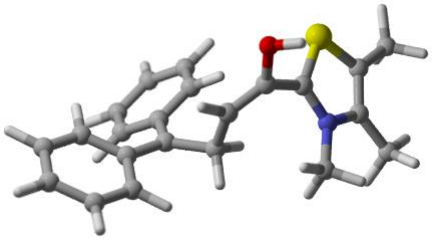
thermodynamic data

Zero-point correction= 0.398760 (Hartree/Particle)
Thermal correction to Energy= 0.422775
Thermal correction to Enthalpy= 0.423719
Thermal correction to Gibbs Free Energy= 0.340884
Sum of electronic and zero-point Energies= -1379.273975
Sum of electronic and thermal Energies= -1379.249961
Sum of electronic and thermal Enthalpies= -1379.249017
Sum of electronic and thermal Free Energies= -1379.331852

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	265.295	91.855	174.341

uM062X/6-31++G**/PCM	**Konformation 2offenpr**





xyz-matrix

48

XYZ file generated by gabedit : coordinates in Angstrom

C	4.2187410000	0.3032940000	0.1461610000
C	3.8051480000	-0.4252720000	-0.9297380000
N	2.6567410000	-1.1617480000	-0.6528740000
C	2.1764800000	-0.9962450000	0.5780500000
S	3.1536590000	0.0642290000	1.4816220000
C	2.1008450000	-2.0973780000	-1.6426460000
H	2.9148250000	-2.7108490000	-2.0272370000
H	1.6398280000	-1.5350910000	-2.4562390000
H	1.3620540000	-2.7272160000	-1.1538260000
C	5.4098710000	1.2075520000	0.2354810000
H	6.3109210000	0.6778920000	-0.0821840000
H	5.5632290000	1.5575160000	1.2568960000
H	5.2723840000	2.0807160000	-0.4078640000
C	4.4512090000	-0.5005610000	-2.2729300000
H	3.7272200000	-0.3065460000	-3.0684790000
H	4.8992060000	-1.4839900000	-2.4429220000
H	5.2399310000	0.2487860000	-2.3392690000
C	0.9676180000	-1.6193030000	1.1474700000

C	-0.2471480000	-1.5588890000	0.5881220000
C	-0.6238630000	-0.7969680000	-0.6558160000
H	-0.8462220000	-1.5044400000	-1.4650600000
H	0.2079000000	-0.1815950000	-1.0082760000
C	-1.8264160000	0.0835030000	-0.3961450000
C	-3.1310630000	-0.5315130000	-0.2541110000
C	-4.1721860000	0.0984640000	0.4720150000
C	-5.4107160000	-0.5082180000	0.6321860000
C	-5.6619390000	-1.7675750000	0.0814550000
C	-4.6455290000	-2.4178140000	-0.6200760000
C	-3.4017360000	-1.8178650000	-0.7794250000
H	-3.9898650000	1.0592590000	0.9412330000
H	-6.1832990000	-0.0002880000	1.2012330000
H	-6.6315190000	-2.2382570000	0.2071110000
H	-4.8212850000	-3.3997110000	-1.0486350000
H	-2.6407850000	-2.3517920000	-1.3378930000
C	-1.6036370000	1.5144910000	-0.2367510000
C	-2.5565710000	2.4669650000	-0.6591500000
C	-2.3085400000	3.8299990000	-0.5443220000
C	-1.1068130000	4.2885220000	-0.0000760000
C	-0.1493440000	3.3637930000	0.4202620000
C	-0.3902160000	2.0002590000	0.2974910000
H	-3.4834890000	2.1279050000	-1.1115070000
H	-3.0530690000	4.5392820000	-0.8925100000
H	-0.9169500000	5.3531480000	0.0901360000
H	0.7875040000	3.7061040000	0.8494390000
H	0.3590170000	1.2983970000	0.6525690000
H	-1.0515810000	-2.0510170000	1.1316140000

O	1.1267570000	-2.1319340000	2.4092690000
H	1.8990780000	-2.7136280000	2.4566470000

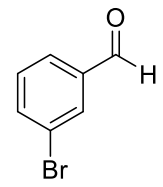
thermodynamic data

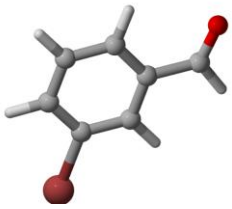
Zero-point correction= 0.399308 (Hartree/Particle)
Thermal correction to Energy= 0.423184
Thermal correction to Enthalpy= 0.424128
Thermal correction to Gibbs Free Energy= 0.343323
Sum of electronic and zero-point Energies= -1379.342854
Sum of electronic and thermal Energies= -1379.318979
Sum of electronic and thermal Enthalpies= -1379.318034
Sum of electronic and thermal Free Energies= -1379.398839

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	265.552	91.718	170.068

SI Computerchemie Reaktionsdiagramm meta-Verbindungen M062X /PCM

M062X/6-311+G**/PCM	***m*-Br-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

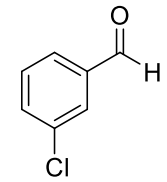
C	-0.5624340000	0.2350150000	0.0000000000
C	-0.3170280000	1.6026020000	-0.0000010000
C	1.0005030000	2.0599240000	0.0000000000
C	2.0541430000	1.1586430000	0.0000010000
C	1.7888480000	-0.2117660000	0.0000020000
C	0.4770950000	-0.6840140000	0.0000010000
C	2.8979660000	-1.1967730000	0.0000040000
O	4.0667910000	-0.8946860000	-0.0000030000
Br	-2.3589980000	-0.3870080000	0.0000000000
H	-1.1424820000	2.3028100000	-0.0000030000
H	1.1915010000	3.1258190000	0.0000000000
H	3.0827690000	1.4984810000	0.0000020000
H	0.2774600000	-1.7497090000	0.0000020000
H	2.5867890000	-2.2564280000	-0.0000080000

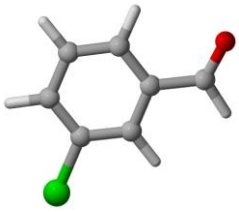
thermodynamic data

Zero-point correction= 0.100434 (Hartree/Particle)
Thermal correction to Energy= 0.108142
Thermal correction to Enthalpy= 0.109086
Thermal correction to Gibbs Free Energy= 0.066568
Sum of electronic and zero-point Energies= -2918.993383
Sum of electronic and thermal Energies= -2918.985675
Sum of electronic and thermal Enthalpies= -2918.984731
Sum of electronic and thermal Free Energies= -2919.027249

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.860	28.037	89.487

M062X/6-311+G**/PCM	***m*-Cl-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.1932610000	-0.0025400000	0.0000000000
C	-1.0985380000	1.3828040000	-0.0000010000
C	0.1608290000	1.9809510000	0.0000000000
C	1.3069410000	1.1998770000	0.0000010000
C	1.1923790000	-0.1911770000	0.0000010000
C	-0.0598200000	-0.8027500000	0.0000010000
C	2.4018660000	-1.0496380000	0.0000030000
O	3.5307920000	-0.6223500000	-0.0000020000
Cl	-2.7705030000	-0.7530730000	0.0000000000
H	-1.9977760000	1.9860110000	-0.0000020000
H	0.2349080000	3.0612670000	0.0000000000
H	2.2926390000	1.6492540000	0.0000010000
H	-0.1485600000	-1.8834650000	0.0000010000
H	2.2086210000	-2.1371920000	-0.0000090000

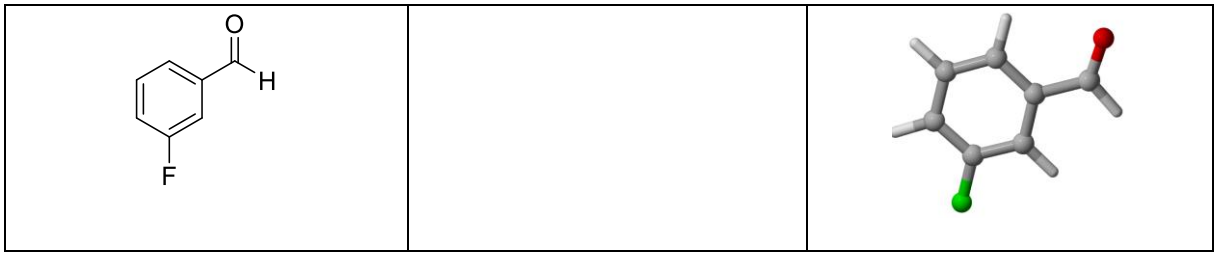
thermodynamic data

Zero-point correction= 0.100978 (Hartree/Particle)
Thermal correction to Energy= 0.108456
Thermal correction to Enthalpy= 0.109400
Thermal correction to Gibbs Free Energy= 0.068159
Sum of electronic and zero-point Energies= -805.021263

Sum of electronic and thermal Energies= -805.013785
Sum of electronic and thermal Enthalpies= -805.012841
Sum of electronic and thermal Free Energies= -805.054082

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.057	27.600	86.801

M062X/6-311+G**/PCM	***m*-F-PhCHO**



xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

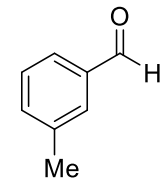
C	1.5346440000	-0.3933300000	0.0000010000
C	1.6998120000	0.9800890000	0.0000010000
C	0.5650400000	1.7905690000	-0.0000010000
C	-0.7011320000	1.2228680000	0.0000000000
C	-0.8353920000	-0.1666650000	0.0000000000
C	0.2887020000	-0.9916590000	0.0000000000
C	-2.1784300000	-0.7963160000	-0.0000020000
O	-3.2138610000	-0.1756270000	0.0000010000
F	2.6291870000	-1.1777330000	-0.0000010000
H	2.6987090000	1.3981780000	0.0000010000
H	0.6810850000	2.8670870000	-0.0000010000
H	-1.5915680000	1.8395030000	0.0000000000
H	0.2013050000	-2.0725320000	-0.0000010000
H	-2.1807800000	-1.9009640000	0.0000060000

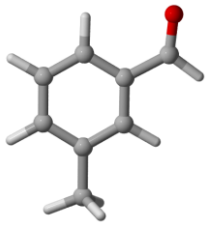
thermodynamic data

Zero-point correction= 0.102432 (Hartree/Particle)
Thermal correction to Energy= 0.109523
Thermal correction to Enthalpy= 0.110467
Thermal correction to Gibbs Free Energy= 0.070579
Sum of electronic and zero-point Energies= -444.661133
Sum of electronic and thermal Energies= -444.654042
Sum of electronic and thermal Enthalpies= -444.653098
Sum of electronic and thermal Free Energies= -444.692986

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.727	26.711	83.953

M062X/6-311+G**/PCM	***m*-Me-PhCHO**





xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

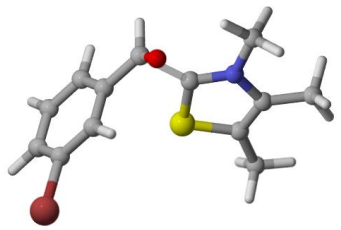
C	1.5553200000	-0.3124770000	-0.0000060000
C	1.5970520000	1.0812500000	0.0000010000
C	0.4275400000	1.8459350000	0.0000000000
C	-0.8095750000	1.2236540000	-0.0000020000
C	-0.8679370000	-0.1732340000	-0.0000060000
C	0.3020410000	-0.9289740000	-0.0000120000
C	-2.1697870000	-0.8754120000	-0.0000040000
O	-3.2445110000	-0.3214660000	0.0000120000
C	2.8146270000	-1.1387990000	0.0000090000
H	2.5597190000	1.5818570000	0.0000060000
H	0.4934840000	2.9273810000	0.0000000000
H	-1.7300190000	1.7953860000	-0.0000020000
H	0.2358660000	-2.0141360000	-0.0000200000
H	-2.1068790000	-1.9789400000	0.0000040000
H	3.7010420000	-0.5044750000	-0.0001380000
H	2.8536600000	-1.7833840000	0.8810250000
H	2.8535330000	-1.7836180000	-0.8808410000

thermodynamic data

Zero-point correction= 0.137964 (Hartree/Particle)
Thermal correction to Energy= 0.146071
Thermal correction to Enthalpy= 0.147015
Thermal correction to Gibbs Free Energy= 0.104952
Sum of electronic and zero-point Energies= -384.691907
Sum of electronic and thermal Energies= -384.683800
Sum of electronic and thermal Enthalpies= -384.682856
Sum of electronic and thermal Free Energies= -384.724919

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.661	29.936	88.530

M062X/6-311+G**/PCM	**TST1 *m*-Br**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.8196250000	0.6587900000	0.3412590000
S	-1.5235250000	-0.9594730000	0.8087220000
N	-2.9956930000	0.6904570000	-0.2751660000
C	-3.7080280000	-0.5179760000	-0.3960440000
C	-3.0329030000	-1.5516500000	0.1581540000
C	-5.0328380000	-0.5315330000	-1.0864270000
C	-3.4084170000	-2.9969250000	0.2424310000
C	-3.5475920000	1.9504520000	-0.7866180000
C	0.7937570000	1.3579590000	0.6489820000
C	0.9249290000	1.0808950000	2.0075500000
C	1.9528930000	0.2606360000	2.4569800000
C	2.8593130000	-0.2892840000	1.5530360000
C	2.7172440000	0.0084210000	0.2028790000
C	1.7001460000	0.8272430000	-0.2649140000
C	-0.3238630000	2.2441770000	0.1588670000
O	-0.3570730000	2.6589460000	-1.0032370000
H	-0.8211600000	2.7969180000	0.9710990000
H	-5.4896330000	-1.5157150000	-1.0060910000
H	-5.7150570000	0.1975210000	-0.6440840000
H	-4.9249030000	-0.2933170000	-2.1473170000
H	-4.4310910000	-3.1516560000	-0.0998340000
H	-3.3362570000	-3.3583830000	1.2696030000
H	-2.7470250000	-3.6073050000	-0.3759450000
H	-2.7715100000	2.7073460000	-0.7188560000
H	-4.4147490000	2.2399210000	-0.1927350000
H	-3.8438920000	1.8259530000	-1.8274910000
H	0.2098700000	1.4992780000	2.7094600000
H	2.0561580000	0.0416340000	3.5129170000
H	3.6617450000	-0.9311690000	1.8928240000
H	1.5942580000	1.0595910000	-1.3175080000
Br	3.9635990000	-0.7220300000	-1.0408680000

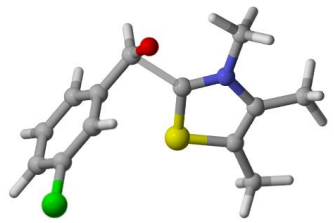
thermodynamic data

Zero-point correction= 0.241341 (Hartree/Particle)
Thermal correction to Energy= 0.258850
Thermal correction to Enthalpy= 0.259794
Thermal correction to Gibbs Free Energy= 0.191849
Sum of electronic and zero-point Energies= -3605.750178

Sum of electronic and thermal Energies= -3605.732669
Sum of electronic and thermal Enthalpies= -3605.731725
Sum of electronic and thermal Free Energies= -3605.799670

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.431	62.770	143.003

M062X/6-311+G**/PCM	**TST1 *m*-Cl**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2229360000	0.6015160000	0.4282610000
S	-1.0057550000	-1.0838800000	0.6234290000
N	-2.4390920000	0.7954020000	-0.0692450000
C	-3.2420340000	-0.3372430000	-0.3035510000
C	-2.5987550000	-1.4807380000	0.0288900000
C	-4.6176710000	-0.1680020000	-0.8614680000
C	-3.0695060000	-2.8978260000	-0.0573200000
C	-2.9390700000	2.1491700000	-0.3357970000
C	1.4486760000	1.0834800000	0.5669770000
C	1.7058390000	0.5743250000	1.8376090000
C	2.7091580000	-0.3705190000	2.0212940000
C	3.4618910000	-0.8152550000	0.9377170000
C	3.1933830000	-0.2902850000	-0.3204690000
C	2.2014540000	0.6572840000	-0.5231830000
C	0.3591200000	2.1066370000	0.3654890000
O	0.2457510000	2.7292840000	-0.6947810000
H	-0.0127200000	2.5297440000	1.3116450000
H	-5.1285040000	-1.1273830000	-0.9042960000
H	-5.2127370000	0.5054020000	-0.2407670000
H	-4.5841510000	0.2446920000	-1.8725420000
H	-4.0649680000	-2.9498450000	-0.4965350000
H	-3.1101550000	-3.3552860000	0.9331760000
H	-2.3959410000	-3.4941880000	-0.6755180000
H	-2.1057380000	2.8387080000	-0.2363570000
H	-3.7265340000	2.3966470000	0.3763110000
H	-3.3340550000	2.2024890000	-1.3494950000
H	1.1087200000	0.9109320000	2.6796420000
H	2.9096060000	-0.7694660000	3.0083790000

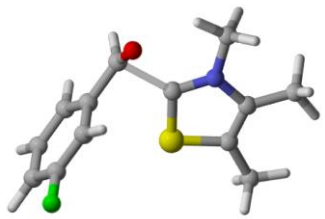
H	4.2433550000	-1.5534080000	1.0657690000
H	2.0029010000	1.0637430000	-1.5075040000
Cl	4.1337260000	-0.8457680000	-1.6900300000

thermodynamic data

Zero-point correction= 0.241634 (Hartree/Particle)
Thermal correction to Energy= 0.258894
Thermal correction to Enthalpy= 0.259839
Thermal correction to Gibbs Free Energy= 0.192894
Sum of electronic and zero-point Energies= -1491.778106
Sum of electronic and thermal Energies= -1491.760846
Sum of electronic and thermal Enthalpies= -1491.759902
Sum of electronic and thermal Free Energies= -1491.826847

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.459	62.434	140.898

M062X/6-311+G**/PCM	**TST1 *m*-F**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.8943670000	0.5307120000	0.4407300000
S	-0.7832810000	-1.1764750000	0.4442660000
N	-2.1276870000	0.8525200000	0.0679350000
C	-3.0252900000	-0.1960350000	-0.2113760000
C	-2.4418640000	-1.4063270000	-0.0511970000
C	-4.4242340000	0.1181440000	-0.6316540000
C	-3.0169130000	-2.7737740000	-0.2418830000
C	-2.5492590000	2.2559280000	-0.0192540000
C	1.8072770000	0.8548950000	0.4334130000
C	2.1461020000	0.1227850000	1.5698720000
C	3.1055570000	-0.8819780000	1.4946080000
C	3.7346700000	-1.1624630000	0.2846200000
C	3.3806060000	-0.4116980000	-0.8241120000
C	2.4351950000	0.5941620000	-0.7813590000
C	0.7683150000	1.9441740000	0.5145440000
O	0.6213450000	2.7643250000	-0.3976970000
H	0.4915520000	2.1968780000	1.5499000000

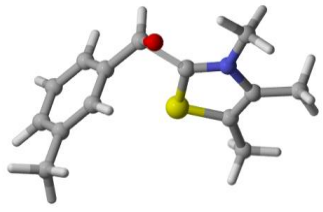
H	-5.0052260000	-0.7970140000	-0.7231910000
H	-4.9181090000	0.7619250000	0.0994760000
H	-4.4402690000	0.6288560000	-1.5974160000
H	-4.0647650000	-2.7162330000	-0.5341470000
H	-2.9523880000	-3.3543920000	0.6801970000
H	-2.4774070000	-3.3169110000	-1.0201560000
H	-1.6623450000	2.8767160000	0.0728490000
H	-3.2571850000	2.4772160000	0.7797020000
H	-3.0211900000	2.4367040000	-0.9842530000
H	1.6483660000	0.3356750000	2.5107430000
H	3.3689310000	-1.4518040000	2.3775060000
H	4.4847660000	-1.9378570000	0.1926640000
F	3.9914030000	-0.6771550000	-2.0000720000
H	2.1834210000	1.1648430000	-1.6671600000

thermodynamic data

Zero-point correction= 0.243315 (Hartree/Particle)
Thermal correction to Energy= 0.260075
Thermal correction to Enthalpy= 0.261019
Thermal correction to Gibbs Free Energy= 0.196664
Sum of electronic and zero-point Energies= -1131.417707
Sum of electronic and thermal Energies= -1131.400947
Sum of electronic and thermal Enthalpies= -1131.400002
Sum of electronic and thermal Free Energies= -1131.464358

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.200	61.458	135.447

M062X/6-311+G**/PCM	**TST1 *m*-Me**

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9186000000	0.5438070000	-0.4294930000
S	0.7807490000	-1.1610420000	-0.4569170000
N	2.1542100000	0.8425330000	-0.0458320000
C	3.0343490000	-0.2231210000	0.2238870000
C	2.4333980000	-1.4221500000	0.0440540000
C	4.4358930000	0.0643160000	0.6546320000
C	2.9864800000	-2.8005660000	0.2209640000

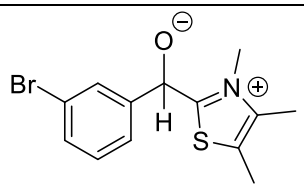
C	2.5946870000	2.2386080000	0.0620360000
C	-1.7743740000	0.8870730000	-0.4492000000
C	-2.0963850000	0.2156000000	-1.6248730000
C	-3.0765500000	-0.7729950000	-1.6092590000
C	-3.7301830000	-1.0856060000	-0.4219100000
C	-3.4228580000	-0.4128620000	0.7662330000
C	-2.4417560000	0.5761550000	0.7339660000
C	-0.7110200000	1.9551000000	-0.4601350000
O	-0.5609300000	2.7337730000	0.4922170000
H	-0.4243450000	2.2603370000	-1.4798040000
H	5.0027840000	-0.8605040000	0.7365240000
H	4.9425390000	0.7103320000	-0.0657310000
H	4.4552990000	0.5619240000	1.6271820000
H	4.0347460000	-2.7628930000	0.5151370000
H	2.9139850000	-3.3704640000	-0.7071870000
H	2.4373210000	-3.3432290000	0.9928300000
H	1.7155510000	2.8720400000	-0.0186160000
H	3.3049490000	2.4624960000	-0.7341790000
H	3.0696150000	2.3984530000	1.0292450000
H	-1.5727560000	0.4601000000	-2.5446520000
H	-3.3316560000	-1.3003880000	-2.5212890000
H	-4.4927720000	-1.8582730000	-0.4131230000
H	-2.1791260000	1.1215470000	1.6348140000
C	-4.1437280000	-0.7599670000	2.0437850000
H	-3.8082530000	-0.1309490000	2.8687240000
H	-3.9688650000	-1.8035920000	2.3164280000
H	-5.2223470000	-0.6285270000	1.9293240000

thermodynamic data

Zero-point correction= 0.278457 (Hartree/Particle)
Thermal correction to Energy= 0.296411
Thermal correction to Enthalpy= 0.297355
Thermal correction to Gibbs Free Energy= 0.228516
Sum of electronic and zero-point Energies= -1071.446298
Sum of electronic and thermal Energies= -1071.428344
Sum of electronic and thermal Enthalpies= -1071.427399
Sum of electronic and thermal Free Energies= -1071.496238

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.001	64.712	144.883

M062X/6-311+G**/PCM	**Zwitterion *m*-Br**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

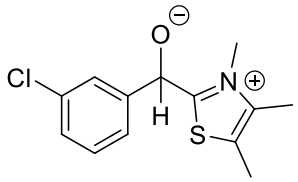
C	-1.4686230000	-1.6868460000	-1.7652480000
C	-2.6644510000	-1.0176300000	-1.5102640000
C	-2.7842050000	-0.3153230000	-0.3192500000
C	-1.7541610000	-0.2581780000	0.6102360000
C	-0.5638990000	-0.9243770000	0.3430180000
C	-0.4275000000	-1.6435340000	-0.8451530000
C	0.5649150000	-0.8577230000	1.4024100000
C	1.8355660000	-0.3741270000	0.6685170000
O	0.3137360000	-0.0912300000	2.4666400000
S	3.2412440000	-1.3093760000	0.5032140000
C	4.0868710000	-0.0161180000	-0.2949090000
C	3.2756960000	1.0650420000	-0.4014820000
N	2.0146830000	0.8340230000	0.1619220000
C	5.5029390000	-0.1938720000	-0.7411540000
C	3.5769000000	2.3876970000	-1.0253510000
C	0.9495730000	1.8486730000	0.1636650000
H	-3.4807510000	-1.0463960000	-2.2202220000
H	-1.3582540000	-2.2433040000	-2.6885820000
Br	-4.4154820000	0.6036600000	0.0507780000
H	-1.8399400000	0.2927230000	1.5392010000
H	0.4970640000	-2.1740020000	-1.0538130000
H	0.7940950000	-1.9213410000	1.6374830000
H	5.8950620000	0.7379120000	-1.1448450000
H	6.1354900000	-0.4919840000	0.0964520000
H	5.5759220000	-0.9618200000	-1.5131730000
H	2.8059660000	2.6577030000	-1.7495220000
H	3.6326480000	3.1764870000	-0.2717210000
H	4.5305560000	2.3456600000	-1.5458550000
H	1.4015630000	2.8285120000	0.2958680000
H	0.4126290000	1.8075060000	-0.7848330000
H	0.2895330000	1.6238240000	0.9981140000

thermodynamic data

Zero-point correction= 0.243780 (Hartree/Particle)
Thermal correction to Energy= 0.260679
Thermal correction to Enthalpy= 0.261623
Thermal correction to Gibbs Free Energy= 0.197533
Sum of electronic and zero-point Energies= -3605.765095
Sum of electronic and thermal Energies= -3605.748196
Sum of electronic and thermal Enthalpies= -3605.747251
Sum of electronic and thermal Free Energies= -3605.811342

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.579	62.820	134.890

M062X/6-311+G**/PCM	**Zwitterion *m*-Cl**



xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

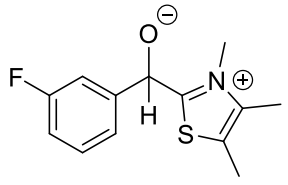
C	-2.1656370000	-1.5272390000	-1.7059130000
C	-3.3044510000	-0.7619310000	-1.4632560000
C	-3.3619110000	-0.0199110000	-0.2923510000
C	-2.3255140000	-0.0193450000	0.6308910000
C	-1.1913440000	-0.7805730000	0.3769560000
C	-1.1172550000	-1.5383230000	-0.7930540000
C	-0.0533610000	-0.7720430000	1.4288320000
C	1.2342620000	-0.3619770000	0.6787250000
O	-0.2552150000	0.0104170000	2.4918870000
S	2.5733800000	-1.3838720000	0.4752490000
C	3.4828240000	-0.1410150000	-0.3314860000
C	2.7423670000	0.9922020000	-0.4088060000
N	1.4813060000	0.8371660000	0.1793330000
C	4.8739510000	-0.4084090000	-0.8102300000
C	3.1178840000	2.3019970000	-1.0190210000
C	0.4830180000	1.9171660000	0.2089900000
H	-4.1279380000	-0.7436350000	-2.1654750000
H	-2.1051180000	-2.1163430000	-2.6134430000
Cl	-4.7866650000	0.9535440000	0.0252980000
H	-2.3686210000	0.5607380000	1.5448640000
H	-0.2371680000	-2.1427620000	-0.9927220000
H	0.1208690000	-1.8456300000	1.6658630000
H	5.2825460000	0.4690510000	-1.3079250000
H	5.5278900000	-0.6598400000	0.0265400000
H	4.8888850000	-1.2407140000	-1.5157010000
H	2.3589770000	2.6297850000	-1.7319490000
H	3.2279910000	3.0745780000	-0.2546800000
H	4.0639990000	2.2104520000	-1.5467490000
H	0.9973050000	2.8652830000	0.3435530000
H	-0.0709450000	1.9201470000	-0.7306280000
H	-0.1758630000	1.7234980000	1.0523040000

thermodynamic data

Zero-point correction= 0.243996 (Hartree/Particle)
Thermal correction to Energy= 0.259955
Thermal correction to Enthalpy= 0.260899
Thermal correction to Gibbs Free Energy= 0.199225
Sum of electronic and zero-point Energies= -1491.793165
Sum of electronic and thermal Energies= -1491.777207
Sum of electronic and thermal Enthalpies= -1491.776263
Sum of electronic and thermal Free Energies= -1491.837937

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.124	60.508	129.804

M062X/6-311+G**/PCM	**Zwitterion *m*-F**



xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.5900070000	-1.3239130000	-1.6550380000
C	-3.6799400000	-0.4866800000	-1.4230230000
C	-3.6701830000	0.2798170000	-0.2726580000
C	-2.6346050000	0.2524370000	0.6437940000
C	-1.5513810000	-0.5825760000	0.4002270000
C	-1.5346020000	-1.3739100000	-0.7509020000
C	-0.4091020000	-0.6196050000	1.4459760000
C	0.9016490000	-0.3268250000	0.6806180000
O	-0.5479410000	0.2090380000	2.4839600000
S	2.1561160000	-1.4545900000	0.4943040000
C	3.1602410000	-0.3015590000	-0.3330090000
C	2.5116870000	0.8852100000	-0.4293140000
N	1.2415220000	0.8395060000	0.1591910000
C	4.5258510000	-0.6860080000	-0.8055440000
C	2.9878390000	2.1544730000	-1.0544620000
C	0.3332580000	1.9962330000	0.1641510000
H	-4.5159580000	-0.4283410000	-2.1083430000
H	-2.5719930000	-1.9393940000	-2.5467350000
F	-4.7232460000	1.0960840000	-0.0338880000
H	-2.6469640000	0.8627890000	1.5389500000
H	-0.6950900000	-2.0357940000	-0.9415060000
H	-0.3095670000	-1.6944440000	1.7177580000
H	4.9951050000	0.1417240000	-1.3341450000
H	5.1638300000	-0.9567580000	0.0376200000
H	4.4762030000	-1.5401430000	-1.4827090000

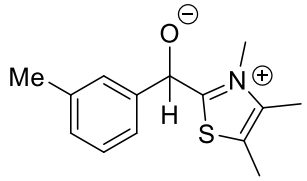
H	2.2615970000	2.5272590000	-1.7792950000
H	3.1457330000	2.9274280000	-0.2989390000
H	3.9299420000	1.9880950000	-1.5708070000
H	0.9160360000	2.8974840000	0.3393350000
H	-0.1724140000	2.0593370000	-0.8001760000
H	-0.3764550000	1.8480240000	0.9742090000

thermodynamic data

Zero-point correction= 0.245714 (Hartree/Particle)
Thermal correction to Energy= 0.262133
Thermal correction to Enthalpy= 0.263077
Thermal correction to Gibbs Free Energy= 0.199898
Sum of electronic and zero-point Energies= -1131.432747
Sum of electronic and thermal Energies= -1131.416327
Sum of electronic and thermal Enthalpies= -1131.415383
Sum of electronic and thermal Free Energies= -1131.478562

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.491	61.591	132.971

M062X/6-311+G**/PCM	**Zwitterion *m*-Me**	



xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.5376410000	-1.3600210000	-1.6714090000
C	-3.6383930000	-0.5434460000	-1.4291080000
C	-3.6996100000	0.2423840000	-0.2756420000
C	-2.6320420000	0.1918870000	0.6226090000
C	-1.5249800000	-0.6175700000	0.3900860000
C	-1.4828820000	-1.4002940000	-0.7638680000
C	-0.3846300000	-0.6467990000	1.4376970000
C	0.9240700000	-0.3315890000	0.6787840000
O	-0.5270120000	0.1721090000	2.4857650000
S	2.1974580000	-1.4388210000	0.4922080000
C	3.1853830000	-0.2674490000	-0.3298590000
C	2.5180540000	0.9088180000	-0.4240710000
N	1.2473890000	0.8412120000	0.1613540000
C	4.5586310000	-0.6279880000	-0.7991560000
C	2.9753260000	2.1871290000	-1.0449510000
C	0.3206390000	1.9829040000	0.1675270000

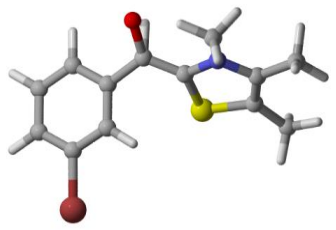
H	-4.4594800000	-0.5174310000	-2.1387870000
H	-2.5044360000	-1.9689150000	-2.5681370000
H	-2.6386890000	0.7866460000	1.5301970000
H	-0.6302110000	-2.0463820000	-0.9550090000
H	-0.2684560000	-1.7218480000	1.7034260000
H	5.0092660000	0.2025030000	-1.3395820000
H	5.2034460000	-0.8737360000	0.0465730000
H	4.5272510000	-1.4920110000	-1.4647680000
H	2.2451020000	2.5499660000	-1.7708460000
H	3.1189330000	2.9608590000	-0.2873520000
H	3.9214800000	2.0369280000	-1.5589220000
H	0.8876610000	2.8921010000	0.3537160000
H	-0.1789520000	2.0445300000	-0.8000850000
H	-0.3935000000	1.8166660000	0.9702260000
C	-4.8965140000	1.1221090000	-0.0166680000
H	-4.8051180000	1.6380810000	0.9395380000
H	-5.8165410000	0.5328770000	-0.0010550000
H	-5.0051770000	1.8745050000	-0.8018840000

thermodynamic data

Zero-point correction= 0.281342 (Hartree/Particle)
Thermal correction to Energy= 0.298792
Thermal correction to Enthalpy= 0.299736
Thermal correction to Gibbs Free Energy= 0.233998
Sum of electronic and zero-point Energies= -1071.459810
Sum of electronic and thermal Energies= -1071.442360
Sum of electronic and thermal Enthalpies= -1071.441416
Sum of electronic and thermal Free Energies= -1071.507155

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	187.495	64.733	138.358

M062X/6-311+G**/PCM	**TST2 *m*-Br**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	1.6059970000	0.5893390000	-0.0697790000
S	1.4088320000	-0.8632610000	-1.0180350000

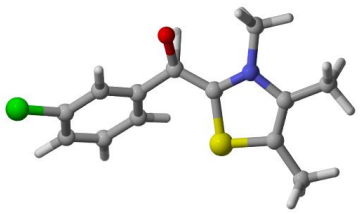
N	2.8161230000	0.5820440000	0.5268630000
C	3.6377550000	-0.5125100000	0.1879540000
C	3.0386010000	-1.3922230000	-0.6339590000
C	5.0165180000	-0.5851420000	0.7585100000
C	3.5390630000	-2.6785640000	-1.2065750000
C	3.1768610000	1.4576310000	1.6486560000
C	-0.7721210000	1.4148240000	-0.3140970000
C	-1.5650640000	2.3994710000	-0.9169560000
C	-2.9306370000	2.2146110000	-1.0742720000
C	-3.5469800000	1.0447090000	-0.6318340000
C	-2.7582780000	0.0845650000	-0.0173770000
C	-1.3907220000	0.2535480000	0.1579860000
C	0.6825740000	1.6685850000	-0.1346440000
O	1.0360890000	2.9550440000	0.4129640000
H	1.1588170000	2.5169450000	-0.8249150000
H	4.9924330000	-0.5961400000	1.8503590000
H	5.5153470000	-1.4898150000	0.4193800000
H	5.6149620000	0.2723330000	0.4421020000
H	4.5294150000	-2.9122920000	-0.8195380000
H	3.6010680000	-2.6262750000	-2.2956530000
H	2.8703810000	-3.5022690000	-0.9471720000
H	3.0967250000	0.8963140000	2.5812870000
H	2.4945730000	2.3027590000	1.6549340000
H	4.2007850000	1.8044420000	1.5201520000
H	-1.0972510000	3.3133810000	-1.2636840000
H	-3.5286860000	2.9816140000	-1.5517560000
H	-4.6105520000	0.8905310000	-0.7581630000
Br	-3.5703330000	-1.5142590000	0.6312280000
H	-0.8206570000	-0.5080110000	0.6748110000

thermodynamic data

Zero-point correction= 0.238263 (Hartree/Particle)
Thermal correction to Energy= 0.255534
Thermal correction to Enthalpy= 0.256478
Thermal correction to Gibbs Free Energy= 0.191009
Sum of electronic and zero-point Energies= -3605.693184
Sum of electronic and thermal Energies= -3605.675913
Sum of electronic and thermal Enthalpies= -3605.674968
Sum of electronic and thermal Free Energies= -3605.740438

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.350	63.767	137.792

M062X/6-311+G**/PCM	**TST2 *m*-Cl**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.1691430000	0.3592400000	0.2061920000
S	-1.3388990000	-1.3129590000	-0.2012820000
N	-2.3679120000	0.9701530000	0.1437240000
C	-3.4408160000	0.1374670000	-0.2170640000
C	-3.0631620000	-1.1404660000	-0.4281470000
C	-4.8190090000	0.7031830000	-0.3324470000
C	-3.8760080000	-2.3382530000	-0.8031650000
C	-2.5585120000	2.3444540000	0.6177330000
C	1.3086340000	0.1966380000	0.5365660000
C	1.4224420000	-0.9698720000	1.3052360000
C	2.6053340000	-1.6962820000	1.3165100000
C	3.7083120000	-1.2744150000	0.5762270000
C	3.5882900000	-0.1080430000	-0.1644660000
C	2.4165890000	0.6342810000	-0.1944820000
C	0.0678280000	1.0082780000	0.4994020000
O	0.2177560000	2.3624890000	-0.0135800000
H	-0.0032060000	1.9680110000	1.2120680000
H	-4.8272870000	1.5722810000	-0.9934710000
H	-5.4924710000	-0.0422740000	-0.7479840000
H	-5.2110670000	1.0072620000	0.6406220000
H	-3.5532340000	-2.7446560000	-1.7638030000
H	-4.9310700000	-2.0815070000	-0.8783200000
H	-3.7718140000	-3.1242990000	-0.0523690000
H	-3.6208830000	2.5309040000	0.7333660000
H	-2.1131320000	3.0525960000	-0.0732450000
H	-2.0731040000	2.4447990000	1.5910520000
H	0.5903090000	-1.2950140000	1.9193230000
H	2.6808280000	-2.5934490000	1.9194090000
H	4.6381110000	-1.8281230000	0.5866020000
Cl	4.9678520000	0.4565250000	-1.0891240000
H	2.3455740000	1.5516640000	-0.7636100000

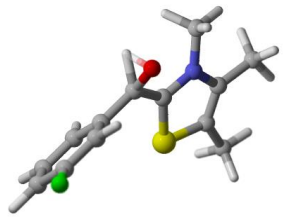
thermodynamic data

Zero-point correction= 0.239438 (Hartree/Particle)
Thermal correction to Energy= 0.256245
Thermal correction to Enthalpy= 0.257189
Thermal correction to Gibbs Free Energy= 0.194101

Sum of electronic and zero-point Energies= -1491.723326
Sum of electronic and thermal Energies= -1491.706518
Sum of electronic and thermal Enthalpies= -1491.705574
Sum of electronic and thermal Free Energies= -1491.768663

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.796	63.023	132.781

M062X/6-311+G**/PCM	**TST2 *m*-F**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8492450000	0.3752140000	-0.1607440000
S	0.9902140000	-1.3170700000	0.1698240000
N	2.0675180000	0.9492280000	-0.1410000000
C	3.1328380000	0.0725170000	0.1261160000
C	2.7287720000	-1.2016410000	0.3091100000
C	4.5321250000	0.5935260000	0.1836120000
C	3.5248210000	-2.4348730000	0.5943390000
C	2.2731260000	2.3343980000	-0.5754600000
C	-1.6477440000	0.2986790000	-0.3536900000
C	-1.8430810000	-0.8345780000	-1.1565920000
C	-3.0480530000	-1.5242210000	-1.1260610000
C	-4.0929710000	-1.0988200000	-0.3070910000
C	-3.8817670000	0.0305470000	0.4607920000
C	-2.6962820000	0.7414190000	0.4570860000
C	-0.3812380000	1.0705990000	-0.3575510000
O	-0.4599080000	2.4067820000	0.2163500000
H	-0.3177560000	2.0567130000	-1.0343800000
H	4.6043250000	1.4359280000	0.8744760000
H	5.2040550000	-0.1864730000	0.5328880000
H	4.8783370000	0.9228590000	-0.7985760000
H	3.2342130000	-2.8752310000	1.5502860000
H	4.5885530000	-2.2074550000	0.6333240000
H	3.3677750000	-3.1846800000	-0.1838380000
H	3.3351300000	2.5045540000	-0.7160050000
H	1.8613250000	3.0269820000	0.1508620000
H	1.7612530000	2.4759400000	-1.5304000000
H	-1.0578240000	-1.1618520000	-1.8281340000

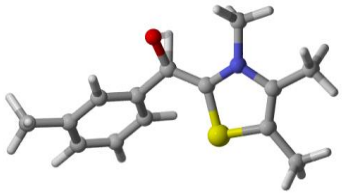
H	-3.1864470000	-2.3941130000	-1.7569120000
H	-5.0452390000	-1.6121370000	-0.2725570000
F	-4.8872500000	0.4671990000	1.2549150000
H	-2.5779700000	1.6318250000	1.0605360000

thermodynamic data

Zero-point correction= 0.240533 (Hartree/Particle)
Thermal correction to Energy= 0.256928
Thermal correction to Enthalpy= 0.257872
Thermal correction to Gibbs Free Energy= 0.196320
Sum of electronic and zero-point Energies= -1131.363526
Sum of electronic and thermal Energies= -1131.347131
Sum of electronic and thermal Enthalpies= -1131.346187
Sum of electronic and thermal Free Energies= -1131.407739

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.225	62.204	129.547

M062X/6-311+G**/PCM	**TST2 *m*-Me**

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.8627720000	0.3866660000	-0.1652060000
S	0.9864760000	-1.3086490000	0.1679240000
N	2.0864490000	0.9527110000	-0.1231190000
C	3.1406160000	0.0664940000	0.1585000000
C	2.7248210000	-1.2043150000	0.3350220000
C	4.5429660000	0.5768870000	0.2368220000
C	3.5073640000	-2.4427050000	0.6351040000
C	2.3090030000	2.3315670000	-0.5669350000
C	-1.6266400000	0.3014250000	-0.4005560000
C	-1.8090930000	-0.8021470000	-1.2446980000
C	-3.0047330000	-1.5073070000	-1.2215540000
C	-4.0372120000	-1.1184380000	-0.3691290000
C	-3.8844050000	-0.0098100000	0.4631120000
C	-2.6757520000	0.6904640000	0.4340090000
C	-0.3601730000	1.0799720000	-0.3900280000
O	-0.4464940000	2.4294360000	0.1509430000
H	-0.2733110000	2.0501060000	-1.0879540000

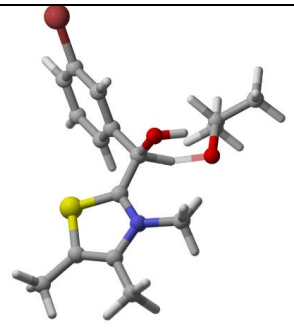
H	4.6116430000	1.4184780000	0.9291370000
H	5.2043240000	-0.2082480000	0.5947490000
H	4.9057250000	0.9047260000	-0.7399640000
H	3.2020380000	-2.8762970000	1.5896910000
H	4.5725900000	-2.2243800000	0.6853990000
H	3.3529720000	-3.1952400000	-0.1410600000
H	3.3751230000	2.4976570000	-0.6792450000
H	1.8796960000	3.0341740000	0.1392290000
H	1.8240420000	2.4647600000	-1.5374630000
H	-1.0223230000	-1.0939740000	-1.9320310000
H	-3.1399530000	-2.3582160000	-1.8796710000
H	-4.9695620000	-1.6733300000	-0.3600420000
H	-2.5349610000	1.5643760000	1.0605670000
C	-5.0074980000	0.4509150000	1.3575710000
H	-4.6273650000	0.7924520000	2.3219820000
H	-5.7277970000	-0.3495330000	1.5316850000
H	-5.5419120000	1.2884010000	0.9002840000

thermodynamic data

Zero-point correction= 0.276397 (Hartree/Particle)
Thermal correction to Energy= 0.293799
Thermal correction to Enthalpy= 0.294744
Thermal correction to Gibbs Free Energy= 0.230722
Sum of electronic and zero-point Energies= -1071.390716
Sum of electronic and thermal Energies= -1071.373314
Sum of electronic and thermal Enthalpies= -1071.372369
Sum of electronic and thermal Free Energies= -1071.436391

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	184.362	65.295	134.745

M062X/6-311+G**/PCM	**TST2 mit Isopropanol *m*-Br**

xyz-matrix

43
XYZ file generated by gabedit : coordinates in Angstrom
C -1.8055130000 -0.2598330000 -0.1238050000

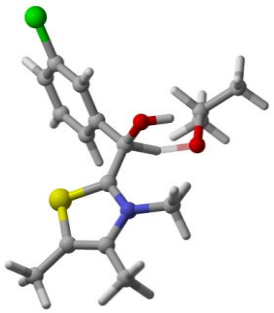
S	-1.8675520000	-1.7928710000	0.6302470000
N	-3.0076240000	0.0865680000	-0.5756070000
C	-4.0166350000	-0.8617870000	-0.3680930000
C	-3.5677430000	-1.9497920000	0.3009020000
C	-5.3998610000	-0.5982710000	-0.8655350000
C	-4.3118710000	-3.1671030000	0.7491510000
C	-3.2724990000	1.3807530000	-1.2231850000
C	0.6284380000	-0.0320490000	0.3490890000
C	0.7081490000	-0.1630110000	1.7393470000
C	1.8425140000	-0.6993400000	2.3347560000
C	2.9284440000	-1.0983830000	1.5587340000
C	2.8408090000	-0.9480830000	0.1816990000
C	1.7121540000	-0.4277990000	-0.4365350000
C	-0.5963020000	0.5687430000	-0.2775060000
O	-0.4168550000	0.9016030000	-1.6473000000
H	-0.7890520000	1.7096910000	0.1906370000
H	-5.3827210000	-0.3085740000	-1.9179570000
H	-6.0042530000	-1.4974220000	-0.7733210000
H	-5.8832350000	0.1997590000	-0.2974300000
H	-4.1097500000	-3.3755740000	1.8008650000
H	-4.0173090000	-4.0421610000	0.1666530000
H	-5.3847860000	-3.0220560000	0.6356240000
H	-4.2869710000	1.6831360000	-0.9774010000
H	-3.1631310000	1.2789880000	-2.3023900000
H	-2.5709950000	2.1204140000	-0.8410430000
H	-0.1192810000	0.1714350000	2.3568520000
H	1.8950870000	-0.7953770000	3.4127130000
Br	4.3256550000	-1.4628070000	-0.8986630000
H	1.6671700000	-0.3120860000	-1.5112770000
C	0.8093990000	4.7835210000	-0.5092140000
C	0.4863220000	3.5430240000	0.3249000000
H	0.6720450000	4.5684750000	-1.5721840000
H	1.8383650000	5.1216650000	-0.3532770000
H	0.1316940000	5.5982190000	-0.2350340000
C	0.6896280000	3.8250740000	1.8157670000
H	0.4701070000	2.9258500000	2.3983090000
H	0.0057280000	4.6172200000	2.1375950000
H	1.7148700000	4.1387960000	2.0359460000
O	-0.8092120000	3.0977730000	0.0642130000
H	1.2227000000	2.7606030000	0.0436830000
H	-0.4351930000	1.8732190000	-1.6526920000
H	3.8211100000	-1.5050250000	2.0154920000

thermodynamic data

Zero-point correction= 0.349389 (Hartree/Particle)
Thermal correction to Energy= 0.372864
Thermal correction to Enthalpy= 0.373808
Thermal correction to Gibbs Free Energy= 0.293425
Sum of electronic and zero-point Energies= -3799.974262
Sum of electronic and thermal Energies= -3799.950787
Sum of electronic and thermal Enthalpies= -3799.949843
Sum of electronic and thermal Free Energies= -3800.030227

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.976	85.683	169.182

M062X/6-311+G**/PCM	**TST2 mit Isopropanol *m*-Cl**



xyz-matrix

43
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3965750000	-0.1007920000	-0.1314930000
S	-1.7212940000	-1.6407740000	0.5366740000
N	-2.5294220000	0.5129740000	-0.4617450000
C	-3.6958140000	-0.2258450000	-0.2270530000
C	-3.4362980000	-1.4282610000	0.3379230000
C	-5.0249160000	0.3476760000	-0.5937670000
C	-4.3829000000	-2.5023600000	0.7704580000
C	-2.5666300000	1.8783260000	-1.0080410000
C	1.0544010000	-0.4147970000	0.1466510000
C	1.2240690000	-0.6323340000	1.5177940000
C	2.2502990000	-1.4453410000	1.9818710000
C	3.1359880000	-2.0448960000	1.0899810000
C	2.9625600000	-1.8095210000	-0.2666310000
C	1.9392960000	-1.0088120000	-0.7535660000
C	-0.0550740000	0.4738300000	-0.3364980000
O	0.0946630000	0.8634490000	-1.6955120000
H	0.0235420000	1.5883030000	0.2175970000
H	-5.0204430000	0.7013340000	-1.6265150000
H	-5.7959330000	-0.4132620000	-0.5001140000
H	-5.2903780000	1.1854870000	0.0549030000
H	-5.4083480000	-2.1376830000	0.7519620000
H	-4.1589930000	-2.8258810000	1.7881220000
H	-4.3131040000	-3.3720750000	0.1142780000
H	-3.4718330000	2.3626560000	-0.6515530000
H	-2.5689530000	1.8368630000	-2.0966910000
H	-1.6970040000	2.4286470000	-0.6525450000
H	0.5534610000	-0.1508810000	2.2223040000
H	2.3757420000	-1.6066110000	3.0458300000
Cl	4.0690180000	-2.5509980000	-1.4052920000

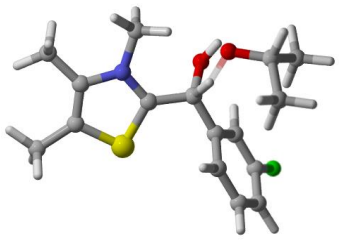
H	1.8288560000	-0.8345480000	-1.8158050000
C	2.1236810000	4.3234490000	-0.4850950000
C	1.6378190000	3.1403650000	0.3545890000
H	1.8631930000	4.1721590000	-1.5361550000
H	3.2074160000	4.4566560000	-0.4121420000
H	1.6374770000	5.2422340000	-0.1415880000
C	2.0172830000	3.3310230000	1.8255340000
H	1.6889360000	2.4682450000	2.4118500000
H	1.5214040000	4.2233840000	2.2210520000
H	3.0978480000	3.4468710000	1.9564530000
O	0.2639930000	2.9594110000	0.2027540000
H	2.1828580000	2.2410600000	-0.0029950000
H	0.2796310000	1.8153970000	-1.6451900000
H	3.9455980000	-2.6729620000	1.4384680000

thermodynamic data

Zero-point correction= 0.349600 (Hartree/Particle)
Thermal correction to Energy= 0.372875
Thermal correction to Enthalpy= 0.373819
Thermal correction to Gibbs Free Energy= 0.294839
Sum of electronic and zero-point Energies= -1686.002363
Sum of electronic and thermal Energies= -1685.979088
Sum of electronic and thermal Enthalpies= -1685.978144
Sum of electronic and thermal Free Energies= -1686.057124

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.983	85.392	166.229

M062X/6-311+G**/PCM	**TST2 mit Isopropanol *m*-F**

xyz-matrix

43
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2078320000	-0.0160960000	-0.1652510000
S	-1.6781720000	-1.5511500000	0.4271790000
N	-2.2774010000	0.7403070000	-0.3985700000
C	-3.5095270000	0.1244610000	-0.1408340000
C	-3.3644340000	-1.1329260000	0.3380140000
C	-4.7791010000	0.8699770000	-0.3922110000

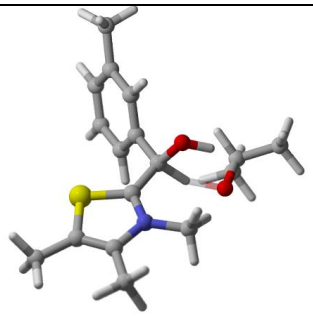
C	-4.4030810000	-2.1159460000	0.7748990000
C	-2.1837840000	2.1310810000	-0.8696800000
C	1.2000070000	-0.6372430000	-0.0743100000
C	1.3819650000	-1.0379500000	1.2545280000
C	2.3392960000	-1.9899290000	1.5828260000
C	3.1468890000	-2.5514170000	0.5963980000
C	2.9569320000	-2.1278430000	-0.7054850000
C	2.0085220000	-1.1889160000	-1.0679420000
C	0.1805860000	0.4103810000	-0.4115260000
O	0.3026700000	0.8917960000	-1.7427830000
H	0.4341030000	1.4709420000	0.2139260000
H	-4.7870790000	1.2932240000	-1.3983050000
H	-5.6286110000	0.1974800000	-0.3018560000
H	-4.9103700000	1.6834670000	0.3248460000
H	-4.3552600000	-3.0271810000	0.1761920000
H	-5.3995140000	-1.6903720000	0.6714670000
H	-4.2581290000	-2.3891620000	1.8216850000
H	-3.0222770000	2.6859920000	-0.4573670000
H	-2.2209610000	2.1517270000	-1.9582390000
H	-1.2508440000	2.5657550000	-0.5129450000
H	0.7797690000	-0.5868040000	2.0362920000
H	2.4718210000	-2.2896900000	2.6152940000
F	3.7358670000	-2.6569050000	-1.6758370000
H	1.9042630000	-0.8846120000	-2.1012060000
C	2.4073840000	2.5766270000	1.9766400000
C	2.0264270000	3.1543360000	0.6092910000
H	1.7041780000	2.9166850000	2.7410830000
H	3.4167660000	2.8757500000	2.2754630000
H	2.3712660000	1.4824400000	1.9369190000
C	3.0223600000	2.6760830000	-0.4547350000
H	2.7573640000	3.0879940000	-1.4329430000
H	2.9967000000	1.5821530000	-0.5233850000
H	4.0470100000	2.9797430000	-0.2195350000
O	0.7144190000	2.8337100000	0.2623200000
H	2.1235970000	4.2526100000	0.6781820000
H	0.6151530000	1.8048370000	-1.6305980000
H	3.9084470000	-3.2867070000	0.8226740000

thermodynamic data

Zero-point correction= 0.351119 (Hartree/Particle)
Thermal correction to Energy= 0.373775
Thermal correction to Enthalpy= 0.374719
Thermal correction to Gibbs Free Energy= 0.298472
Sum of electronic and zero-point Energies= -1325.642623
Sum of electronic and thermal Energies= -1325.619966
Sum of electronic and thermal Enthalpies= -1325.619022
Sum of electronic and thermal Free Energies= -1325.695270

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.547	84.405	160.477

M062X/6-311+G**/PCM	**TST2 mit Isopropanol *m*-Me**



xyz-matrix

46
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2218480000	0.0084890000	-0.1571380000
S	-1.7774040000	-1.4948510000	0.4419490000
N	-2.2463520000	0.8261940000	-0.3872390000
C	-3.5115890000	0.2827400000	-0.1278230000
C	-3.4379210000	-0.9801660000	0.3531360000
C	-4.7353950000	1.1007780000	-0.3800760000
C	-4.5315860000	-1.8991800000	0.7949590000
C	-2.0668180000	2.2129320000	-0.8434380000
C	1.1415250000	-0.7483440000	-0.0352570000
C	1.3451480000	-1.0651760000	1.3122180000
C	2.2212110000	-2.0838820000	1.6638680000
C	2.9147280000	-2.7840740000	0.6785910000
C	2.7381620000	-2.4716360000	-0.6695850000
C	1.8439790000	-1.4538050000	-1.0111930000
C	0.1875500000	0.3549330000	-0.3962480000
O	0.3433440000	0.8222250000	-1.7316430000
H	0.4821890000	1.3923170000	0.2393300000
H	-4.7120370000	1.5324600000	-1.3823820000
H	-5.6227610000	0.4772800000	-0.3018380000
H	-4.8257740000	1.9148500000	0.3427150000
H	-4.4057180000	-2.1704160000	1.8447800000
H	-4.5331280000	-2.8171120000	0.2047380000
H	-5.5023130000	-1.4193310000	0.6840310000
H	-2.8610490000	2.8187110000	-0.4152270000
H	-2.1115360000	2.2518040000	-1.9312520000
H	-1.1031680000	2.5786680000	-0.4922130000
H	0.8209700000	-0.5053770000	2.0809900000
H	2.3746580000	-2.3274890000	2.7090050000
H	1.6935440000	-1.1955160000	-2.0538230000
C	2.9707500000	3.7461830000	-0.4385150000
C	2.3509080000	2.6179520000	0.3888470000
H	2.6039830000	3.7050400000	-1.4678550000
H	4.0632000000	3.6848370000	-0.4573420000
H	2.6847060000	4.7136630000	-0.0133310000
C	2.8760340000	2.6547860000	1.8265100000

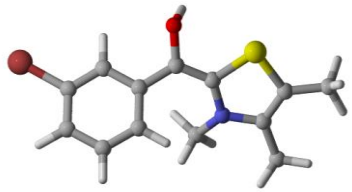
H	2.4433390000	1.8331770000	2.4037960000
H	2.5852710000	3.5976960000	2.3008850000
H	3.9665300000	2.5682840000	1.8649210000
O	0.9589670000	2.6859410000	0.3521110000
H	2.6969930000	1.6602660000	-0.0535500000
H	0.6955650000	1.7202720000	-1.6303960000
H	3.6009340000	-3.5760660000	0.9597350000
C	3.5099220000	-3.1977090000	-1.7418100000
H	4.3726000000	-2.6059920000	-2.0605800000
H	2.8893020000	-3.3740970000	-2.6221110000
H	3.8795850000	-4.1579260000	-1.3795710000

thermodynamic data

Zero-point correction= 0.386475 (Hartree/Particle)
Thermal correction to Energy= 0.410468
Thermal correction to Enthalpy= 0.411413
Thermal correction to Gibbs Free Energy= 0.330583
Sum of electronic and zero-point Energies= -1265.670379
Sum of electronic and thermal Energies= -1265.646385
Sum of electronic and thermal Enthalpies= -1265.645441
Sum of electronic and thermal Free Energies= -1265.726271

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.573	87.759	170.121

M062X/6-311+G**/PCM	**Breslowintermediat *m*-Br**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.0381650000	0.2716170000	-0.1820310000
C	-2.9613660000	1.5138670000	-0.8000870000
C	-1.7068970000	1.9600320000	-1.2104000000
C	-0.5710680000	1.1926170000	-0.9954870000
C	-0.6548390000	-0.0488760000	-0.3436080000
C	-1.9219390000	-0.5150000000	0.0453390000
C	0.5164110000	-0.8959890000	-0.1406960000
C	1.8120920000	-0.4998500000	-0.0278880000
O	0.2772200000	-2.2661820000	-0.2410290000
Br	-4.7441950000	-0.3690060000	0.3855840000

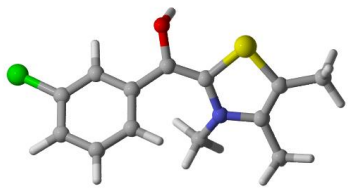
S	3.1342510000	-1.6493750000	-0.2717560000
C	4.3286430000	-0.3663380000	-0.0206650000
C	3.7325220000	0.8028740000	0.2589560000
N	2.3240380000	0.7431820000	0.3026760000
C	1.5650980000	1.6825900000	1.1242990000
C	5.7792400000	-0.6986550000	-0.1547860000
C	4.3986810000	2.1186440000	0.5151240000
H	-3.8506670000	2.1056900000	-0.9704870000
H	-1.6234710000	2.9123750000	-1.7208540000
H	0.3883790000	1.5367930000	-1.3637560000
H	-2.0168380000	-1.4817330000	0.5224230000
H	0.5515970000	-2.7039730000	0.5725810000
H	2.2183110000	2.1057580000	1.8851360000
H	1.1315780000	2.4931110000	0.5351190000
H	0.7564600000	1.1429110000	1.6180330000
H	6.0496690000	-1.5185300000	0.5156340000
H	6.0253490000	-1.0084960000	-1.1735590000
H	6.3981820000	0.1603430000	0.1017430000
H	5.4288090000	2.0961250000	0.1658950000
H	3.8756520000	2.9187380000	-0.0131640000
H	4.4093030000	2.3681010000	1.5789750000

thermodynamic data

Zero-point correction= 0.243553 (Hartree/Particle)
Thermal correction to Energy= 0.260977
Thermal correction to Enthalpy= 0.261922
Thermal correction to Gibbs Free Energy= 0.197589
Sum of electronic and zero-point Energies= -3605.778812
Sum of electronic and thermal Energies= -3605.761388
Sum of electronic and thermal Enthalpies= -3605.760444
Sum of electronic and thermal Free Energies= -3605.824776

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.766	64.913	135.400

M062X/6-311+G**/PCM	**Breslowintermediat *m*-Cl**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

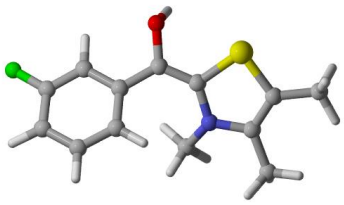
C	-3.6790250000	0.0939880000	-0.0232390000
C	-3.6561260000	1.3389380000	-0.6384560000
C	-2.4241380000	1.8332250000	-1.0610200000
C	-1.2576160000	1.1091870000	-0.8605960000
C	-1.2865420000	-0.1351000000	-0.2082590000
C	-2.5307010000	-0.6478040000	0.1937190000
C	-0.0848740000	-0.9425320000	-0.0243020000
C	1.2031020000	-0.5098940000	0.0264830000
O	-0.2854630000	-2.3214630000	-0.0818620000
Cl	-5.2194260000	-0.5665220000	0.4941750000
S	2.5446080000	-1.6313300000	-0.2433940000
C	3.7116850000	-0.3069200000	-0.0987460000
C	3.0965470000	0.8537120000	0.1748970000
N	1.6945200000	0.7556460000	0.2959320000
C	0.9600310000	1.6924200000	1.1438020000
C	5.1618850000	-0.6045370000	-0.3006110000
C	3.7318090000	2.1976420000	0.3494100000
H	-4.5721780000	1.8923580000	-0.7975260000
H	-2.3820650000	2.7878480000	-1.5721300000
H	-0.3177860000	1.4892250000	-1.2432250000
H	-2.5896640000	-1.6182980000	0.6688820000
H	0.0027000000	-2.7265790000	0.7437800000
H	1.6336060000	2.1068760000	1.8922910000
H	0.5165100000	2.5092080000	0.5709960000
H	0.1616880000	1.1527820000	1.6527840000
H	5.5059990000	-1.3539570000	0.4170540000
H	5.3517910000	-0.9942120000	-1.3037650000
H	5.7641210000	0.2925430000	-0.1623830000
H	4.7485520000	2.1903220000	-0.0373820000
H	3.1649820000	2.9585740000	-0.1915690000
H	3.7740940000	2.4937090000	1.4004010000

thermodynamic data

Zero-point correction= 0.243843 (Hartree/Particle)
Thermal correction to Energy= 0.261138
Thermal correction to Enthalpy= 0.262082
Thermal correction to Gibbs Free Energy= 0.198262
Sum of electronic and zero-point Energies= -1491.806783
Sum of electronic and thermal Energies= -1491.789487
Sum of electronic and thermal Enthalpies= -1491.788543
Sum of electronic and thermal Free Energies= -1491.852364

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.867	64.553	134.322

M062X/6-311+G**/PCM	**Breslowintermediat *m*-F**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-4.0042720000	-0.0919100000	0.1151480000
C	-4.0517690000	1.1334880000	-0.5258210000
C	-2.8474290000	1.6585860000	-0.9908610000
C	-1.6521860000	0.9786380000	-0.8029410000
C	-1.6222120000	-0.2520830000	-0.1234710000
C	-2.8365970000	-0.7969050000	0.3230700000
C	-0.3870420000	-1.0109750000	0.0458730000
C	0.8834250000	-0.5273070000	0.0565630000
O	-0.5363430000	-2.3972900000	0.0228320000
F	-5.1626200000	-0.6296850000	0.5633220000
S	2.2650350000	-1.5970410000	-0.2259720000
C	3.3766640000	-0.2201480000	-0.1449210000
C	2.7197680000	0.9186640000	0.1226830000
N	1.3276360000	0.7631930000	0.2874330000
C	0.5806680000	1.6847150000	1.1412610000
C	4.8318910000	-0.4597610000	-0.3845770000
C	3.2989670000	2.2932000000	0.2469470000
H	-4.9977560000	1.6400420000	-0.6660130000
H	-2.8492290000	2.6017400000	-1.5241870000
H	-0.7349180000	1.3826130000	-1.2141680000
H	-2.8673390000	-1.7546870000	0.8263030000
H	-0.2137140000	-2.7732590000	0.8495570000
H	1.2533870000	2.1204170000	1.8787290000
H	0.1070160000	2.4854760000	0.5699050000
H	-0.1959580000	1.1270010000	1.6634020000
H	5.2277700000	-1.1809870000	0.3352610000
H	5.0092520000	-0.8594330000	-1.3861210000
H	5.3989890000	0.4642590000	-0.2795490000
H	4.3070150000	2.3197850000	-0.1611240000
H	2.6877560000	3.0124570000	-0.3027750000
H	3.3488050000	2.6211490000	1.2880250000

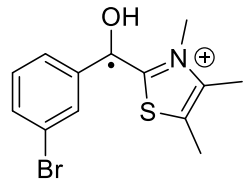
thermodynamic data

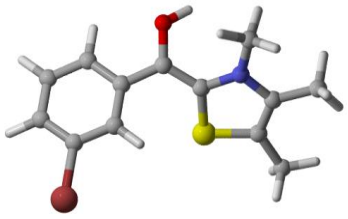
Zero-point correction= 0.245225 (Hartree/Particle)
Thermal correction to Energy= 0.262124
Thermal correction to Enthalpy= 0.263068
Thermal correction to Gibbs Free Energy= 0.200880

Sum of electronic and zero-point Energies= -1131.446631
Sum of electronic and thermal Energies= -1131.429733
Sum of electronic and thermal Enthalpies= -1131.428788
Sum of electronic and thermal Free Energies= -1131.490976

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.485	63.736	130.885

M062X/6-311+G**/PCM	**Breslowintermediat rad *m*-Br**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.7640270000	0.1177300000	-0.0026490000
C	-3.4980740000	1.1224150000	-0.6233870000
C	-2.8442880000	2.2867740000	-1.0178210000
C	-1.4822350000	2.4373010000	-0.8096100000
C	-0.7473150000	1.4076770000	-0.2030640000
C	-1.4036060000	0.2430630000	0.2235020000
C	0.6839260000	1.5859470000	-0.0044670000
Br	-3.6539360000	-1.4595250000	0.5691070000
C	1.6112100000	0.5298990000	-0.0145280000
O	1.0747270000	2.8616410000	0.1411270000
S	1.3505890000	-0.9426070000	-0.8823260000
C	2.9723790000	-1.4634850000	-0.5771590000
C	3.6505490000	-0.5379070000	0.1569570000
N	2.8731890000	0.5624080000	0.4861410000
C	3.4308170000	-2.7908050000	-1.0861780000
C	5.0627010000	-0.6173790000	0.6336430000
C	3.3433440000	1.5701980000	1.4499970000
H	-4.5606740000	1.0006400000	-0.7884880000
H	-3.4072010000	3.0775940000	-1.4976290000
H	-0.9747700000	3.3393670000	-1.1249490000
H	-0.8720890000	-0.5335470000	0.7580820000
H	1.9877000000	3.0012920000	-0.1402810000
H	4.4953400000	-2.9228620000	-0.9048960000
H	2.8952610000	-3.5979750000	-0.5824110000
H	3.2505680000	-2.8794740000	-2.1583800000
H	5.5843780000	0.3239010000	0.4537650000
H	5.1042360000	-0.8377360000	1.7031010000
H	5.5912160000	-1.4071370000	0.1058420000

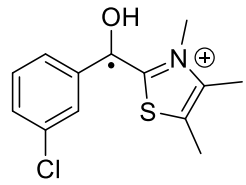
H	3.9448970000	1.0696540000	2.2039420000
H	3.9507440000	2.3264670000	0.9507740000
H	2.4863200000	2.0263410000	1.9365820000

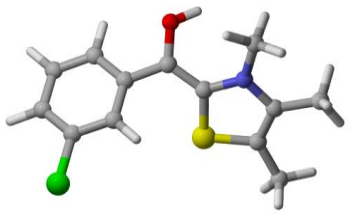
thermodynamic data

Zero-point correction= 0.244893 (Hartree/Particle)
Thermal correction to Energy= 0.262131
Thermal correction to Enthalpy= 0.263075
Thermal correction to Gibbs Free Energy= 0.197286
Sum of electronic and zero-point Energies= -3605.607976
Sum of electronic and thermal Energies= -3605.590738
Sum of electronic and thermal Enthalpies= -3605.589794
Sum of electronic and thermal Free Energies= -3605.655582

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.490	63.894	138.464

M062X/6-311+G**/PCM	**Breslowintermediat rad *m*-Cl**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	3.1849750000	0.5416800000	0.2578960000
C	4.0722590000	-0.2603790000	-0.4499870000
C	3.6081130000	-1.4511560000	-1.0016890000
C	2.2813780000	-1.8270510000	-0.8571950000
C	1.3907760000	-0.9981500000	-0.1603320000
C	1.8551160000	0.1909420000	0.4185810000
C	-0.0028740000	-1.4087210000	-0.0321150000
Cl	3.7604290000	2.0191000000	0.9845410000
C	-1.0747130000	-0.5030010000	-0.0160710000
O	-0.1874450000	-2.7368230000	0.0116310000
S	-0.9817000000	1.0662190000	-0.7384270000
C	-2.6725690000	1.3304360000	-0.4931150000
C	-3.2502820000	0.2574140000	0.1163760000
N	-2.3452930000	-0.7535740000	0.3979810000
C	-3.2942560000	2.6277410000	-0.8983300000
C	-4.6823640000	0.1108840000	0.5088210000
C	-2.7166420000	-1.9096690000	1.2278260000
H	5.1066780000	0.0391800000	-0.5589440000

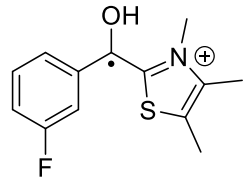
H	4.2914750000	-2.0853050000	-1.5522430000
H	1.9212350000	-2.7504170000	-1.2915980000
H	1.2062110000	0.8144780000	1.0202380000
H	-1.0633670000	-3.0033370000	-0.2939680000
H	-4.3634950000	2.5030270000	-1.0616240000
H	-3.1492680000	3.3804170000	-0.1202490000
H	-2.8518880000	3.0020310000	-1.8217700000
H	-4.8044610000	0.2075790000	1.5903270000
H	-5.2775230000	0.8872660000	0.0344280000
H	-5.0728400000	-0.8601720000	0.2004220000
H	-3.1304270000	-2.7100720000	0.6124700000
H	-1.8418550000	-2.2547560000	1.7722420000
H	-3.4674590000	-1.5903380000	1.9449840000

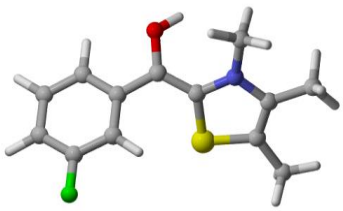
thermodynamic data

Zero-point correction= 0.245364 (Hartree/Particle)
Thermal correction to Energy= 0.262279
Thermal correction to Enthalpy= 0.263223
Thermal correction to Gibbs Free Energy= 0.199147
Sum of electronic and zero-point Energies= -1491.635899
Sum of electronic and thermal Energies= -1491.618984
Sum of electronic and thermal Enthalpies= -1491.618040
Sum of electronic and thermal Free Energies= -1491.682116

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.582	63.551	134.859

M062X/6-311+G**/PCM	**Breslowintermediat rad *m*-F**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	3.3067800000	1.0007920000	0.5564940000
C	4.3267100000	0.3656140000	-0.1317980000
C	4.0281780000	-0.8133860000	-0.8090600000
C	2.7398080000	-1.3276170000	-0.8005310000
C	1.7186010000	-0.6546550000	-0.1117580000
C	2.0140110000	0.5216550000	0.5932960000
C	0.3744540000	-1.2128740000	-0.1238770000
F	3.5892380000	2.1258060000	1.2373160000

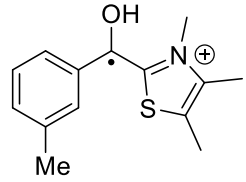
C	-0.7947420000	-0.4350490000	-0.0434310000
O	0.3227630000	-2.5464390000	-0.2696700000
S	-0.8703720000	1.2064760000	-0.5815710000
C	-2.5863710000	1.2481240000	-0.3617670000
C	-3.0463960000	0.0532590000	0.1014860000
N	-2.0336080000	-0.8738940000	0.2972290000
C	-3.3404210000	2.5016960000	-0.6637990000
C	-4.4571210000	-0.3106710000	0.4259720000
C	-2.2870910000	-2.1475330000	0.9891000000
H	5.3247910000	0.7845730000	-0.1226640000
H	4.8106810000	-1.3299580000	-1.3503760000
H	2.5093740000	-2.2396000000	-1.3345420000
H	1.2774350000	1.0362790000	1.1967060000
H	-0.5000860000	-2.8421380000	-0.6794370000
H	-4.3987390000	2.3726220000	-0.4474930000
H	-2.9668850000	3.3279610000	-0.0563000000
H	-3.2323150000	2.7755110000	-1.7146610000
H	-4.7050000000	-1.2922480000	0.0193480000
H	-4.6183830000	-0.3320870000	1.5065210000
H	-5.1394770000	0.4176580000	-0.0045690000
H	-3.0373680000	-1.9785090000	1.7568050000
H	-2.6550460000	-2.8988050000	0.2890060000
H	-1.3714120000	-2.4844840000	1.4657360000

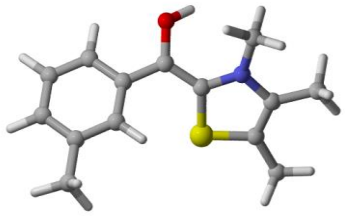
thermodynamic data

Zero-point correction= 0.246337 (Hartree/Particle)
Thermal correction to Energy= 0.262130
Thermal correction to Enthalpy= 0.263074
Thermal correction to Gibbs Free Energy= 0.202411
Sum of electronic and zero-point Energies= -1131.276536
Sum of electronic and thermal Energies= -1131.260744
Sum of electronic and thermal Enthalpies= -1131.259799
Sum of electronic and thermal Free Energies= -1131.320462

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.489	60.868	127.675

M062X/6-311+G**/PCM	**Breslowintermediat rad *m*-Me**





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

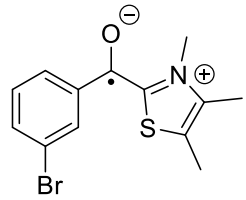
C	3.3333170000	0.9775580000	0.5243940000
C	4.3000520000	0.2800710000	-0.2016200000
C	3.9857870000	-0.9069200000	-0.8625080000
C	2.6967030000	-1.4106510000	-0.8221600000
C	1.7030040000	-0.7109270000	-0.1177410000
C	2.0375650000	0.4673230000	0.5631790000
C	0.3501280000	-1.2455780000	-0.0946850000
C	-0.8021670000	-0.4453250000	-0.0260890000
O	0.2692740000	-2.5830210000	-0.1981930000
S	-0.8480290000	1.1861430000	-0.6029790000
C	-2.5649800000	1.2605110000	-0.3910700000
C	-3.0460380000	0.0871520000	0.1028120000
N	-2.0507950000	-0.8526110000	0.3260470000
C	-3.3031710000	2.5118410000	-0.7403490000
C	-4.4649460000	-0.2410220000	0.4300820000
C	-2.3253170000	-2.0977630000	1.0597380000
C	3.6716580000	2.2413470000	1.2708780000
H	5.3137030000	0.6635990000	-0.2419490000
H	4.7535600000	-1.4356510000	-1.4142860000
H	2.4424940000	-2.3263960000	-1.3398020000
H	1.2930180000	0.9747310000	1.1671430000
H	-0.5641230000	-2.8722540000	-0.5905800000
H	-4.3253990000	2.4687810000	-0.3698770000
H	-2.8170050000	3.3803800000	-0.2936180000
H	-3.3301790000	2.6565070000	-1.8222250000
H	-4.7321740000	-1.2260400000	0.0444420000
H	-4.6309590000	-0.2352640000	1.5101030000
H	-5.1299710000	0.4914710000	-0.0203090000
H	-3.0816330000	-1.8942380000	1.8131350000
H	-2.6944500000	-2.8709400000	0.3842780000
H	-1.4178390000	-2.4267280000	1.5575530000
H	4.7145130000	2.5187700000	1.1189520000
H	3.0428960000	3.0691460000	0.9362270000
H	3.5038210000	2.1125830000	2.3425260000

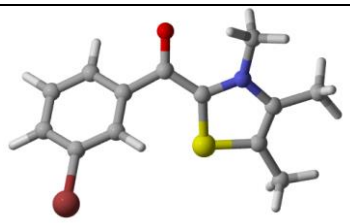
thermodynamic data

Zero-point correction= 0.281693 (Hartree/Particle)
Thermal correction to Energy= 0.298645
Thermal correction to Enthalpy= 0.299589
Thermal correction to Gibbs Free Energy= 0.235999
Sum of electronic and zero-point Energies= -1071.308161
Sum of electronic and thermal Energies= -1071.291209
Sum of electronic and thermal Enthalpies= -1071.290265
Sum of electronic and thermal Free Energies= -1071.353855

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	187.403	64.197	133.838

M062X/6-311+G**/PCM	**Breslowintermediat radde *m*-Br**





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.7620280000	0.1622620000	-0.0381530000
C	-3.4334060000	1.1140450000	-0.7930990000
C	-2.7294350000	2.2361890000	-1.2243620000
C	-1.3857620000	2.3884510000	-0.9114420000
C	-0.7143840000	1.4117960000	-0.1701710000
C	-1.4182280000	0.2936690000	0.2850940000
C	0.7312720000	1.6448910000	0.1495810000
Br	-3.7152290000	-1.3693330000	0.5766420000
C	1.6279680000	0.5404460000	0.0926890000
O	1.1172900000	2.8128050000	0.3962270000
S	1.2797770000	-0.9912650000	-0.6718900000
C	2.9510720000	-1.4929220000	-0.5290360000
C	3.6887530000	-0.5397650000	0.0844730000
N	2.9502870000	0.5829750000	0.4542910000
C	3.3515100000	-2.8376420000	-1.0440180000
C	5.1524120000	-0.5961650000	0.3860020000
C	3.5253770000	1.6734100000	1.2452870000
H	-4.4809420000	0.9870930000	-1.0332750000
H	-3.2404730000	2.9916800000	-1.8089540000
H	-0.8373910000	3.2638590000	-1.2372390000
H	-0.9364220000	-0.4518220000	0.9055470000
H	4.4116830000	-3.0177380000	-0.8743460000
H	2.7910900000	-3.6278470000	-0.5387220000
H	3.1574580000	-2.9221130000	-2.1155330000
H	5.6551210000	0.3072630000	0.0351360000
H	5.3350260000	-0.6931620000	1.4588420000
H	5.6052130000	-1.4503650000	-0.1112980000
H	4.3836690000	1.2910530000	1.7909720000
H	3.8312350000	2.4988180000	0.6025110000
H	2.7802640000	2.0349050000	1.9472080000

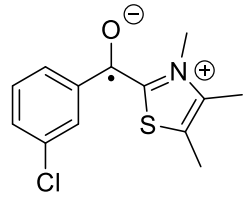
thermodynamic data

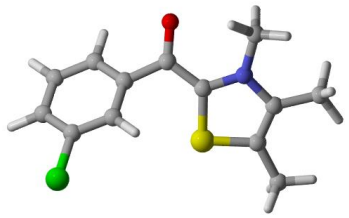
Zero-point correction= 0.231424 (Hartree/Particle)
Thermal correction to Energy= 0.248704
Thermal correction to Enthalpy= 0.249648
Thermal correction to Gibbs Free Energy= 0.183250
Sum of electronic and zero-point Energies= -3605.191141

Sum of electronic and thermal Energies= -3605.173861
Sum of electronic and thermal Enthalpies= -3605.172917
Sum of electronic and thermal Free Energies= -3605.239315

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.064	62.846	139.747

M062X/6-311+G**/PCM	**Breslowintermediat radde *m*-Cl**





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.2078350000	-0.4710380000	0.2270040000
C	-4.0346230000	0.2842970000	-0.5924140000
C	-3.5133300000	1.4326150000	-1.1837030000
C	-2.1948990000	1.8052920000	-0.9592830000
C	-1.3656080000	1.0235050000	-0.1499870000
C	-1.8852830000	-0.1206950000	0.4594680000
C	0.0409550000	1.4877870000	0.0786650000
Cl	-3.8525810000	-1.9009060000	1.0061110000
C	1.0818990000	0.5170500000	0.0720760000
O	0.2633370000	2.7150960000	0.2116270000
S	0.9274480000	-1.1022320000	-0.5644910000
C	2.6556600000	-1.3587140000	-0.4466400000
C	3.2708410000	-0.2692260000	0.0670170000
N	2.3942960000	0.7683750000	0.3798150000
C	3.2262530000	-2.6692480000	-0.8838080000
C	4.7357890000	-0.1029160000	0.3169940000
C	2.8262260000	1.9802320000	1.0795010000
H	-5.0617820000	-0.0146160000	-0.7574400000
H	-4.1470060000	2.0362620000	-1.8223730000
H	-1.7897340000	2.7039760000	-1.4080410000
H	-1.2812770000	-0.7203280000	1.1295950000
H	4.2970030000	-2.7102200000	-0.6915420000
H	2.7557100000	-3.4943280000	-0.3439940000
H	3.0630440000	-2.8323490000	-1.9515690000
H	5.0970920000	0.8356260000	-0.1080450000
H	4.9601670000	-0.1021800000	1.3862620000
H	5.2885620000	-0.9179010000	-0.1438720000
H	3.7451840000	1.7629660000	1.6171630000
H	2.9896360000	2.7961870000	0.3760740000

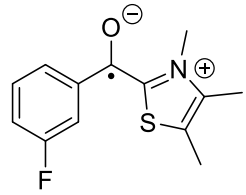
H 2.0550760000 2.2749940000 1.7847010000

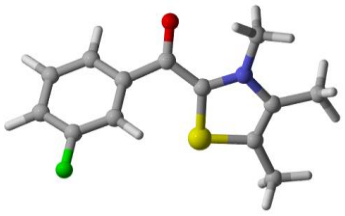
thermodynamic data

Zero-point correction= 0.232266 (Hartree/Particle)
Thermal correction to Energy= 0.249287
Thermal correction to Enthalpy= 0.250231
Thermal correction to Gibbs Free Energy= 0.185101
Sum of electronic and zero-point Energies= -1491.218716
Sum of electronic and thermal Energies= -1491.201695
Sum of electronic and thermal Enthalpies= -1491.200751
Sum of electronic and thermal Free Energies= -1491.265881

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.430	62.344	137.077

M062X/6-311+G**/PCM	**Breslowintermediat radde *m*-F**





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.3517860000	-0.9030100000	0.5363130000
C	-4.2955180000	-0.3381540000	-0.3010500000
C	-3.9240930000	0.7849430000	-1.0369520000
C	-2.6418650000	1.3083110000	-0.9278830000
C	-1.6980890000	0.7059670000	-0.0903810000
C	-2.0652030000	-0.4123650000	0.6625660000
C	-0.3389660000	1.3289600000	0.0068050000
F	-3.7030650000	-1.9768090000	1.2765270000
C	0.7965430000	0.4716400000	0.0574090000
O	-0.2368090000	2.5790130000	-0.0153400000
S	0.7900030000	-1.2183790000	-0.3871450000
C	2.5389460000	-1.2847560000	-0.3285250000
C	3.0546550000	-0.0876220000	0.0323100000
N	2.0862410000	0.8861030000	0.2702140000
C	3.2267080000	-2.5728860000	-0.6476170000
C	4.5017740000	0.2518380000	0.1957370000
C	2.4170820000	2.2089230000	0.8044980000
H	-5.2885400000	-0.7646840000	-0.3642330000
H	-4.6448570000	1.2492500000	-1.6990350000
H	-2.3550760000	2.1877760000	-1.4910180000

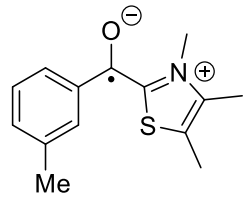
H	-1.3843200000	-0.8827310000	1.3617650000
H	4.3047370000	-2.4771720000	-0.5291200000
H	2.8840850000	-3.3691100000	0.0172500000
H	3.0215940000	-2.8830970000	-1.6747780000
H	4.7534910000	1.1555480000	-0.3629340000
H	4.7550800000	0.4183980000	1.2454890000
H	5.1216120000	-0.5604080000	-0.1756710000
H	3.3663260000	2.1450040000	1.3295370000
H	2.4840050000	2.9449150000	0.0034910000
H	1.6390510000	2.5161000000	1.4966770000

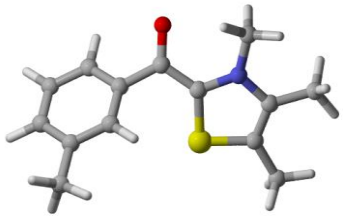
thermodynamic data

Zero-point correction= 0.233720 (Hartree/Particle)
Thermal correction to Energy= 0.250181
Thermal correction to Enthalpy= 0.251125
Thermal correction to Gibbs Free Energy= 0.188165
Sum of electronic and zero-point Energies= -1130.858521
Sum of electronic and thermal Energies= -1130.842060
Sum of electronic and thermal Enthalpies= -1130.841116
Sum of electronic and thermal Free Energies= -1130.904077

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.991	61.399	132.512

M062X/6-311+G**/PCM	**Breslowintermediat radde *m*-Me**





xyz-matrix

33
XYZ file generated by gabedit : coordinates in Angstrom

C	3.3701450000	0.8770350000	0.5150350000
C	4.2643790000	0.2520510000	-0.3579860000
C	3.8821580000	-0.8726040000	-1.0823510000
C	2.5963630000	-1.3859800000	-0.9519360000
C	1.6789240000	-0.7619950000	-0.1050120000
C	2.0810550000	0.3583950000	0.6296330000
C	0.3116020000	-1.3598730000	0.0229650000
C	-0.8076520000	-0.4801980000	0.0651180000
O	0.1813580000	-2.6076940000	0.0365020000
S	-0.7726240000	1.1971480000	-0.4274500000
C	-2.5208730000	1.2967440000	-0.3614790000

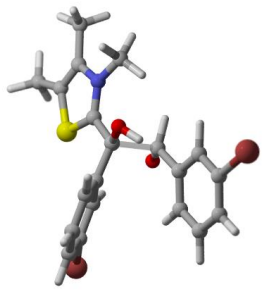
C	-3.0559870000	0.1214990000	0.0399170000
N	-2.1046900000	-0.8627290000	0.3019020000
C	-3.1878330000	2.5866380000	-0.7156760000
C	-4.5079590000	-0.1860860000	0.2241820000
C	-2.4553440000	-2.1586610000	0.8858710000
C	3.8009940000	2.0777000000	1.3177550000
H	5.2701460000	0.6466740000	-0.4622250000
H	4.5895890000	-1.3494780000	-1.7510780000
H	2.2913770000	-2.2675030000	-1.5034860000
H	1.3887320000	0.8198460000	1.3268190000
H	-4.2675900000	2.5109240000	-0.5979320000
H	-2.8347050000	3.3949810000	-0.0710580000
H	-2.9755990000	2.8669610000	-1.7500430000
H	-4.7778810000	-1.1073050000	-0.2960230000
H	-4.7581730000	-0.3057910000	1.2810670000
H	-5.1164470000	0.6206640000	-0.1769430000
H	-3.3915410000	-2.0551840000	1.4281960000
H	-2.5572850000	-2.9194720000	0.1119340000
H	-1.6702210000	-2.4621660000	1.5715850000
H	4.6569120000	1.8343510000	1.9515590000
H	4.1037910000	2.8950520000	0.6590040000
H	2.9930080000	2.4357400000	1.9562870000

thermodynamic data

Zero-point correction= 0.269172 (Hartree/Particle)
Thermal correction to Energy= 0.286748
Thermal correction to Enthalpy= 0.287692
Thermal correction to Gibbs Free Energy= 0.222180
Sum of electronic and zero-point Energies= -1070.887586
Sum of electronic and thermal Energies= -1070.870010
Sum of electronic and thermal Enthalpies= -1070.869066
Sum of electronic and thermal Free Energies= -1070.934578

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.937	64.651	137.882

M062X/6-311+G**/PCM	**TST3 *m*-Br**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	-1.3982310000	3.0528930000	0.2661730000
C	-2.6299020000	3.6678820000	-0.0156100000
C	-0.2049890000	3.8929230000	0.4762140000
C	-3.6283840000	2.7777690000	-0.1982260000
S	-3.0338590000	1.1590600000	0.0120910000
C	-1.4466030000	1.7135020000	0.3481610000
C	-2.7223440000	5.1578910000	-0.0808480000
C	-5.0688480000	3.0011940000	-0.5321480000
C	-0.3336190000	0.8048930000	0.5544780000
C	-0.6631650000	-0.5938140000	0.9787510000
O	0.6372280000	1.4026490000	1.3724610000
C	-1.4515790000	-1.4364180000	0.1813360000
C	-1.6611720000	-2.7484560000	0.5770630000
C	-1.1135520000	-3.2743780000	1.7385840000
C	-0.3233550000	-2.4370100000	2.5196590000
C	-0.0970200000	-1.1171260000	2.1473960000
C	0.3299570000	0.7034690000	-1.2704300000
O	-0.5415340000	0.2302810000	-2.0661180000
C	1.5975350000	-0.0886410000	-1.0266060000
C	2.7763520000	0.5616560000	-0.6566880000
C	3.9237210000	-0.1869720000	-0.4141820000
C	3.9333970000	-1.5676150000	-0.5388070000
C	2.7565820000	-2.2067250000	-0.9325080000
C	1.6016670000	-1.4777090000	-1.1797480000
H	-0.1790800000	4.2421790000	1.5084570000
H	0.6881640000	3.3238990000	0.2648590000
H	-0.2666250000	4.7397910000	-0.2009630000
H	-2.2883490000	5.6164220000	0.8093630000
H	-3.7654290000	5.4590810000	-0.1389100000
H	-2.2051040000	5.5523900000	-0.9583820000
H	-5.7136570000	2.6795830000	0.2880560000
H	-5.2589950000	4.0552040000	-0.7256660000
H	-5.3493480000	2.4387480000	-1.4244810000
H	1.4833450000	0.9683650000	1.2000160000
H	-1.8352380000	-1.0860760000	-0.7663040000
Br	-2.7300310000	-3.8725660000	-0.5330260000
H	-1.2968290000	-4.3019180000	2.0242800000
H	0.1163830000	-2.8207250000	3.4327040000
H	0.5180450000	-0.4856430000	2.7748050000
H	0.5619170000	1.7870340000	-1.3198180000
H	2.8074260000	1.6443260000	-0.5844710000
Br	5.5248090000	0.7215400000	0.0802130000
H	4.8366610000	-2.1321010000	-0.3464020000
H	2.7547310000	-3.2842880000	-1.0482300000
H	0.6904980000	-1.9668720000	-1.5029040000

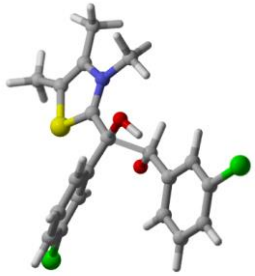
thermodynamic data

Zero-point correction= 0.346332 (Hartree/Particle)
Thermal correction to Energy= 0.371578
Thermal correction to Enthalpy= 0.372522

Thermal correction to Gibbs Free Energy= 0.288397
Sum of electronic and zero-point Energies= -6524.763859
Sum of electronic and thermal Energies= -6524.738614
Sum of electronic and thermal Enthalpies= -6524.737670
Sum of electronic and thermal Free Energies= -6524.821795

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.169	94.645	177.057

M062X/6-311+G**/PCM	**TST3 *m*-Cl**



xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	2.4289210000	-1.8181080000	0.3310340000
C	3.7956710000	-1.7245670000	0.0188920000
C	1.8509470000	-3.1490500000	0.5882270000
C	4.1927200000	-0.4555040000	-0.2138130000
S	2.8554210000	0.6353890000	-0.0181820000
C	1.7814130000	-0.6428700000	0.3751870000
C	4.6289720000	-2.9635620000	-0.0316510000
C	5.5339110000	0.0791160000	-0.6025420000
C	0.3614180000	-0.4208930000	0.5669110000
C	-0.0732450000	0.9748530000	0.8954050000
O	-0.1796400000	-1.3740730000	1.4428320000
C	0.1485460000	2.0359920000	0.0064420000
C	-0.3415750000	3.2950160000	0.3134980000
C	-1.0543820000	3.5542010000	1.4751790000
C	-1.2813080000	2.4959130000	2.3481630000
C	-0.8020160000	1.2219080000	2.0647110000
C	-0.2410540000	-0.8099970000	-1.2496950000
O	0.3197250000	-0.0575390000	-2.1067890000
C	-1.7353020000	-0.6932990000	-1.0406960000
C	-2.4667360000	-1.7741940000	-0.5446250000
C	-3.8323260000	-1.6318490000	-0.3225510000
C	-4.4952310000	-0.4454340000	-0.5944310000
C	-3.7630360000	0.6188470000	-1.1207620000
C	-2.3990830000	0.4975000000	-1.3483910000

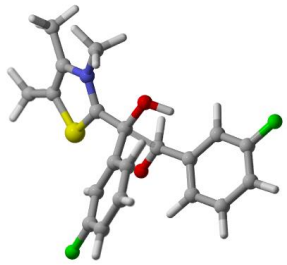
H	2.2075290000	-3.5170230000	1.5507420000
H	0.7735600000	-3.0841370000	0.6045440000
H	2.1742320000	-3.8188210000	-0.2054780000
H	4.5294200000	-3.5413520000	0.8887610000
H	5.6765090000	-2.6990900000	-0.1521680000
H	4.3412520000	-3.6020710000	-0.8698420000
H	5.9049120000	0.7846680000	0.1430910000
H	6.2566900000	-0.7289630000	-0.6980890000
H	5.4776690000	0.5979200000	-1.5613950000
H	-1.1332920000	-1.4120640000	1.2898300000
H	0.6363870000	1.8606110000	-0.9429220000
Cl	-0.0683110000	4.6000660000	-0.8244700000
H	-1.4216230000	4.5500890000	1.6865300000
H	-1.8351180000	2.6700760000	3.2630160000
H	-0.9867020000	0.4158700000	2.7623190000
H	0.0730850000	-1.8719840000	-1.1846790000
H	-1.9858140000	-2.7294900000	-0.3581690000
Cl	-4.7367240000	-2.9961950000	0.3017470000
H	-5.5591510000	-0.3594490000	-0.4140890000
H	-4.2733910000	1.5455660000	-1.3555320000
H	-1.8302440000	1.3145160000	-1.7755880000

thermodynamic data

Zero-point correction= 0.346879 (Hartree/Particle)
Thermal correction to Energy= 0.371796
Thermal correction to Enthalpy= 0.372740
Thermal correction to Gibbs Free Energy= 0.289363
Sum of electronic and zero-point Energies= -2296.820048
Sum of electronic and thermal Energies= -2296.795132
Sum of electronic and thermal Enthalpies= -2296.794188
Sum of electronic and thermal Free Energies= -2296.877565

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.305	94.083	175.482

M062X/6-311+G**/PCM	**TST3 *m*-F**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	2.5680870000	-1.0245390000	0.8634970000
C	3.8629470000	-0.9672920000	0.3304280000
C	2.3232910000	-1.7326550000	2.1342030000
C	3.9664300000	-0.0859440000	-0.6872240000
S	2.4201840000	0.6193890000	-1.0400250000
C	1.6617660000	-0.2593350000	0.2294580000
C	4.9543380000	-1.8250710000	0.8862490000
C	5.1620890000	0.2757730000	-1.5115590000
C	0.2260180000	-0.2428810000	0.4594420000
C	-0.4291480000	1.0626220000	0.7564260000
O	-0.1440560000	-1.2795640000	1.3252570000
C	-0.2220650000	2.2049350000	-0.0287020000
C	-0.9488920000	3.3470800000	0.2477320000
C	-1.8814400000	3.4365880000	1.2636600000
C	-2.0828740000	2.2994970000	2.0400630000
C	-1.3741390000	1.1304840000	1.7917770000
C	-0.4426160000	-0.7111410000	-1.3623840000
O	-0.1505800000	0.2033560000	-2.1857010000
C	-1.8940130000	-0.9459200000	-1.0219080000
C	-2.3306080000	-2.2115920000	-0.6238990000
C	-3.6689570000	-2.3861920000	-0.3076780000
C	-4.5937310000	-1.3632600000	-0.3755350000
C	-4.1490880000	-0.1072340000	-0.7903950000
C	-2.8152410000	0.1013700000	-1.1139400000
H	1.6520050000	-1.1423640000	2.7472360000
H	1.8834010000	-2.7099080000	1.9488430000
H	3.2757450000	-1.8396840000	2.6434040000
H	5.2891800000	-1.4745680000	1.8653330000
H	5.8074600000	-1.8086640000	0.2114310000
H	4.6235540000	-2.8604040000	0.9855000000
H	6.0808730000	0.0479990000	-0.9728520000
H	5.1682780000	-0.2715880000	-2.4565900000
H	5.1630930000	1.3426050000	-1.7397700000
H	-1.0295040000	-1.5745880000	1.0761420000
H	0.4468680000	2.2195500000	-0.8760410000
F	-0.7372350000	4.4341470000	-0.5305360000
H	-2.4183420000	4.3606790000	1.4342540000
H	-2.8014600000	2.3269820000	2.8506170000
H	-1.5496380000	0.2616030000	2.4115710000
H	0.1246270000	-1.6639150000	-1.3817040000
H	-1.6548780000	-3.0605080000	-0.5876320000
F	-4.0845250000	-3.6151570000	0.0693920000
H	-5.6293800000	-1.5527600000	-0.1228850000
H	-4.8582700000	0.7090680000	-0.8602820000
H	-2.4646600000	1.0717720000	-1.4440950000

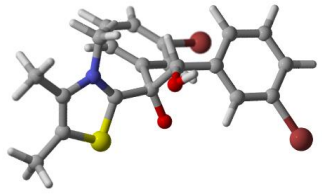
thermodynamic data

Zero-point correction= 0.349766 (Hartree/Particle)
Thermal correction to Energy= 0.373679
Thermal correction to Enthalpy= 0.374624

Thermal correction to Gibbs Free Energy= 0.295304
Sum of electronic and zero-point Energies= -1576.096443
Sum of electronic and thermal Energies= -1576.072530
Sum of electronic and thermal Enthalpies= -1576.071585
Sum of electronic and thermal Free Energies= -1576.150905

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.487	92.301	166.942

M062X/6-311+G**/PCM	**Zwitterion2 *m*-Br**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.9678960000	2.0256680000	0.4166790000
C	-3.7753970000	1.2044190000	1.1960110000
C	-3.1650850000	0.2589900000	2.0134360000
C	-1.7784030000	0.1428500000	2.0389780000
C	-0.9838220000	0.9638720000	1.2400840000
C	-1.5854660000	1.9236080000	0.4240530000
C	0.5146740000	0.8087350000	1.2385090000
C	1.0280300000	0.1371070000	-0.1074390000
C	0.7266350000	-1.3833010000	-0.0435590000
C	2.5673160000	0.3640180000	-0.1501660000
O	0.5199070000	0.6989290000	-1.2030080000
S	3.1414940000	0.9510700000	-1.6317900000
C	4.7686510000	1.0162220000	-1.0311590000
C	4.8146530000	0.6204130000	0.2644330000
N	3.5468120000	0.2414970000	0.7350260000
C	-0.5924180000	-1.7444920000	-0.3376250000
C	-0.9654030000	-3.0762070000	-0.2948950000
C	-0.0582330000	-4.0886800000	-0.0006110000
C	1.2598220000	-3.7306040000	0.2474680000
C	1.6499830000	-2.3912160000	0.2289390000
C	5.8815770000	1.4942200000	-1.9102060000
C	5.9966700000	0.5684400000	1.1767300000
H	-4.8526950000	1.3060940000	1.1695590000
H	-0.3703670000	-5.1248280000	0.0171330000
Br	-3.7876980000	3.3268210000	-0.7130640000
H	-3.7774850000	-0.3842530000	2.6340540000
H	-1.3103650000	-0.5987980000	2.6778860000

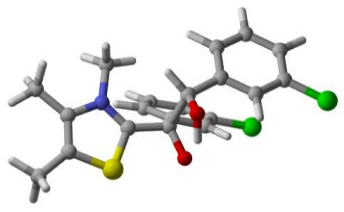
H	-0.9676660000	2.5505430000	-0.2038360000
H	0.7803550000	0.1849570000	2.0973440000
H	-1.3007760000	-0.9737700000	-0.6129710000
Br	-2.7792950000	-3.5344320000	-0.6695070000
H	1.9927990000	-4.5026190000	0.4497240000
H	2.6946480000	-2.1615100000	0.4030750000
H	6.8468110000	1.3468380000	-1.4291330000
H	5.8882320000	0.9468670000	-2.8539860000
H	5.7674910000	2.5562060000	-2.1361710000
H	5.8044570000	1.1228500000	2.0973900000
H	6.2536260000	-0.4601020000	1.4405180000
H	6.8580440000	1.0181120000	0.6886970000
C	3.3489370000	-0.1646120000	2.1326600000
H	4.2413360000	-0.6782110000	2.4792800000
H	2.5097800000	-0.8489230000	2.1965160000
H	3.1616880000	0.7223650000	2.7385460000
O	1.1839600000	2.0603010000	1.3278030000
H	0.7933860000	2.5664400000	2.0475380000

thermodynamic data

Zero-point correction= 0.348376 (Hartree/Particle)
Thermal correction to Energy= 0.373767
Thermal correction to Enthalpy= 0.374711
Thermal correction to Gibbs Free Energy= 0.290481
Sum of electronic and zero-point Energies= -6524.773761
Sum of electronic and thermal Energies= -6524.748370
Sum of electronic and thermal Enthalpies= -6524.747426
Sum of electronic and thermal Free Energies= -6524.831656

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.542	95.427	177.277

M062X/6-311+G**/PCM	**Zwitterion2 *m*-Cl**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

C	3.6143580000	-1.5753170000	0.3082390000
C	3.9804890000	-0.8472670000	1.4320910000
C	2.9754190000	-0.3900170000	2.2797250000

C	1.6406520000	-0.6448950000	1.9879920000
C	1.2868330000	-1.3563700000	0.8409550000
C	2.2875610000	-1.8461230000	0.0049380000
C	-0.1650780000	-1.5223250000	0.4617920000
C	-0.6884170000	-0.3096210000	-0.5043330000
C	-0.0177520000	1.0498390000	-0.2375760000
C	-2.2120250000	-0.2266680000	-0.2702950000
O	-0.4948250000	-0.7195170000	-1.7730570000
S	-3.1877900000	-0.4596390000	-1.6358630000
C	-4.6354650000	-0.3074860000	-0.6918750000
C	-4.3318670000	-0.1035710000	0.6138480000
N	-2.9449070000	-0.0605090000	0.8235540000
C	1.2820680000	1.2015630000	-0.7345760000
C	1.9700940000	2.3796660000	-0.5198050000
C	1.3972090000	3.4591250000	0.1451900000
C	0.0879590000	3.3304050000	0.5829660000
C	-0.6148460000	2.1394970000	0.3925710000
C	-5.9780000000	-0.4190650000	-1.3422180000
C	-5.2581290000	0.0722220000	1.7716480000
H	5.0242720000	-0.6511360000	1.6416500000
H	1.9549960000	4.3743980000	0.2954610000
Cl	4.8673090000	-2.1620510000	-0.7669490000
H	3.2416470000	0.1683090000	3.1692610000
H	0.8692720000	-0.2749890000	2.6559170000
H	2.0264400000	-2.4126030000	-0.8801820000
H	-0.7564510000	-1.5799780000	1.3772520000
H	1.7417110000	0.3936170000	-1.2865410000
Cl	3.6140470000	2.5172900000	-1.1135620000
H	-0.3966050000	4.1660820000	1.0734390000
H	-1.6442670000	2.1028700000	0.7248690000
H	-6.7729010000	-0.3007480000	-0.6082800000
H	-6.1021960000	0.3505580000	-2.1058080000
H	-6.0956070000	-1.3931630000	-1.8202150000
H	-5.0372660000	-0.6442080000	2.5651790000
H	-5.1834460000	1.0794520000	2.1878670000
H	-6.2850290000	-0.0850380000	1.4515030000
C	-2.4100270000	0.1298480000	2.1803390000
H	-2.9058190000	0.9851390000	2.6361710000
H	-1.3456220000	0.3263810000	2.1291050000
H	-2.6009940000	-0.7661330000	2.7710000000
O	-0.3965150000	-2.6699080000	-0.3009120000
H	-0.4316880000	-2.2653260000	-1.2179760000

thermodynamic data

Zero-point correction= 0.349300 (Hartree/Particle)
Thermal correction to Energy= 0.373884
Thermal correction to Enthalpy= 0.374829
Thermal correction to Gibbs Free Energy= 0.290871
Sum of electronic and zero-point Energies= -2296.838851
Sum of electronic and thermal Energies= -2296.814266
Sum of electronic and thermal Enthalpies= -2296.813322
Sum of electronic and thermal Free Energies= -2296.897280

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.616	93.430	176.704

M062X/6-311+G**/PCM	**Zwitterion2 *m*-F**

xyz-matrix

thermodynamic data

M062X/6-311+G**/PCM	**Zwitterion2 *m*-Me**

xyz-matrix

51
XYZ file generated by gabedit : coordinates in Angstrom

C	4.0106380000	-1.7468080000	0.0288790000
C	4.4725360000	-0.9290230000	1.0641810000
C	3.5770500000	-0.3126880000	1.9317610000
C	2.2073000000	-0.4934260000	1.7644370000
C	1.7257070000	-1.2870480000	0.7253550000
C	2.6350030000	-1.9201780000	-0.1218720000
C	0.2389930000	-1.4053490000	0.4907880000
C	-0.3327450000	-0.2709800000	-0.5217170000
C	0.2905470000	1.1275500000	-0.3607160000
C	-1.8511570000	-0.2233650000	-0.2341410000
O	-0.1810330000	-0.7533600000	-1.7733490000
S	-2.8664220000	-0.5867900000	-1.5418530000
C	-4.2842730000	-0.4174050000	-0.5551050000
C	-3.9417180000	-0.1124210000	0.7203100000
N	-2.5501440000	-0.0042060000	0.8721260000
C	1.5971630000	1.3008440000	-0.8255320000
C	2.2551240000	2.5253330000	-0.7479880000
C	1.5708860000	3.6216300000	-0.2176160000
C	0.2547080000	3.4840330000	0.2037420000
C	-0.3834520000	2.2468680000	0.1315290000

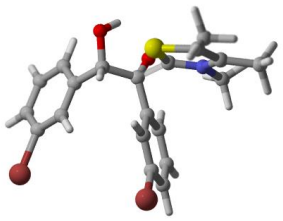
C	-5.6446610000	-0.6094460000	-1.1475800000
C	-4.8315810000	0.1105610000	1.8983970000
H	5.5404670000	-0.7833500000	1.1947580000
H	2.0654400000	4.5851230000	-0.1506620000
H	3.9462730000	0.3102310000	2.7386450000
H	1.5115170000	-0.0004870000	2.4373930000
H	2.2580010000	-2.5510730000	-0.9194480000
H	-0.2642480000	-1.3608400000	1.4584260000
H	2.1115990000	0.4513070000	-1.2599830000
H	-0.2854630000	4.3429890000	0.5852520000
H	-1.4193630000	2.1901140000	0.4430290000
H	-6.4172970000	-0.4907450000	-0.3901840000
H	-5.8265140000	0.1233240000	-1.9358120000
H	-5.7412360000	-1.6056240000	-1.5826440000
H	-4.5398850000	-0.5238690000	2.7374300000
H	-4.7990880000	1.1518490000	2.2276650000
H	-5.8595480000	-0.1286760000	1.6370690000
C	-1.9703530000	0.3295760000	2.1821260000
H	-2.4923750000	1.1961100000	2.5846400000
H	-0.9210920000	0.5756460000	2.0635990000
H	-2.0869860000	-0.5183270000	2.8568540000
O	-0.1141340000	-2.6099650000	-0.1370800000
H	-0.1607150000	-2.3083800000	-1.0848220000
C	4.9875400000	-2.4213270000	-0.9007130000
H	4.4691630000	-3.0252550000	-1.6459860000
H	5.6673640000	-3.0721070000	-0.3454080000
H	5.5983810000	-1.6821470000	-1.4249270000
C	3.6795520000	2.6441900000	-1.2281010000
H	4.0591600000	3.6580080000	-1.0959000000
H	3.7561540000	2.3850730000	-2.2869670000
H	4.3285690000	1.9590660000	-0.6763670000

thermodynamic data

Zero-point correction= 0.422878 (Hartree/Particle)
Thermal correction to Energy= 0.446941
Thermal correction to Enthalpy= 0.447885
Thermal correction to Gibbs Free Energy= 0.368838
Sum of electronic and zero-point Energies= -1456.174190
Sum of electronic and thermal Energies= -1456.150128
Sum of electronic and thermal Enthalpies= -1456.149183
Sum of electronic and thermal Free Energies= -1456.228230

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	280.460	94.064	166.368

M062X/6-311+G**/PCM	**TST5 *m*-Br**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	3.5108760000	-0.6482930000	0.6403440000
C	4.6947320000	-0.3302740000	-0.0546060000
C	3.3830510000	-0.3870760000	2.0792370000
C	4.5953290000	-0.6255470000	-1.3708870000
S	3.0096110000	-1.2938220000	-1.6774400000
C	2.4955290000	-1.1573870000	-0.0515140000
C	5.8560230000	0.2529610000	0.6832920000
C	5.6027180000	-0.4645320000	-2.4644710000
C	0.4454850000	-1.5488180000	0.9086940000
C	0.1936540000	-0.1043320000	1.2715460000
O	0.6417110000	-2.3876400000	1.7866970000
C	0.3233310000	0.9273080000	0.3400090000
C	0.0227290000	2.2236230000	0.7244660000
C	-0.4058690000	2.5259440000	2.0130710000
C	-0.5315580000	1.4905170000	2.9319550000
C	-0.2332730000	0.1810210000	2.5652370000
C	-0.1718300000	-2.0549230000	-0.4147600000
O	0.3287930000	-3.3392960000	-0.6779770000
C	-1.6839670000	-2.0507420000	-0.2402830000
C	-2.4223940000	-0.9299980000	-0.6199010000
C	-3.7925800000	-0.9129820000	-0.3977500000
C	-4.4529020000	-1.9858480000	0.1857410000
C	-3.7070610000	-3.1024230000	0.5534170000
C	-2.3325960000	-3.1360380000	0.3457090000
H	3.2324540000	0.6803840000	2.2511500000
H	2.5290080000	-0.9476720000	2.4494130000
H	4.2848980000	-0.7167190000	2.5923750000
H	6.2813560000	-0.4689050000	1.3848180000
H	5.5559280000	1.1374550000	1.2493220000
H	6.6372610000	0.5472060000	-0.0143200000
H	5.2426960000	0.2307710000	-3.2252980000
H	6.5439890000	-0.0825460000	-2.0708650000
H	5.8026870000	-1.4209760000	-2.9510870000
H	0.6769450000	0.7258170000	-0.6642030000
Br	0.2197240000	3.6286340000	-0.5447680000
H	-0.6330150000	3.5473500000	2.2900830000
H	-0.8660710000	1.7100690000	3.9386520000
H	-0.3319420000	-0.6307260000	3.2756260000
H	0.0924650000	-1.3940220000	-1.2422810000
H	0.6595720000	-3.6717270000	0.1706630000
H	-1.9336920000	-0.0799630000	-1.0824580000

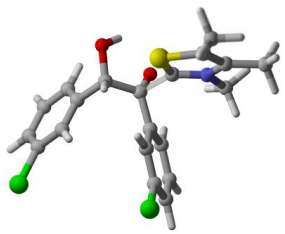
Br	-4.7925730000	0.6267490000	-0.9060930000
H	-5.5224730000	-1.9530370000	0.3472710000
H	-4.2077760000	-3.9492480000	1.0073270000
H	-1.7598360000	-4.0099470000	0.6315980000

thermodynamic data

Zero-point correction= 0.346309 (Hartree/Particle)
Thermal correction to Energy= 0.371814
Thermal correction to Enthalpy= 0.372758
Thermal correction to Gibbs Free Energy= 0.286767
Sum of electronic and zero-point Energies= -6524.768608
Sum of electronic and thermal Energies= -6524.743103
Sum of electronic and thermal Enthalpies= -6524.742159
Sum of electronic and thermal Free Energies= -6524.828149

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.317	94.775	180.983

M062X/6-311+G**/PCM	**TST5 *m*-Cl**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	3.1435990000	-0.2571060000	0.6891420000
C	4.3731040000	-0.1526490000	0.0082620000
C	2.9989320000	0.2325910000	2.0652290000
C	4.2871440000	-0.6312350000	-1.2537520000
S	2.6563330000	-1.1938870000	-1.5297080000
C	2.1068980000	-0.7755570000	0.0365990000
C	5.5604430000	0.4284440000	0.7050660000
C	5.3392990000	-0.7264100000	-2.3122380000
C	0.0221380000	-0.9852520000	1.0089490000
C	-0.2365090000	0.4985410000	1.1013570000
O	0.2064160000	-1.6513290000	2.0262940000
C	-0.1235920000	1.3418230000	-0.0044780000
C	-0.4485240000	2.6802890000	0.1354900000
C	-0.8807020000	3.2081690000	1.3479200000
C	-0.9868520000	2.3598190000	2.4429600000
C	-0.6678270000	1.0099110000	2.3219970000
C	-0.5719040000	-1.7247650000	-0.2105110000

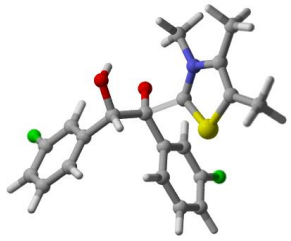
O	-0.1287280000	-3.0567100000	-0.1810030000
C	-2.0862950000	-1.6191270000	-0.1126440000
C	-2.7682030000	-0.6855260000	-0.8895220000
C	-4.1424200000	-0.5546750000	-0.7434180000
C	-4.8594700000	-1.3336870000	0.1529640000
C	-4.1695900000	-2.2690510000	0.9195600000
C	-2.7930330000	-2.4116350000	0.7909730000
H	2.9836970000	1.3236880000	2.0699450000
H	2.0669910000	-0.1556880000	2.4661720000
H	3.8316870000	-0.1222090000	2.6706570000
H	5.8908620000	-0.2141510000	1.5247970000
H	5.3291210000	1.4122270000	1.1191180000
H	6.3884560000	0.5411280000	0.0085880000
H	5.0523560000	-0.1579120000	-3.1989370000
H	6.2893340000	-0.3353800000	-1.9497190000
H	5.4936200000	-1.7642490000	-2.6137810000
H	0.2359230000	0.9697730000	-0.9566890000
Cl	-0.3029150000	3.7376540000	-1.2509920000
H	-1.1262590000	4.2595080000	1.4267190000
H	-1.3250410000	2.7551040000	3.3931640000
H	-0.7538240000	0.3395310000	3.1685130000
H	-0.2432550000	-1.2600000000	-1.1416330000
H	0.1743550000	-3.2115500000	0.7271670000
H	-2.2387170000	-0.0646870000	-1.6034950000
Cl	-4.9903520000	0.6242530000	-1.7222700000
H	-5.9312610000	-1.2135440000	0.2461010000
H	-4.7163910000	-2.8865830000	1.6218710000
H	-2.2623570000	-3.1412870000	1.3913030000

thermodynamic data

Zero-point correction= 0.346749 (Hartree/Particle)
Thermal correction to Energy= 0.372130
Thermal correction to Enthalpy= 0.373074
Thermal correction to Gibbs Free Energy= 0.286165
Sum of electronic and zero-point Energies= -2296.824950
Sum of electronic and thermal Energies= -2296.799569
Sum of electronic and thermal Enthalpies= -2296.798625
Sum of electronic and thermal Free Energies= -2296.885535

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.515	94.153	182.917

M062X/6-311+G**/PCM	**TST5 *m*-F**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	2.9200780000	-1.1201650000	0.3342740000
C	4.1229870000	-0.7860250000	-0.3185250000
C	2.8326660000	-2.3135990000	1.1848760000
C	3.9918640000	0.3371480000	-1.0605510000
S	2.3591310000	0.9330180000	-0.9014790000
C	1.8663550000	-0.3352520000	0.1390120000
C	5.3343240000	-1.6394780000	-0.1269460000
C	5.0048450000	1.0523130000	-1.8970350000
C	-0.1870240000	-0.5972480000	0.9867730000
C	-0.4550220000	0.8859130000	1.0616490000
O	-0.0728030000	-1.2580110000	2.0264080000
C	-0.7254340000	1.6451680000	-0.0780230000
C	-0.9634030000	2.9978420000	0.0715660000
C	-0.9510200000	3.6337510000	1.3002310000
C	-0.6890590000	2.8637510000	2.4292170000
C	-0.4454230000	1.4991840000	2.3126330000
C	-0.7125740000	-1.3678410000	-0.2485080000
O	-0.2499080000	-2.6966430000	-0.1610750000
C	-2.2333380000	-1.3047750000	-0.2709280000
C	-2.8882300000	-0.7695190000	-1.3774060000
C	-4.2717320000	-0.7291070000	-1.3790360000
C	-5.0366300000	-1.1997880000	-0.3295470000
C	-4.3721530000	-1.7376280000	0.7704590000
C	-2.9835680000	-1.7901730000	0.8025680000
H	3.6790310000	-2.3338060000	1.8699020000
H	1.9054690000	-2.2555360000	1.7467640000
H	2.8419160000	-3.2100110000	0.5640640000
H	5.1150880000	-2.6869330000	-0.3438950000
H	5.7026810000	-1.5763030000	0.8998560000
H	6.1319350000	-1.3152500000	-0.7919000000
H	4.6479110000	1.1710210000	-2.9215960000
H	5.2078790000	2.0467110000	-1.4944040000
H	5.9431600000	0.4997490000	-1.9256970000
H	-0.7470570000	1.2192700000	-1.0737600000
F	-1.2186850000	3.7293720000	-1.0339120000
H	-1.1453120000	4.6971050000	1.3600640000
H	-0.6774930000	3.3350710000	3.4044630000
H	-0.2424380000	0.8936040000	3.1866600000
H	-0.3235010000	-0.9431150000	-1.1734640000
H	-0.1474130000	-2.8705430000	0.7875470000

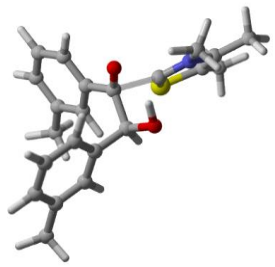
H	-2.3429990000	-0.3936430000	-2.2361840000
F	-4.8972950000	-0.2103240000	-2.4577830000
H	-6.1167640000	-1.1461450000	-0.3795440000
H	-4.9476680000	-2.1142170000	1.6073640000
H	-2.4761510000	-2.2061930000	1.6652320000

thermodynamic data

Zero-point correction= 0.350185 (Hartree/Particle)
Thermal correction to Energy= 0.374408
Thermal correction to Enthalpy= 0.375352
Thermal correction to Gibbs Free Energy= 0.293536
Sum of electronic and zero-point Energies= -1576.102980
Sum of electronic and thermal Energies= -1576.078758
Sum of electronic and thermal Enthalpies= -1576.077813
Sum of electronic and thermal Free Energies= -1576.159630

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.944	92.054	172.197

M062X/6-311+G**/PCM	**TST5 *m*-Me**



xyz-matrix

51
XYZ file generated by gabedit : coordinates in Angstrom

N	2.9368600000	-1.1330400000	0.2364140000
C	4.1340470000	-0.7193190000	-0.3812350000
C	2.8720380000	-2.3996390000	0.9764080000
C	3.9839730000	0.4669660000	-1.0131320000
S	2.3424840000	1.0200220000	-0.8020190000
C	1.8708610000	-0.3507480000	0.1126180000
C	5.3574980000	-1.5702660000	-0.2740650000
C	4.9833850000	1.2719860000	-1.7816500000
C	-0.1238560000	-0.6859370000	0.9518480000
C	-0.4326050000	0.7815530000	1.1252920000
O	0.0131570000	-1.4138300000	1.9499580000
C	-0.7192080000	1.6099900000	0.0386460000
C	-1.0097260000	2.9616530000	0.2126420000
C	-1.0187840000	3.4777680000	1.5114030000
C	-0.7424230000	2.6598830000	2.6018220000

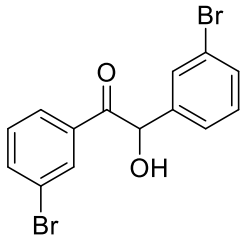
C	-0.4507270000	1.3123610000	2.4122280000
C	-0.6805330000	-1.3886850000	-0.3132420000
O	-0.2010580000	-2.7174520000	-0.3131150000
C	-2.2004260000	-1.3389190000	-0.2960080000
C	-2.8933880000	-0.7187830000	-1.3315420000
C	-4.2899130000	-0.6526510000	-1.3437490000
C	-4.9881340000	-1.2285700000	-0.2839170000
C	-4.3069740000	-1.8592520000	0.7565740000
C	-2.9193160000	-1.9154440000	0.7543860000
H	3.7231170000	-2.4666340000	1.6524730000
H	1.9477230000	-2.4053190000	1.5458220000
H	2.8919480000	-3.2361100000	0.2772870000
H	5.1542140000	-2.5919230000	-0.6018240000
H	5.7217100000	-1.6111000000	0.7552220000
H	6.1523270000	-1.1668550000	-0.8976760000
H	5.9408720000	0.7551360000	-1.8327340000
H	4.6370450000	1.4489580000	-2.8016170000
H	5.1462610000	2.2426610000	-1.3091620000
H	-0.7152630000	1.2089820000	-0.9696100000
H	-1.2496630000	4.5267770000	1.6667520000
H	-0.7600540000	3.0730390000	3.6038760000
H	-0.2395290000	0.6602330000	3.2508390000
H	-0.3182360000	-0.9093800000	-1.2224420000
H	-0.0774140000	-2.9383260000	0.6233270000
H	-2.3385530000	-0.2730610000	-2.1537380000
H	-6.0721940000	-1.1849300000	-0.2711930000
H	-4.8640370000	-2.3038030000	1.5735230000
H	-2.3887500000	-2.3985830000	1.5675670000
C	-1.2824000000	3.8505450000	-0.9730500000
H	-2.0530400000	4.5881110000	-0.7426100000
H	-1.6074300000	3.2672770000	-1.8358840000
H	-0.3787390000	4.3961150000	-1.2594380000
C	-5.0108080000	0.0098020000	-2.4896720000
H	-6.0507570000	0.2163720000	-2.2341740000
H	-5.0030870000	-0.6325780000	-3.3743930000
H	-4.5285030000	0.9503730000	-2.7631740000

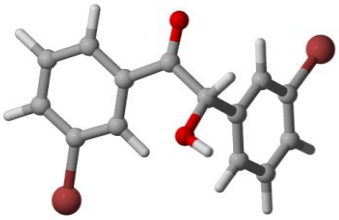
thermodynamic data

Zero-point correction= 0.421192 (Hartree/Particle)
Thermal correction to Energy= 0.447566
Thermal correction to Enthalpy= 0.448511
Thermal correction to Gibbs Free Energy= 0.361228
Sum of electronic and zero-point Energies= -1456.160779
Sum of electronic and thermal Energies= -1456.134405
Sum of electronic and thermal Enthalpies= -1456.133461
Sum of electronic and thermal Free Energies= -1456.220743

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	280.852	98.396	183.701

M062X/6-311+G**/PCM	***m*-Br-Benzoin**





xyz-matrix

28
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.1525840000	0.0420180000	-0.5311940000
C	-3.7704600000	0.9712530000	-1.3579450000
C	-3.2161240000	2.2439400000	-1.4720590000
C	-2.0631840000	2.5707040000	-0.7731980000
C	-1.4566810000	1.6283360000	0.0607540000
C	-2.0064840000	0.3505800000	0.1870570000
C	-0.1992530000	2.0291840000	0.7654070000
C	0.3743400000	1.1691150000	1.8991070000
O	0.4118660000	3.0198920000	0.4334560000
C	1.2249530000	0.0516190000	1.3011790000
O	-0.6759990000	0.7021940000	2.7148030000
C	2.3328470000	0.3941580000	0.5228460000
C	3.1149080000	-0.6146090000	-0.0174880000
C	2.8282750000	-1.9582800000	0.1951300000
C	1.7251670000	-2.2849170000	0.9747590000
C	0.9237860000	-1.2883400000	1.5252080000
Br	-3.9015510000	-1.6983620000	-0.3615520000
Br	4.6270660000	-0.1471230000	-1.0741520000
H	-4.6682370000	0.7084590000	-1.9027340000
H	-3.6907450000	2.9764110000	-2.1130280000
H	-1.6215730000	3.5553520000	-0.8625130000
H	-1.5571360000	-0.3888920000	0.8334100000
H	1.0293730000	1.8441530000	2.4572700000
H	-0.3180860000	0.4674440000	3.5770680000
H	2.5782020000	1.4354520000	0.3467190000
H	3.4540100000	-2.7287350000	-0.2357420000
H	1.4897190000	-3.3271460000	1.1533140000
H	0.0674960000	-1.5557690000	2.1324240000

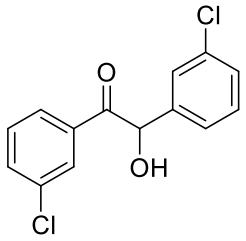
thermodynamic data

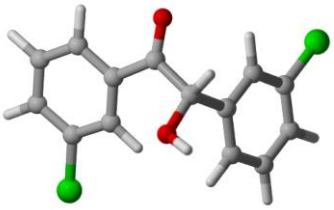
Zero-point correction= 0.205342 (Hartree/Particle)
Thermal correction to Energy= 0.221419
Thermal correction to Enthalpy= 0.222363
Thermal correction to Gibbs Free Energy= 0.157933
Sum of electronic and zero-point Energies= -5838.003692
Sum of electronic and thermal Energies= -5837.987615

Sum of electronic and thermal Enthalpies= -5837.986671
Sum of electronic and thermal Free Energies= -5838.051100

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.942	60.025	135.603

M062X/6-311+G**/PCM	***m*-Cl-Benzoin**





xyz-matrix

28
XYZ file generated by gabedit : coordinates in Angstrom

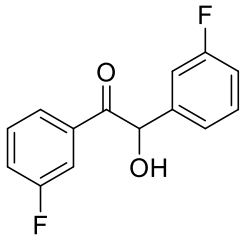
C	-3.0238080000	-0.6589630000	-0.4935450000
C	-3.8678290000	0.1931820000	-1.1929370000
C	-3.5509120000	1.5470140000	-1.2631140000
C	-2.4046800000	2.0298540000	-0.6482740000
C	-1.5694610000	1.1617680000	0.0590820000
C	-1.8828080000	-0.1959940000	0.1439860000
C	-0.3286000000	1.7320430000	0.6690510000
C	0.4674450000	0.9368600000	1.7118060000
O	0.0908700000	2.8150140000	0.3284960000
C	1.4241880000	-0.0148180000	0.9987160000
O	-0.4263560000	0.2858520000	2.5856750000
C	2.3939920000	0.5202460000	0.1493930000
C	3.2719650000	-0.3357900000	-0.4959150000
C	3.2160660000	-1.7130190000	-0.3189390000
C	2.2486130000	-2.2327190000	0.5321460000
C	1.3542620000	-1.3916490000	1.1889820000
Cl	-3.4100970000	-2.3611960000	-0.4069590000
Cl	4.4858270000	0.3386140000	-1.5586040000
H	-4.7570060000	-0.1966630000	-1.6721310000
H	-4.2041410000	2.2201130000	-1.8041890000
H	-2.1445370000	3.0794300000	-0.7051570000
H	-1.2567550000	-0.8844410000	0.6927290000
H	1.0571680000	1.6881600000	2.2450080000
H	0.0345390000	0.0814190000	3.4058060000
H	2.4632250000	1.5913310000	-0.0045530000
H	3.9146280000	-2.3586820000	-0.8352800000
H	2.1924950000	-3.3037840000	0.6836730000
H	0.6062510000	-1.8080060000	1.8526590000

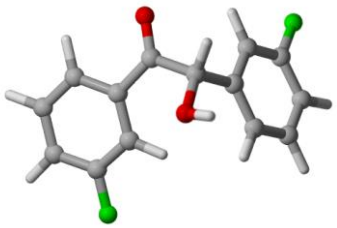
thermodynamic data

Zero-point correction= 0.206198 (Hartree/Particle)
Thermal correction to Energy= 0.221823
Thermal correction to Enthalpy= 0.222767
Thermal correction to Gibbs Free Energy= 0.160538
Sum of electronic and zero-point Energies= -1610.059430
Sum of electronic and thermal Energies= -1610.043805
Sum of electronic and thermal Enthalpies= -1610.042861
Sum of electronic and thermal Free Energies= -1610.105090

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.196	59.254	130.972

M062X/6-311+G**/PCM	***m*-F-Benzoin**





xyz-matrix

28
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.8293360000	1.2564550000	0.3387390000
C	-3.8394530000	0.5853920000	1.0041250000
C	-3.7295130000	-0.7947010000	1.1522380000
C	-2.6264580000	-1.4672250000	0.6446240000
C	-1.6237530000	-0.7654630000	-0.0303790000
C	-1.7243550000	0.6181240000	-0.1905780000
C	-0.4467230000	-1.5425750000	-0.5277560000
C	0.5492370000	-0.9132090000	-1.5104010000
O	-0.2341810000	-2.6689400000	-0.1386580000
C	1.5791510000	-0.1042920000	-0.7277480000
O	-0.1515070000	-0.1572840000	-2.4718200000
C	2.3641970000	-0.7614050000	0.2210760000
C	3.3009170000	-0.0292680000	0.9228570000
C	3.4979360000	1.3270810000	0.7265800000
C	2.7118990000	1.9665570000	-0.2237280000
C	1.7547430000	1.2589580000	-0.9485000000
F	-2.9286160000	2.5929810000	0.1933190000
F	4.0610780000	-0.6666650000	1.8366270000
H	-4.6869220000	1.1369330000	1.3917230000
H	-4.5099910000	-1.3400020000	1.6679570000
H	-2.5289180000	-2.5391130000	0.7613700000

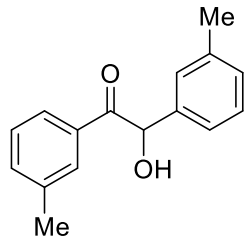
H	-0.9735350000	1.1940760000	-0.7125670000
H	1.0559670000	-1.7627410000	-1.9773610000
H	0.4067900000	-0.0490290000	-3.2484530000
H	2.2546060000	-1.8231490000	0.4121950000
H	4.2484510000	1.8538570000	1.3018620000
H	2.8464340000	3.0264370000	-0.4017950000
H	1.1495380000	1.7691010000	-1.6875210000

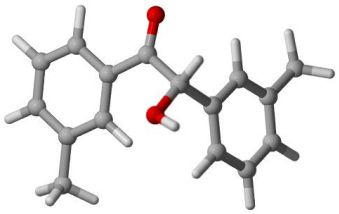
thermodynamic data

Zero-point correction= 0.209027 (Hartree/Particle)
Thermal correction to Energy= 0.223843
Thermal correction to Enthalpy= 0.224787
Thermal correction to Gibbs Free Energy= 0.165379
Sum of electronic and zero-point Energies= -889.339478
Sum of electronic and thermal Energies= -889.324662
Sum of electronic and thermal Enthalpies= -889.323717
Sum of electronic and thermal Free Energies= -889.383126

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	140.464	57.469	125.036

M062X/6-311+G**/PCM	***m*-Me-Benzoin**





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.8287980000	1.2311440000	0.4104690000
C	-3.7942280000	0.4839540000	1.0848050000
C	-3.6796900000	-0.9006940000	1.2032670000
C	-2.5900140000	-1.5563320000	0.6522970000
C	-1.6131820000	-0.8247500000	-0.0316610000
C	-1.7401560000	0.5600920000	-0.1493670000
C	-0.4425980000	-1.5728630000	-0.5788770000
C	0.5308480000	-0.9033490000	-1.5580590000
O	-0.2122940000	-2.7139070000	-0.2382360000
C	1.5447740000	-0.0704430000	-0.7799320000
O	-0.1995390000	-0.1651240000	-2.5150260000
C	2.3467780000	-0.7020360000	0.1744190000
C	3.2942140000	0.0075700000	0.9072380000

C	3.4344180000	1.3784160000	0.6636730000
C	2.6465640000	2.0122710000	-0.2866730000
C	1.6965000000	1.2920940000	-1.0106650000
C	-2.9586390000	2.7248810000	0.2613100000
C	4.1555520000	-0.6744570000	1.9381000000
H	-4.6464930000	0.9906540000	1.5257840000
H	-4.4419700000	-1.4615530000	1.7308760000
H	-2.4799840000	-2.6300900000	0.7420400000
H	-0.9868370000	1.1286240000	-0.6792670000
H	1.0574810000	-1.7349040000	-2.0358090000
H	0.3652100000	-0.0130870000	-3.2794770000
H	2.2278790000	-1.7681310000	0.3473320000
H	4.1698350000	1.9465560000	1.2241240000
H	2.7677240000	3.0739380000	-0.4686050000
H	1.0798980000	1.7913490000	-1.7486140000
H	-3.6652200000	3.1329820000	0.9845940000
H	-1.9943340000	3.2163890000	0.4021050000
H	-3.3162760000	2.9805060000	-0.7396340000
H	3.9241490000	-1.7376620000	2.0053930000
H	5.2140860000	-0.5685120000	1.6893610000
H	4.0054540000	-0.2277940000	2.9238340000

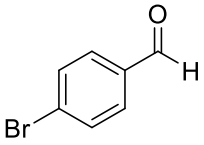
thermodynamic data

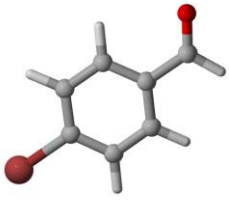
Zero-point correction= 0.280512 (Hartree/Particle)
Thermal correction to Energy= 0.297410
Thermal correction to Enthalpy= 0.298354
Thermal correction to Gibbs Free Energy= 0.233884
Sum of electronic and zero-point Energies= -769.398480
Sum of electronic and thermal Energies= -769.381583
Sum of electronic and thermal Enthalpies= -769.380639
Sum of electronic and thermal Free Energies= -769.445108

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.627	63.743	135.688

Computerchemie Reaktionsdiagramm M062X/PCM

M062X/6-311+G**/PCM	***p*-Br-PhCHO**





xyz-matrix

XYZ file generated by gabedit : coordinates in Angstrom

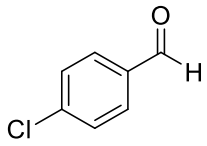
C	-0.0516110000	1.2915860000	-0.0000010000
C	-0.6471740000	0.0365590000	0.0000000000
C	0.1029600000	-1.1384140000	0.0000000000
C	1.4854640000	-1.0462910000	0.0000000000
C	2.1052500000	0.2051600000	0.0000000000
C	1.3361810000	1.3677190000	0.0000000000
C	3.5815020000	0.3130730000	0.0000000000
O	4.3288620000	-0.6362640000	0.0000000000
Br	-2.5415740000	-0.0832320000	0.0000000000
H	-0.6574420000	2.1880470000	-0.0000020000
H	-0.3898940000	-2.1018050000	-0.0000010000
H	2.0962680000	-1.9415160000	0.0000000000
H	1.8214940000	2.3381470000	0.0000000000
H	3.9783390000	1.3439940000	0.0000080000

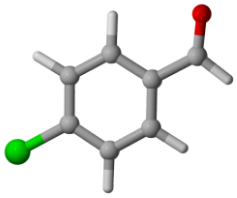
thermodynamic data

Zero-point correction= 0.100481 (Hartree/Particle)
Thermal correction to Energy= 0.108169
Thermal correction to Enthalpy= 0.109113
Thermal correction to Gibbs Free Energy= 0.066673
Sum of electronic and zero-point Energies= -2918.994224
Sum of electronic and thermal Energies= -2918.986536
Sum of electronic and thermal Enthalpies= -2918.985592
Sum of electronic and thermal Free Energies= -2919.028033

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.877	27.986	89.324

M062X/6-311+G**/PCM	***p*-Cl-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.7456480000	1.2553530000	-0.0000010000
C	-1.3187800000	-0.0097690000	0.0000000000
C	-0.5479400000	-1.1708230000	0.0000000000
C	0.8320900000	-1.0547330000	0.0000000000
C	1.4298090000	0.2077030000	0.0000000000
C	0.6399300000	1.3565320000	0.0000000000

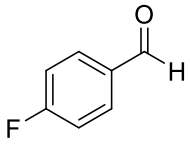
C	2.9034970000	0.3417710000	0.0000000000
O	3.6681030000	-0.5938510000	0.0000000000
Cl	-3.0559340000	-0.1517280000	0.0000000000
H	-1.3715340000	2.1382140000	-0.0000020000
H	-1.0285070000	-2.1405410000	0.0000000000
H	1.4588210000	-1.9387680000	0.0000000000
H	1.1076690000	2.3354780000	0.0000000000
H	3.2818590000	1.3796130000	0.0000080000

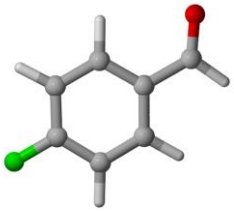
thermodynamic data

Zero-point correction= 0.100982 (Hartree/Particle)
Thermal correction to Energy= 0.108458
Thermal correction to Enthalpy= 0.109402
Thermal correction to Gibbs Free Energy= 0.068183
Sum of electronic and zero-point Energies= -805.022235
Sum of electronic and thermal Energies= -805.014759
Sum of electronic and thermal Enthalpies= -805.013815
Sum of electronic and thermal Free Energies= -805.055034

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.058	27.575	86.751

M062X/6-311+G**/PCM	***p*-F-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2207970000	1.1999720000	-0.0000010000
C	-1.7430930000	-0.0816360000	0.0000000000
C	-0.9548510000	-1.2247690000	0.0000000000
C	0.4209940000	-1.0692960000	0.0000010000
C	0.9829530000	0.2108180000	0.0000010000
C	0.1612070000	1.3383850000	0.0000000000
C	2.4502640000	0.3877370000	0.0000020000
O	3.2447560000	-0.5233590000	-0.0000030000
F	-3.0780900000	-0.2295970000	0.0000000000
H	-1.8850380000	2.0543200000	-0.0000030000
H	-1.4238380000	-2.2003190000	-0.0000010000
H	1.0738170000	-1.9340370000	0.0000010000
H	0.6029710000	2.3291870000	-0.0000010000

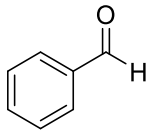
H 2.7967810000 1.4368280000 0.0000070000

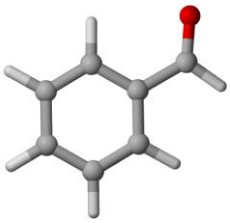
thermodynamic data

Zero-point correction= 0.102260 (Hartree/Particle)
Thermal correction to Energy= 0.109370
Thermal correction to Enthalpy= 0.110314
Thermal correction to Gibbs Free Energy= 0.070377
Sum of electronic and zero-point Energies= -444.662941
Sum of electronic and thermal Energies= -444.655832
Sum of electronic and thermal Enthalpies= -444.654887
Sum of electronic and thermal Free Energies= -444.694824

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.631	26.732	84.054

M062X/6-311+G**/PCM	***p*-H-PhCHO**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom
C -1.7239590000 1.0627530000 -0.0000010000
C -2.2089310000 -0.2418360000 0.0000010000
C -1.3278220000 -1.3250330000 0.0000000000
C 0.0412290000 -1.1035220000 0.0000000000
C 0.5303670000 0.2056660000 0.0000000000
C -0.3510110000 1.2866660000 0.0000000000
C 1.9864720000 0.4671540000 0.0000000000
O 2.8339810000 -0.3948890000 -0.0000010000
H -2.4115200000 1.8994990000 -0.0000020000
H -3.2780310000 -0.4189740000 0.0000020000
H -1.7146370000 -2.3368340000 -0.0000010000
H 0.7429140000 -1.9296070000 0.0000000000
H 0.0401680000 2.2990210000 -0.0000010000
H 2.2711910000 1.5349230000 0.0000080000

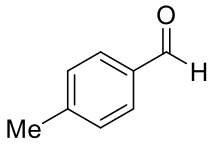
thermodynamic data

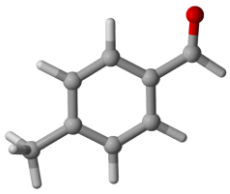
Zero-point correction= 0.110510 (Hartree/Particle)
Thermal correction to Energy= 0.116837
Thermal correction to Enthalpy= 0.117781

Thermal correction to Gibbs Free Energy= 0.079890
Sum of electronic and zero-point Energies= -345.412239
Sum of electronic and thermal Energies= -345.405912
Sum of electronic and thermal Enthalpies= -345.404967
Sum of electronic and thermal Free Energies= -345.442859

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.316	23.801	79.749

M062X/6-311+G**/PCM	***p*-Me-PhCHO**





xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

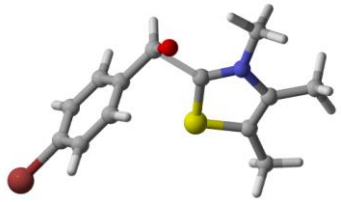
C	1.1559200000	1.2049810000	-0.0000030000
C	1.7473860000	-0.0584490000	-0.0000050000
C	0.9193450000	-1.1915770000	-0.0000050000
C	-0.4579770000	-1.0654750000	0.0000000000
C	-1.0407100000	0.2065710000	0.0000010000
C	-0.2284560000	1.3390170000	0.0000010000
C	-2.5072270000	0.3687460000	0.0000020000
O	-3.2975370000	-0.5477950000	0.0000020000
C	3.2427140000	-0.2219160000	0.0000050000
H	1.7835570000	2.0892200000	-0.0000060000
H	1.3718900000	-2.1777320000	-0.0000110000
H	-1.0985350000	-1.9399990000	-0.0000020000
H	-0.6804930000	2.3259560000	-0.0000010000
H	-2.8634010000	1.4151430000	-0.0000080000
H	3.7483630000	0.7434400000	-0.0002480000
H	3.5664880000	-0.7823040000	0.8803150000
H	3.5664540000	-0.7827510000	-0.8800320000

thermodynamic data

Zero-point correction= 0.137800 (Hartree/Particle)
Thermal correction to Energy= 0.145123
Thermal correction to Enthalpy= 0.146068
Thermal correction to Gibbs Free Energy= 0.105798
Sum of electronic and zero-point Energies= -384.693012
Sum of electronic and thermal Energies= -384.685689
Sum of electronic and thermal Enthalpies= -384.684745
Sum of electronic and thermal Free Energies= -384.725015

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.066	27.893	84.755

M062X/6-311+G**/PCM	**TST1 *p*-Br**



xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

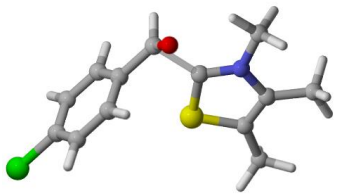
C	1.9643690000	-0.5194060000	0.3697340000
S	1.3782660000	1.0818520000	0.2333410000
N	3.2773640000	-0.4855590000	0.1726400000
C	3.8737990000	0.7663520000	-0.0714860000
C	2.9572580000	1.7623140000	-0.0744660000
C	5.3489800000	0.8538250000	-0.2920700000
C	3.1459860000	3.2288500000	-0.2998910000
C	4.0815730000	-1.7115510000	0.2352990000
C	-0.5305060000	-1.5833820000	0.1417900000
C	-1.0854090000	-1.0372310000	1.2969680000
C	-2.2810510000	-0.3312800000	1.2445570000
C	-2.9130220000	-0.1819950000	0.0149170000
C	-2.3864650000	-0.7302970000	-1.1483890000
C	-1.1894120000	-1.4354360000	-1.0749240000
C	0.7729040000	-2.3356120000	0.2148260000
O	1.2015030000	-2.9815780000	-0.7472910000
H	1.0580880000	-2.6033080000	1.2447540000
H	5.6627010000	1.8943040000	-0.3421620000
H	5.8946090000	0.3738290000	0.5231800000
H	5.6378230000	0.3656010000	-1.2259740000
H	4.1915440000	3.4577230000	-0.5027620000
H	2.8347840000	3.8014820000	0.5759290000
H	2.5541260000	3.5684520000	-1.1519810000
H	3.4012330000	-2.5583450000	0.2482940000
H	4.6970620000	-1.7035480000	1.1351410000
H	4.7218090000	-1.7747120000	-0.6436230000
H	-0.5705320000	-1.1515460000	2.2463900000
H	-2.7122380000	0.0982290000	2.1395180000
Br	-4.5393370000	0.8052550000	-0.0712140000
H	-2.9000260000	-0.6074770000	-2.0933990000
H	-0.7540280000	-1.8736140000	-1.9656190000

thermodynamic data

Zero-point correction= 0.241621 (Hartree/Particle)
Thermal correction to Energy= 0.258904
Thermal correction to Enthalpy= 0.259848
Thermal correction to Gibbs Free Energy= 0.193295
Sum of electronic and zero-point Energies= -3605.749592
Sum of electronic and thermal Energies= -3605.732309
Sum of electronic and thermal Enthalpies= -3605.731365
Sum of electronic and thermal Free Energies= -3605.797918

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.465	62.696	140.072

M062X/6-311+G**/PCM	**TST1 *p*-Cl**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.3248740000	0.5286610000	0.4009630000
S	-0.8975840000	-1.1248770000	0.3031520000
N	-2.6261780000	0.6229770000	0.1512090000
C	-3.3326110000	-0.5657240000	-0.1066930000
C	-2.5214160000	-1.6477970000	-0.0639540000
C	-4.8004120000	-0.5179750000	-0.3802440000
C	-2.8647220000	-3.0916690000	-0.2585120000
C	-3.3090310000	1.9217520000	0.1641310000
C	1.2588950000	1.3436470000	0.1729850000
C	1.7876110000	0.7195540000	1.3005330000
C	2.9137010000	-0.0887350000	1.2011260000
C	3.5011240000	-0.2617910000	-0.0465680000
C	2.9965060000	0.3573150000	-1.1834400000
C	1.8717630000	1.1652000000	-1.0638900000
C	0.0361890000	2.2156830000	0.2939300000
O	-0.3336060000	2.9401210000	-0.6376800000
H	-0.2063790000	2.4736110000	1.3369990000
H	-5.1977520000	-1.5270880000	-0.4690520000
H	-5.3328460000	-0.0148750000	0.4300720000
H	-5.0133760000	0.0177740000	-1.3083200000
H	-3.7786220000	-3.1951360000	-0.8433510000
H	-3.0127350000	-3.5899970000	0.7021900000

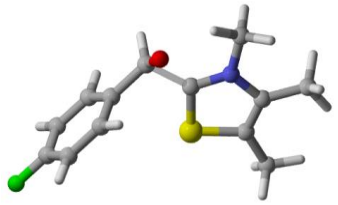
H	-2.0660170000	-3.6125030000	-0.7878790000
H	-2.5524690000	2.6968230000	0.2454190000
H	-3.9956060000	1.9673920000	1.0095890000
H	-3.8639790000	2.0524710000	-0.7642120000
H	1.3086820000	0.8575790000	2.2655270000
H	3.3310060000	-0.5769570000	2.0725800000
Cl	4.9166070000	-1.2807660000	-0.1885040000
H	3.4779780000	0.2088530000	-2.1419020000
H	1.4568980000	1.6625860000	-1.9327540000

thermodynamic data

Zero-point correction= 0.242115 (Hartree/Particle)
Thermal correction to Energy= 0.259243
Thermal correction to Enthalpy= 0.260187
Thermal correction to Gibbs Free Energy= 0.194626
Sum of electronic and zero-point Energies= -1491.777357
Sum of electronic and thermal Energies= -1491.760229
Sum of electronic and thermal Enthalpies= -1491.759285
Sum of electronic and thermal Free Energies= -1491.824845

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.677	62.293	137.984

M062X/6-311+G**/PCM	**TST1 *p*-F**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9542610000	-0.4623780000	0.3945770000
S	0.7890190000	1.2435710000	0.2503950000
N	2.2331500000	-0.7843290000	0.1774840000
C	3.1263120000	0.2753910000	-0.0912490000
C	2.4967550000	1.4815740000	-0.0917820000
C	4.5778240000	-0.0081500000	-0.3343390000
C	3.0550520000	2.8494230000	-0.3459970000
C	2.6658020000	-2.1947140000	0.2248240000
C	-1.6560080000	-0.9137840000	0.2034840000
C	-2.2033160000	-0.2090760000	1.2807630000
C	-3.3603570000	0.5558610000	1.1228220000
C	-3.9605720000	0.5952710000	-0.1307910000

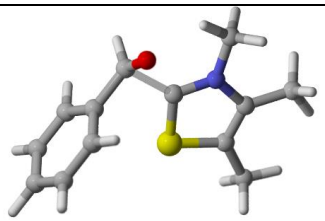
C	-3.4480270000	-0.1039970000	-1.2189140000
C	-2.2914670000	-0.8613390000	-1.0409440000
C	-0.4066820000	-1.7755530000	0.3590690000
O	-0.1175070000	-2.6051090000	-0.5550000000
H	-0.2884610000	-2.0753100000	1.4284260000
H	5.1382110000	0.9249590000	-0.4194760000
H	5.0182340000	-0.5885930000	0.4845300000
H	4.7333090000	-0.5732950000	-1.2614940000
H	4.1404550000	2.8165010000	-0.4751980000
H	2.8391050000	3.5295160000	0.4860630000
H	2.6257250000	3.2922860000	-1.2525880000
H	1.7838550000	-2.8033550000	-0.0094840000
H	3.0662880000	-2.4269070000	1.2162840000
H	3.4389090000	-2.3605450000	-0.5267810000
H	-1.7254930000	-0.2644060000	2.2575830000
H	-3.8029650000	1.1061600000	1.9471180000
F	-5.0844250000	1.3311810000	-0.2940110000
H	-3.9592990000	-0.0528860000	-2.1753010000
H	-1.8618090000	-1.4418950000	-1.8514270000

thermodynamic data

Zero-point correction= 0.243217 (Hartree/Particle)
Thermal correction to Energy= 0.258892
Thermal correction to Enthalpy= 0.259837
Thermal correction to Gibbs Free Energy= 0.200200
Sum of electronic and zero-point Energies= -1131.418460
Sum of electronic and thermal Energies= -1131.402785
Sum of electronic and thermal Enthalpies= -1131.401840
Sum of electronic and thermal Free Energies= -1131.461477

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.457	60.437	125.516

M062X/6-311+G**/PCM	**TST1 *p*-H**



xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.5882200000	0.4859570000	-0.3752620000
S	0.5370790000	-1.2165320000	-0.2154080000

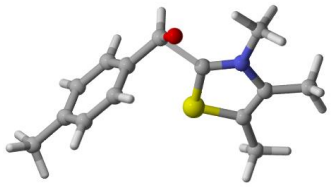
N	1.8448250000	0.8708590000	-0.1846520000
C	2.8059400000	-0.1253630000	0.0728900000
C	2.2502260000	-1.3593550000	0.0920830000
C	4.2326090000	0.2603140000	0.2926590000
C	2.8918870000	-2.6877690000	0.3383880000
C	2.2210770000	2.2868650000	-0.2729330000
C	-2.1138460000	0.7233060000	-0.1386170000
C	-2.4849980000	-0.0695250000	-1.2236970000
C	-3.4118110000	-1.0938000000	-1.0605900000
C	-3.9735290000	-1.3282840000	0.1932960000
C	-3.6105850000	-0.5311590000	1.2771950000
C	-2.6844420000	0.4943660000	1.1108170000
C	-1.1097780000	1.8314590000	-0.3258670000
O	-0.9012380000	2.6754580000	0.5551820000
H	-0.9355350000	2.0761060000	-1.3864120000
H	4.8582770000	-0.6275200000	0.3563940000
H	4.6024330000	0.8785150000	-0.5280960000
H	4.3482740000	0.8253420000	1.2207910000
H	3.9718080000	-2.5837880000	0.4376590000
H	2.6905200000	-3.3756000000	-0.4847320000
H	2.5087410000	-3.1395610000	1.2555760000
H	1.3069860000	2.8741420000	-0.2890030000
H	2.8021370000	2.4577160000	-1.1794620000
H	2.8148570000	2.5631920000	0.5974890000
H	-2.0339950000	0.1116420000	-2.1956410000
H	-3.6958280000	-1.7082180000	-1.9071120000
H	-4.6957710000	-2.1257160000	0.3237830000
H	-4.0521160000	-0.7087000000	2.2512480000
H	-2.3937320000	1.1252050000	1.9430010000

thermodynamic data

Zero-point correction= 0.251646 (Hartree/Particle)
Thermal correction to Energy= 0.267540
Thermal correction to Enthalpy= 0.268484
Thermal correction to Gibbs Free Energy= 0.206242
Sum of electronic and zero-point Energies= -1032.166396
Sum of electronic and thermal Energies= -1032.150502
Sum of electronic and thermal Enthalpies= -1032.149558
Sum of electronic and thermal Free Energies= -1032.211801

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.884	58.457	131.001

M062X/6-311+G**/PCM	**TST1 *p*-Me**

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9891780000	0.5270070000	0.3880100000
S	-0.6871900000	-1.1533460000	0.2830990000
N	-2.2818680000	0.7207310000	0.1541130000
C	-3.0804630000	-0.4108970000	-0.0986220000
C	-2.3525070000	-1.5510800000	-0.0644970000
C	-4.5406640000	-0.2424510000	-0.3664660000
C	-2.7876880000	-2.9656750000	-0.2806350000
C	-2.8607870000	2.0688790000	0.1925340000
C	1.6477800000	1.1311150000	0.1665990000
C	2.1304650000	0.4385240000	1.2730530000
C	3.1981540000	-0.4444680000	1.1423480000
C	3.8057240000	-0.6527290000	-0.0974950000
C	3.3186650000	0.0555830000	-1.2011060000
C	2.2537480000	0.9384810000	-1.0733670000
C	0.4910210000	2.0837850000	0.3149430000
O	0.1723370000	2.8667360000	-0.5924240000
H	0.2790630000	2.3357230000	1.3670010000
H	-5.0221030000	-1.2138930000	-0.4565580000
H	-5.0279280000	0.3051070000	0.4432430000
H	-4.7093730000	0.3067080000	-1.2957960000
H	-3.8658820000	-3.0216330000	-0.4257790000
H	-2.5277400000	-3.5871640000	0.5782660000
H	-2.3037000000	-3.3909650000	-1.1620400000
H	-2.0412560000	2.7808610000	0.2350160000
H	-3.5021200000	2.1685900000	1.0685200000
H	-3.4459430000	2.2430370000	-0.7096190000
H	1.6603490000	0.5847320000	2.2420400000
H	3.5656730000	-0.9776250000	2.0130600000
H	3.7853140000	-0.0883450000	-2.1709470000
H	1.8806320000	1.4880620000	-1.9302770000
C	4.9525410000	-1.6178660000	-0.2551480000
H	5.7832530000	-1.1525650000	-0.7900480000
H	4.6440300000	-2.4950260000	-0.8300840000
H	5.3162860000	-1.9603180000	0.7141290000

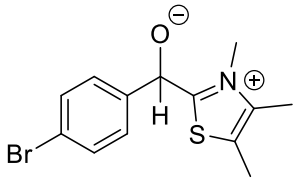
thermodynamic data

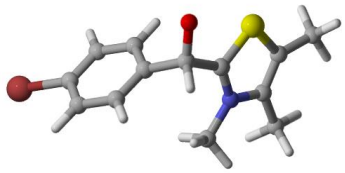
Zero-point correction= 0.279135 (Hartree/Particle)

Thermal correction to Energy= 0.296837
Thermal correction to Enthalpy= 0.297782
Thermal correction to Gibbs Free Energy= 0.231289
Sum of electronic and zero-point Energies= -1071.445724
Sum of electronic and thermal Energies= -1071.428022
Sum of electronic and thermal Enthalpies= -1071.427077
Sum of electronic and thermal Free Energies= -1071.493570

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.268	64.473	139.945

M062X/6-311+G**/PCM	**Zwitterion1 *p*-Br**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.6457700000	0.5106870000	1.1949110000
C	-2.9162410000	0.0592720000	-0.0882820000
C	-1.9608500000	0.1190410000	-1.0977140000
C	-0.7084230000	0.6422150000	-0.8008650000
C	-0.4032390000	1.0950240000	0.4832060000
C	-1.3811690000	1.0271530000	1.4706030000
C	0.9696960000	1.7297720000	0.7670920000
C	2.0392840000	0.6927760000	0.3932700000
O	1.1965560000	2.8671790000	0.0959770000
S	3.1758570000	1.1116170000	-0.7895560000
C	3.9199940000	-0.4585650000	-0.6876620000
C	3.2860770000	-1.2289160000	0.2314220000
N	2.2255020000	-0.5396890000	0.8361610000
C	5.0965630000	-0.7915550000	-1.5495370000
C	3.5829040000	-2.6358290000	0.6343570000
C	1.3545750000	-1.1501400000	1.8475210000
Br	-4.6375220000	-0.6636050000	-0.4741000000
H	-3.4033570000	0.4593730000	1.9667190000
H	-2.1919560000	-0.2363190000	-2.0939850000
H	0.0413980000	0.7076140000	-1.5835580000
H	-1.1608610000	1.3806660000	2.4733130000
H	1.0434410000	1.8160070000	1.8764560000
H	5.4877630000	-1.7774150000	-1.3053650000
H	4.8185080000	-0.7837830000	-2.6051140000
H	5.8973780000	-0.0644120000	-1.4054870000
H	2.6887320000	-3.2585000000	0.5646620000

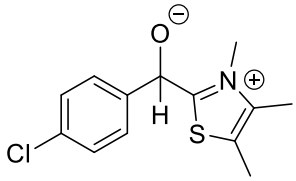
H	4.3396030000	-3.0581640000	-0.0224110000
H	3.9567600000	-2.6839570000	1.6597250000
H	1.9396430000	-1.8419700000	2.4472570000
H	0.9556490000	-0.3683910000	2.4882900000
H	0.5354900000	-1.6756560000	1.3550210000

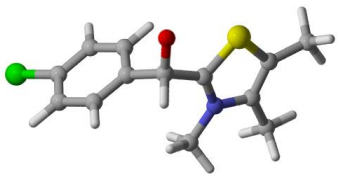
thermodynamic data

Zero-point correction= 0.243466 (Hartree/Particle)
Thermal correction to Energy= 0.260583
Thermal correction to Enthalpy= 0.261527
Thermal correction to Gibbs Free Energy= 0.196456
Sum of electronic and zero-point Energies= -3605.765783
Sum of electronic and thermal Energies= -3605.748666
Sum of electronic and thermal Enthalpies= -3605.747722
Sum of electronic and thermal Free Energies= -3605.812793

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.518	63.028	136.954

M062X/6-311+G**/PCM	**Zwitterion1 *p*-Cl**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.3703830000	0.1899870000	0.9737050000
C	-3.5220190000	-0.2570770000	-0.3301880000
C	-2.4951470000	-0.1460020000	-1.2607820000
C	-1.2923910000	0.4261120000	-0.8652640000
C	-1.1063520000	0.8763030000	0.4425980000
C	-2.1540610000	0.7544840000	1.3506510000
C	0.2020350000	1.5760710000	0.8470450000
C	1.3652940000	0.6591410000	0.4433030000
O	0.3690060000	2.7846410000	0.2918340000
S	2.5251670000	1.2659620000	-0.6303230000
C	3.3837100000	-0.2481840000	-0.6220600000
C	2.7658940000	-1.1427640000	0.1890640000
N	1.6242930000	-0.5912890000	0.7869390000
C	4.6296680000	-0.4125560000	-1.4335240000
C	3.1495750000	-2.5535070000	0.4916960000
C	0.7551610000	-1.3572980000	1.6879870000
Cl	-5.0421400000	-0.9788020000	-0.8173830000

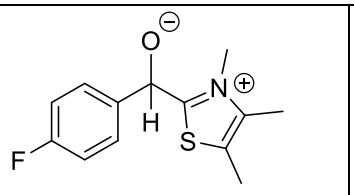
H	-4.1851010000	0.0978840000	1.6808920000
H	-2.6375730000	-0.5020570000	-2.2734400000
H	-0.4895160000	0.5263290000	-1.5895660000
H	-2.0252230000	1.1049250000	2.3699500000
H	0.2207150000	1.5683600000	1.9623930000
H	5.0153350000	-1.4268530000	-1.3475260000
H	4.4354470000	-0.2086400000	-2.4878030000
H	5.4053750000	0.2757650000	-1.0927980000
H	2.3151030000	-3.2331840000	0.3076200000
H	3.9799360000	-2.8573120000	-0.1411320000
H	3.4595890000	-2.6641610000	1.5333920000
H	1.3704460000	-2.0034340000	2.3089670000
H	0.2053070000	-0.6664860000	2.3208590000
H	0.0558780000	-1.9532580000	1.1002370000

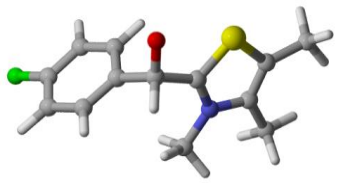
thermodynamic data

Zero-point correction= 0.243914 (Hartree/Particle)
Thermal correction to Energy= 0.260965
Thermal correction to Enthalpy= 0.261909
Thermal correction to Gibbs Free Energy= 0.197191
Sum of electronic and zero-point Energies= -1491.793624
Sum of electronic and thermal Energies= -1491.776573
Sum of electronic and thermal Enthalpies= -1491.775629
Sum of electronic and thermal Free Energies= -1491.840347

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.758	62.671	136.211

M062X/6-311+G**/PCM	**Zwitterion1 *p*-F**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.7015280000	-0.3038750000	0.7094800000
C	-3.7616980000	-0.4998540000	-0.6564650000
C	-2.7360040000	-0.1295040000	-1.5105580000
C	-1.6048400000	0.4606030000	-0.9604320000
C	-1.4985170000	0.6673230000	0.4164570000
C	-2.5541940000	0.2843640000	1.2390210000
C	-0.2649230000	1.3825730000	0.9949180000
C	0.9719540000	0.5972630000	0.5360340000

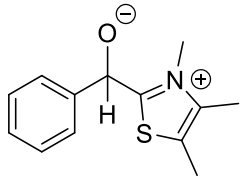
O	-0.1449770000	2.6651380000	0.6242110000
S	2.1360320000	1.4057670000	-0.3910640000
C	3.0790080000	-0.0489460000	-0.5480540000
C	2.4833230000	-1.0772190000	0.1051530000
N	1.2897740000	-0.6733370000	0.7201930000
C	4.3585250000	-0.0406740000	-1.3234310000
C	2.9369560000	-2.4948220000	0.2261930000
C	0.4269030000	-1.5966150000	1.4669100000
F	-4.8659360000	-1.0755910000	-1.1834970000
H	-4.5325040000	-0.6041990000	1.3356040000
H	-2.8325240000	-0.3024360000	-2.5753210000
H	-0.7942510000	0.7703570000	-1.6129120000
H	-2.4864100000	0.4457950000	2.3103290000
H	-0.3050060000	1.2155510000	2.0972370000
H	4.8593340000	-1.0042890000	-1.2494640000
H	4.1720640000	0.1697630000	-2.3781330000
H	5.0373090000	0.7231530000	-0.9405710000
H	2.1480080000	-3.1837660000	-0.0818870000
H	3.8006700000	-2.6649050000	-0.4120090000
H	3.2208640000	-2.7336500000	1.2537780000
H	1.0471150000	-2.3434670000	1.9546160000
H	-0.1221670000	-1.0362270000	2.2191760000
H	-0.2739760000	-2.0750730000	0.7816620000

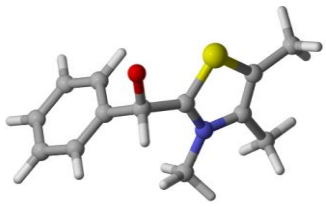
thermodynamic data

Zero-point correction= 0.245478 (Hartree/Particle)
Thermal correction to Energy= 0.261923
Thermal correction to Enthalpy= 0.262867
Thermal correction to Gibbs Free Energy= 0.200706
Sum of electronic and zero-point Energies= -1131.433125
Sum of electronic and thermal Energies= -1131.416680
Sum of electronic and thermal Enthalpies= -1131.415735
Sum of electronic and thermal Free Energies= -1131.477897

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.359	61.671	130.830

M062X/6-311+G**/PCM	**Zwitterion1 *p*-H**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

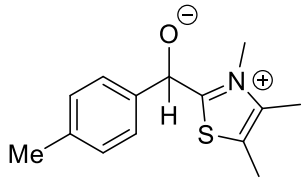
C	4.0097040000	0.7402380000	0.2032330000
C	3.9880250000	0.7040120000	-1.1870670000
C	2.9120630000	0.1092270000	-1.8459780000
C	1.8667960000	-0.4430610000	-1.1146210000
C	1.8770350000	-0.4038500000	0.2813560000
C	2.9559260000	0.1897910000	0.9315980000
C	0.7487970000	-1.0788220000	1.0825610000
C	-0.5763660000	-0.4758180000	0.5963900000
O	0.7042920000	-2.4138610000	0.9606000000
S	-1.7184890000	-1.5113600000	-0.1052240000
C	-2.7917360000	-0.1784620000	-0.4234630000
C	-2.2516250000	0.9843550000	0.0178310000
N	-0.9934570000	0.7793810000	0.5995580000
C	-4.1200860000	-0.4106240000	-1.0723760000
C	-2.8284880000	2.3602770000	-0.0338590000
C	-0.1769850000	1.8804230000	1.1231620000
H	4.8449720000	1.1973650000	0.7215060000
H	4.8036810000	1.1349160000	-1.7558830000
H	2.8909270000	0.0773200000	-2.9293410000
H	1.0361060000	-0.9176040000	-1.6290570000
H	2.9744020000	0.2200630000	2.0171800000
H	0.8540730000	-0.7091220000	2.1294940000
H	-4.5268690000	0.5217710000	-1.4613560000
H	-4.0283180000	-1.1120210000	-1.9024270000
H	-4.8336910000	-0.8242220000	-0.3567470000
H	-2.1284040000	3.0628410000	-0.4901910000
H	-3.7428920000	2.3580350000	-0.6225510000
H	-3.0728890000	2.7213760000	0.9680100000
H	-0.8295400000	2.6083630000	1.5985160000
H	0.5207060000	1.4858330000	1.8564080000
H	0.3750680000	2.3459520000	0.3057110000

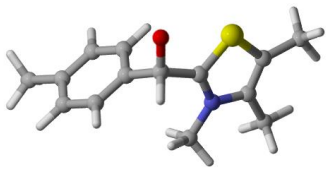
thermodynamic data

Zero-point correction= 0.254395 (Hartree/Particle)
Thermal correction to Energy= 0.269792
Thermal correction to Enthalpy= 0.270736
Thermal correction to Gibbs Free Energy= 0.211436
Sum of electronic and zero-point Energies= -1032.181646
Sum of electronic and thermal Energies= -1032.166248
Sum of electronic and thermal Enthalpies= -1032.165304
Sum of electronic and thermal Free Energies= -1032.224604

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	169.297	58.495	124.808

M062X/6-311+G**/PCM	**Zwitterion1 *p*-Me**





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	3.6810620000	0.1855600000	0.7561100000
C	3.8036780000	0.4974300000	-0.5963530000
C	2.7330500000	0.1870910000	-1.4435720000
C	1.5837220000	-0.4162250000	-0.9516430000
C	1.4632170000	-0.7219040000	0.4062770000
C	2.5237610000	-0.4156300000	1.2516000000
C	0.2131690000	-1.4456060000	0.9332750000
C	-1.0074670000	-0.6211150000	0.5030010000
O	0.0749580000	-2.7081830000	0.4999220000
S	-2.1822220000	-1.3709990000	-0.4594490000
C	-3.1006100000	0.1053840000	-0.5578710000
C	-2.4890410000	1.0955110000	0.1378840000
N	-1.3040640000	0.6461910000	0.7382650000
C	-4.3785630000	0.1491020000	-1.3347070000
C	-2.9174750000	2.5149610000	0.3160360000
C	-0.4260720000	1.5226640000	1.5227900000
C	5.0524570000	1.1381120000	-1.1454700000
H	4.4979320000	0.4159170000	1.4326790000
H	2.8065220000	0.4241280000	-2.5006590000
H	0.7685660000	-0.6569650000	-1.6285380000
H	2.4481140000	-0.6454620000	2.3106410000
H	0.2417290000	-1.3346770000	2.0432870000
H	-4.8448580000	1.1295210000	-1.2546380000
H	-4.1981800000	-0.0599220000	-2.3906670000
H	-5.0848390000	-0.5930260000	-0.9584280000
H	-2.1172160000	3.2013990000	0.0324330000
H	-3.7805420000	2.7254690000	-0.3109100000
H	-3.1936220000	2.7184130000	1.3533260000
H	-1.0329720000	2.2620130000	2.0378220000
H	0.1102590000	0.9229230000	2.2535030000
H	0.2869060000	2.0126390000	0.8584090000
H	5.7143370000	1.4627960000	-0.3418450000
H	5.6046890000	0.4350530000	-1.7745550000
H	4.8081910000	2.0058890000	-1.7620680000

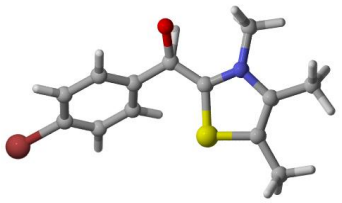
thermodynamic data

Zero-point correction= 0.281100 (Hartree/Particle)
Thermal correction to Energy= 0.298523

Thermal correction to Enthalpy= 0.299467
Thermal correction to Gibbs Free Energy= 0.235171
Sum of electronic and zero-point Energies= -1071.461510
Sum of electronic and thermal Energies= -1071.444087
Sum of electronic and thermal Enthalpies= -1071.443143
Sum of electronic and thermal Free Energies= -1071.507439

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	187.326	64.774	135.322

M062X/6-311+G**/PCM	**TST2 *p*-Br**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.9671490000	0.4428070000	0.0911910000
S	-1.7465610000	-1.2524770000	-0.1760810000
N	-3.2820540000	0.7339500000	0.1262960000
C	-4.1386150000	-0.3670560000	-0.0438930000
C	-3.4716490000	-1.5284920000	-0.2069710000
C	-5.6197480000	-0.1688250000	-0.0314860000
C	-3.9876620000	-2.9190440000	-0.3970130000
C	-3.7644880000	2.0582360000	0.5290490000
C	0.4904160000	0.9102180000	0.1513880000
C	0.9548560000	-0.0939630000	1.0110220000
C	2.2711970000	-0.5321050000	0.9582810000
C	3.1384680000	0.0502310000	0.0407780000
C	2.7148200000	1.0616760000	-0.8096150000
C	1.3923580000	1.4901810000	-0.7449100000
C	-0.9109090000	1.3956090000	0.1929990000
O	-1.1501730000	2.6896810000	-0.4310140000
H	-1.1551770000	2.3758510000	0.8366300000
H	-5.9138200000	0.6055080000	-0.7430070000
H	-6.1199150000	-1.0920400000	-0.3131860000
H	-5.9772040000	0.1205650000	0.9592330000
H	-3.6692710000	-3.3263220000	-1.3587760000
H	-5.0754250000	-2.9359120000	-0.3627370000
H	-3.6147270000	-3.5795710000	0.3885020000
H	-4.8250680000	1.9943770000	0.7475680000
H	-3.5718740000	2.7883920000	-0.2500740000
H	-3.2312220000	2.3573150000	1.4345210000

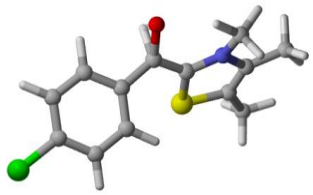
H	0.2877770000	-0.5250700000	1.7496160000
H	2.6215100000	-1.3038240000	1.6316750000
Br	4.9515420000	-0.5341250000	-0.0253300000
H	3.4054680000	1.5122330000	-1.5116020000
H	1.0443600000	2.2905560000	-1.3854100000

thermodynamic data

Zero-point correction= 0.238525 (Hartree/Particle)
Thermal correction to Energy= 0.255783
Thermal correction to Enthalpy= 0.256727
Thermal correction to Gibbs Free Energy= 0.191206
Sum of electronic and zero-point Energies= -3605.695542
Sum of electronic and thermal Energies= -3605.678284
Sum of electronic and thermal Enthalpies= -3605.677340
Sum of electronic and thermal Free Energies= -3605.742861

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.506	63.540	137.900

M062X/6-311+G**/PCM	**TST2 *p*-Cl**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2909790000	0.3910070000	-0.1165240000
S	1.3702250000	-1.3155310000	-0.4781110000
N	2.5158080000	0.8382910000	0.2317170000
C	3.5454270000	-0.1206680000	0.1437260000
C	3.1073500000	-1.3380470000	-0.2227300000
C	4.9452640000	0.2919080000	0.4627420000
C	3.8520350000	-2.6204760000	-0.4073930000
C	2.7456700000	2.1088850000	0.9300090000
C	-1.2344100000	0.6344180000	-0.1896910000
C	-1.5296190000	-0.4382190000	0.6571190000
C	-2.8348780000	-0.8945770000	0.8149910000
C	-3.8589670000	-0.2589360000	0.1305900000
C	-3.6048120000	0.8297360000	-0.6955350000
C	-2.2981390000	1.2685800000	-0.8465250000
C	0.1355510000	1.1786240000	-0.3801700000
O	0.2475060000	2.6153240000	-0.4076520000

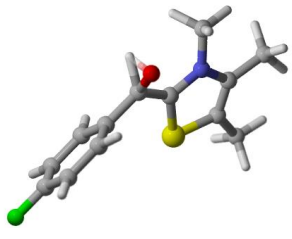
H	0.3338600000	1.7534270000	-1.4061030000
H	5.0200940000	0.6835600000	1.4794480000
H	5.6169510000	-0.5586910000	0.3758930000
H	5.2886170000	1.0682900000	-0.2250450000
H	4.9074920000	-2.4897940000	-0.1745050000
H	3.7716830000	-2.9767150000	-1.4364900000
H	3.4526630000	-3.3965140000	0.2494050000
H	2.8516430000	1.9156720000	1.9991020000
H	1.8953580000	2.7588170000	0.7437480000
H	3.6575250000	2.5668250000	0.5511380000
H	-0.7442670000	-0.9211490000	1.2256250000
H	-3.0524460000	-1.7245870000	1.4753880000
Cl	-5.5043450000	-0.8269910000	0.3201370000
H	-4.4182650000	1.3227840000	-1.2130460000
H	-2.0900490000	2.1213750000	-1.4815570000

thermodynamic data

Zero-point correction= 0.238936 (Hartree/Particle)
Thermal correction to Energy= 0.256003
Thermal correction to Enthalpy= 0.256947
Thermal correction to Gibbs Free Energy= 0.192186
Sum of electronic and zero-point Energies= -1491.720704
Sum of electronic and thermal Energies= -1491.703636
Sum of electronic and thermal Enthalpies= -1491.702692
Sum of electronic and thermal Free Energies= -1491.767453

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.644	63.306	136.301

M062X/6-311+G**/PCM	**TST2 *p*-F**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9136820000	0.4319010000	0.1056830000
S	-0.8678470000	-1.2820440000	-0.1374410000
N	-2.1924610000	0.8606860000	0.1129490000
C	-3.1564570000	-0.1478980000	-0.0599650000
C	-2.6134630000	-1.3744890000	-0.1979010000

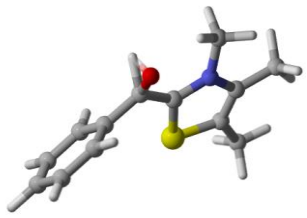
C	-4.6085190000	0.2042990000	-0.0849920000
C	-3.2701030000	-2.7050560000	-0.3824950000
C	-2.5401760000	2.2283520000	0.5105450000
C	1.5794520000	0.6273770000	0.1645030000
C	1.9571570000	-0.4103770000	1.0254020000
C	3.2168160000	-0.9903040000	0.9383390000
C	4.0992500000	-0.5088930000	-0.0134440000
C	3.7753060000	0.5283630000	-0.8669000000
C	2.5089040000	1.0963680000	-0.7681790000
C	0.2364670000	1.2624210000	0.2276210000
O	0.1448460000	2.5896800000	-0.3632240000
H	0.0908310000	2.2468010000	0.8962840000
H	-4.8030360000	0.9913510000	-0.8165300000
H	-5.1958220000	-0.6671990000	-0.3638360000
H	-4.9567330000	0.5482260000	0.8914210000
H	-2.9635240000	-3.1658520000	-1.3236930000
H	-4.3537570000	-2.6029640000	-0.3898650000
H	-2.9999720000	-3.3840520000	0.4290090000
H	-3.6133000000	2.2914810000	0.6545270000
H	-2.2059970000	2.9387430000	-0.2377720000
H	-2.0387580000	2.4501820000	1.4564430000
H	1.2690120000	-0.7583470000	1.7879830000
H	3.5220220000	-1.7897610000	1.6018240000
F	5.3298120000	-1.0651580000	-0.0963630000
H	4.5030940000	0.8828290000	-1.5866450000
H	2.2259300000	1.9230540000	-1.4069810000

thermodynamic data

Zero-point correction= 0.240689 (Hartree/Particle)
Thermal correction to Energy= 0.257234
Thermal correction to Enthalpy= 0.258178
Thermal correction to Gibbs Free Energy= 0.195801
Sum of electronic and zero-point Energies= -1131.362279
Sum of electronic and thermal Energies= -1131.345734
Sum of electronic and thermal Enthalpies= -1131.344789
Sum of electronic and thermal Free Energies= -1131.407166

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.417	62.190	131.283

M062X/6-311+G**/PCM	**TST2 *p*-H**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.5436930000	0.4302440000	0.1155370000
S	-0.5997270000	-1.2931330000	-0.0942430000
N	-1.7961950000	0.9334660000	0.0655850000
C	-2.8146950000	-0.0256610000	-0.0852300000
C	-2.3470810000	-1.2847800000	-0.1833920000
C	-4.2395970000	0.4216850000	-0.1240210000
C	-3.0784640000	-2.5781270000	-0.3484900000
C	-2.1307940000	2.3186270000	0.4189780000
C	1.9596260000	0.4123330000	0.1674940000
C	2.2837350000	-0.6693210000	0.9955890000
C	3.4948930000	-1.3368550000	0.8477800000
C	4.4090040000	-0.9280680000	-0.1211570000
C	4.1037630000	0.1604070000	-0.9338590000
C	2.8926130000	0.8290740000	-0.7865330000
C	0.6719350000	1.1523970000	0.2848900000
O	0.7128590000	2.5326080000	-0.1727280000
H	0.6228870000	2.0765300000	1.0473970000
H	-4.4281870000	1.0548050000	-0.9943390000
H	-4.8992550000	-0.4404560000	-0.1840740000
H	-4.5012120000	0.9885710000	0.7717060000
H	-2.7911870000	-3.0737030000	-1.2781730000
H	-4.1542640000	-2.4130640000	-0.3716420000
H	-2.8555520000	-3.2569660000	0.4773820000
H	-2.9894190000	2.6371330000	-0.1667610000
H	-1.2782620000	2.9493810000	0.1964540000
H	-2.3762490000	2.3669580000	1.4832910000
H	1.5940640000	-0.9771140000	1.7744670000
H	3.7320580000	-2.1688010000	1.5010260000
H	5.3551080000	-1.4447930000	-0.2313730000
H	4.8138480000	0.4943040000	-1.6821260000
H	2.6542900000	1.6904970000	-1.3981330000

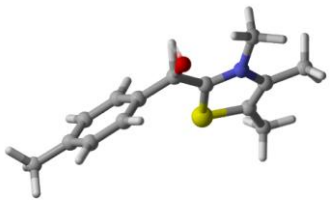
thermodynamic data

Zero-point correction= 0.248901 (Hartree/Particle)
Thermal correction to Energy= 0.264527
Thermal correction to Enthalpy= 0.265471
Thermal correction to Gibbs Free Energy= 0.205619

Sum of electronic and zero-point Energies= -1032.111209
Sum of electronic and thermal Energies= -1032.095582
Sum of electronic and thermal Enthalpies= -1032.094638
Sum of electronic and thermal Free Energies= -1032.154490

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	165.993	59.271	125.969

M062X/6-311+G**/PCM	**TST2 *p*-Me**

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9490530000	0.4632410000	0.1079600000
S	-0.8395950000	-1.2605380000	-0.0841090000
N	-2.2440840000	0.8444350000	0.0469030000
C	-3.1659940000	-0.2088870000	-0.0972400000
C	-2.5806020000	-1.4188500000	-0.1804470000
C	-4.6268350000	0.1009180000	-0.1434900000
C	-3.1845580000	-2.7776310000	-0.3351290000
C	-2.7079170000	2.1929630000	0.3934800000
C	1.5413450000	0.6700940000	0.1883150000
C	1.9581510000	-0.3397880000	1.0597880000
C	3.2235510000	-0.9059300000	0.9396430000
C	4.1172450000	-0.4752490000	-0.0423450000
C	3.7025560000	0.5465270000	-0.9002450000
C	2.4398210000	1.1155540000	-0.7858200000
C	0.1919950000	1.2956040000	0.2759150000
O	0.1141640000	2.6679940000	-0.2018540000
H	0.0514950000	2.2233700000	1.0229620000
H	-4.8725260000	0.7050380000	-1.0202130000
H	-5.2018280000	-0.8203470000	-0.1954790000
H	-4.9426140000	0.6494440000	0.7463520000
H	-2.8312880000	-3.2596950000	-1.2490480000
H	-4.2702610000	-2.7144990000	-0.3848900000
H	-2.9181110000	-3.4184730000	0.5081330000
H	-3.5805770000	2.4368750000	-0.2074010000
H	-1.9117940000	2.8987480000	0.1862720000
H	-2.9754760000	2.2178590000	1.4532880000
H	1.2947860000	-0.6763950000	1.8499280000
H	3.5260670000	-1.6873300000	1.6294080000

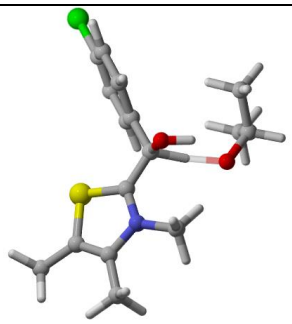
H	4.3823470000	0.9041230000	-1.6678660000
H	2.1341500000	1.9204910000	-1.4432270000
C	5.5003280000	-1.0639070000	-0.1546260000
H	5.7629000000	-1.2515520000	-1.1977270000
H	5.5734860000	-2.0039310000	0.3936900000
H	6.2478440000	-0.3780650000	0.2535110000

thermodynamic data

Zero-point correction= 0.276441 (Hartree/Particle)
Thermal correction to Energy= 0.293900
Thermal correction to Enthalpy= 0.294844
Thermal correction to Gibbs Free Energy= 0.230747
Sum of electronic and zero-point Energies= -1071.390286
Sum of electronic and thermal Energies= -1071.372828
Sum of electronic and thermal Enthalpies= -1071.371884
Sum of electronic and thermal Free Energies= -1071.435981

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	184.425	65.320	134.904

M062X/6-311+G**/PCM	**TST2 mit Isopropanol *p*-Cl**

xyz-matrix

43
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.4646100000	-0.1696390000	-0.2155690000
S	-1.4363840000	-1.8162260000	0.2515710000
N	-2.7179330000	0.2744250000	-0.2790680000
C	-3.7024770000	-0.6793260000	0.0139030000
C	-3.1724570000	-1.8791520000	0.3468530000
C	-5.1458560000	-0.3023240000	-0.0565870000
C	-3.8534600000	-3.1408730000	0.7708670000
C	-3.0559430000	1.6693400000	-0.6023490000
C	1.0168630000	-0.1067150000	-0.3854580000
C	1.4459840000	-0.5314430000	0.8765720000
C	2.6503500000	-1.2048250000	1.0364810000

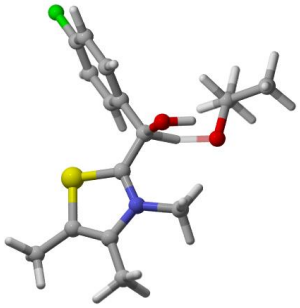
C	3.4410200000	-1.4377760000	-0.0814210000
C	3.0514200000	-1.0116500000	-1.3429040000
C	1.8372800000	-0.3472810000	-1.4877440000
C	-0.2763460000	0.6417650000	-0.5238840000
O	-0.4288600000	1.2517440000	-1.7984040000
H	-0.2531660000	1.6801810000	0.1903540000
H	-5.3724770000	0.1838310000	-1.0072330000
H	-5.7665940000	-1.1912770000	0.0259510000
H	-5.4186240000	0.3792480000	0.7521760000
H	-3.5543480000	-3.9784710000	0.1388180000
H	-4.9344930000	-3.0323790000	0.7044940000
H	-3.5997990000	-3.3869660000	1.8038950000
H	-3.9645110000	1.9310660000	-0.0666020000
H	-3.2126070000	1.7694100000	-1.6757270000
H	-2.2444160000	2.3180410000	-0.2748970000
H	0.8372040000	-0.3225800000	1.7507640000
H	2.9786780000	-1.5313800000	2.0150860000
Cl	4.9657830000	-2.2777870000	0.1088320000
H	3.6865930000	-1.1982040000	-2.1999110000
H	1.5238570000	-0.0013360000	-2.4644220000
C	1.4122350000	3.1458710000	2.0130490000
C	0.8514500000	3.6859470000	0.6933150000
H	0.6707800000	3.2456550000	2.8096500000
H	2.3200240000	3.6776950000	2.3139120000
H	1.6579120000	2.0841980000	1.9011200000
C	1.9023650000	3.5488120000	-0.4155730000
H	1.5109440000	3.9411480000	-1.3585850000
H	2.1541340000	2.4919170000	-0.5610950000
H	2.8220160000	4.0896860000	-0.1727940000
O	-0.3439370000	3.0557650000	0.3470600000
H	0.6623690000	4.7651290000	0.8337590000
H	-0.3586600000	2.2019480000	-1.6070640000

thermodynamic data

Zero-point correction= 0.349688 (Hartree/Particle)
Thermal correction to Energy= 0.372871
Thermal correction to Enthalpy= 0.373816
Thermal correction to Gibbs Free Energy= 0.295166
Sum of electronic and zero-point Energies= -1686.002207
Sum of electronic and thermal Energies= -1685.979024
Sum of electronic and thermal Enthalpies= -1685.978080
Sum of electronic and thermal Free Energies= -1686.056729

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.980	85.377	165.532

M062X/6-311+G**/PCM	**TST2 mit Isopropanol *p*-F**

xyz-matrix

43
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2490280000	-0.0126460000	0.1977570000
S	1.6715380000	-1.6057820000	-0.2594290000
N	2.3307010000	0.7607290000	0.2498070000
C	3.5388570000	0.1134720000	-0.0406810000
C	3.3584800000	-1.1891190000	-0.3613650000
C	4.8210900000	0.8769270000	0.0166650000
C	4.3598360000	-2.2191940000	-0.7759600000
C	2.2632890000	2.1992690000	0.5504610000
C	-1.1519910000	-0.6315640000	0.3561870000
C	-1.5156460000	-1.0803290000	-0.9172580000
C	-2.4706940000	-2.0769810000	-1.0803400000
C	-3.0659930000	-2.6035200000	0.0523480000
C	-2.7448070000	-2.1780110000	1.3279310000
C	-1.7781960000	-1.1870990000	1.4727550000
C	-0.1159600000	0.4483050000	0.4942830000
O	-0.1408470000	1.0833840000	1.7671930000
H	-0.4062820000	1.4189660000	-0.2409810000
H	4.9099880000	1.4126570000	0.9635840000
H	5.6637090000	0.1949820000	-0.0673480000
H	4.8881430000	1.6028460000	-0.7968960000
H	4.3284550000	-3.0845430000	-0.1119750000
H	5.3664930000	-1.8061320000	-0.7507830000
H	4.1596010000	-2.5634390000	-1.7924170000
H	3.0567850000	2.6999400000	0.0021830000
H	2.3913910000	2.3584610000	1.6205080000
H	1.2981280000	2.5843480000	0.2244330000
H	-1.0526980000	-0.6372480000	-1.7933730000
H	-2.7646420000	-2.4314430000	-2.0603150000
F	-4.0041480000	-3.5656530000	-0.0957880000
H	-3.2421000000	-2.6176500000	2.1836600000
H	-1.5127330000	-0.8303190000	2.4599300000
C	-2.7085280000	3.9971900000	0.3076780000
C	-2.2125910000	2.7407040000	-0.4104760000
H	-2.2748940000	4.0563620000	1.3097150000
H	-3.7988180000	4.0099390000	0.4008330000

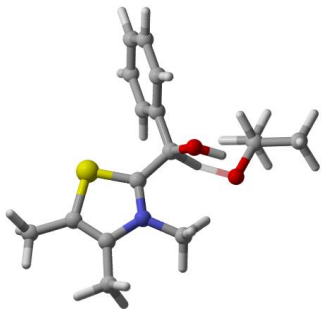
H	-2.3980850000	4.8857860000	-0.2513110000
C	-2.8260970000	2.6450450000	-1.8098380000
H	-2.4827800000	1.7347720000	-2.3086030000
H	-2.5083500000	3.5045410000	-2.4090590000
H	-3.9199180000	2.6300500000	-1.7754920000
O	-0.8196010000	2.7207280000	-0.4627200000
H	-2.5844740000	1.8666490000	0.1644720000
H	-0.4559830000	1.9811860000	1.5768730000

thermodynamic data

Zero-point correction= 0.351145 (Hartree/Particle)
Thermal correction to Energy= 0.373990
Thermal correction to Enthalpy= 0.374934
Thermal correction to Gibbs Free Energy= 0.297534
Sum of electronic and zero-point Energies= -1325.641375
Sum of electronic and thermal Energies= -1325.618530
Sum of electronic and thermal Enthalpies= -1325.617586
Sum of electronic and thermal Free Energies= -1325.694986

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.682	84.461	162.902

M062X/6-311+G**/PCM	**TST2 mit Isopropanol *p*-H**

xyz-matrix

43
XYZ file generated by gabedit : coordinates in Angstrom

C	1.0668840000	-0.0700650000	-0.1925130000
S	1.8674480000	1.3769730000	0.2463660000
N	1.9287730000	-1.0829750000	-0.2409520000
C	3.2599750000	-0.7461370000	0.0371340000
C	3.4035420000	0.5641160000	0.3446430000
C	4.3173260000	-1.7987640000	-0.0218350000
C	4.6287930000	1.3271380000	0.7352370000
C	1.5139320000	-2.4639950000	-0.5313280000
C	-1.1165690000	1.1074000000	-0.3403040000
C	-1.3176710000	1.6444280000	0.9358770000

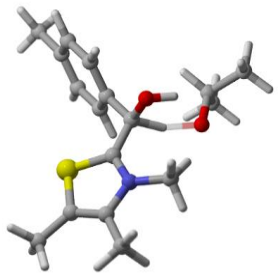
C	-2.0145130000	2.8358560000	1.1018760000
C	-2.5352430000	3.5005410000	-0.0065810000
C	-2.3501810000	2.9649850000	-1.2781760000
C	-1.6431750000	1.7770860000	-1.4458290000
C	-0.3689600000	-0.1872860000	-0.4879110000
O	-0.5472760000	-0.7975100000	-1.7607890000
H	-0.8883900000	-1.0624150000	0.2443110000
H	4.2727900000	-2.3373990000	-0.9703360000
H	5.3010290000	-1.3438930000	0.0644560000
H	4.2045950000	-2.5219000000	0.7890190000
H	4.5082720000	1.7684550000	1.7263310000
H	4.8277190000	2.1329260000	0.0265580000
H	5.4973260000	0.6716250000	0.7602300000
H	2.1623730000	-3.1383450000	0.0217220000
H	1.5979950000	-2.6563810000	-1.6003000000
H	0.4847000000	-2.6011130000	-0.2033970000
H	-0.9349130000	1.1146560000	1.8033290000
H	-2.1634590000	3.2390190000	2.0969950000
H	-3.0857120000	4.4250410000	0.1215800000
H	-2.7573680000	3.4738940000	-2.1444660000
H	-1.5048890000	1.3531560000	-2.4330410000
C	-3.7811850000	-2.9523350000	-0.3054770000
C	-2.9651630000	-1.8733100000	0.4091400000
H	-3.3883160000	-3.1169540000	-1.3125560000
H	-4.8371860000	-2.6768230000	-0.3862190000
H	-3.7102160000	-3.8948480000	0.2468160000
C	-3.5215630000	-1.6185140000	1.8124800000
H	-2.9459820000	-0.8311330000	2.3069670000
H	-3.4410810000	-2.5309500000	2.4123010000
H	-4.5723240000	-1.3128890000	1.7846360000
O	-1.6151990000	-2.2206840000	0.4512260000
H	-3.0976380000	-0.9316870000	-0.1637200000
H	-1.0674820000	-1.5940960000	-1.5685070000

thermodynamic data

Zero-point correction= 0.359479 (Hartree/Particle)
Thermal correction to Energy= 0.381444
Thermal correction to Enthalpy= 0.382388
Thermal correction to Gibbs Free Energy= 0.307358
Sum of electronic and zero-point Energies= -1226.390564
Sum of electronic and thermal Energies= -1226.368600
Sum of electronic and thermal Enthalpies= -1226.367656
Sum of electronic and thermal Free Energies= -1226.442685

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	239.359	81.522	157.913

M062X/6-311+G**/PCM	**TST2 mit Isopropanol *p*-Me**

xyz-matrix

46
XYZ file generated by gabedit : coordinates in Angstrom

C	1.2618710000	-0.0482940000	0.2042670000
S	1.6171280000	-1.6545380000	-0.2665890000
N	2.3752130000	0.6800700000	0.2554420000
C	3.5546240000	-0.0145920000	-0.0451370000
C	3.3195710000	-1.3062050000	-0.3731260000
C	4.8683080000	0.6935450000	0.0144110000
C	4.2765670000	-2.3756580000	-0.7934910000
C	2.3668450000	2.1187910000	0.5610770000
C	-1.1604480000	-0.5744750000	0.3722490000
C	-1.5493700000	-1.0078320000	-0.8994940000
C	-2.5453390000	-1.9642200000	-1.0505200000
C	-3.1970350000	-2.5068160000	0.0609550000
C	-2.8110690000	-2.0643950000	1.3264630000
C	-1.8056600000	-1.1132370000	1.4843240000
C	-0.0816090000	0.4623220000	0.5085200000
O	-0.0756030000	1.1026030000	1.7799740000
H	-0.3349720000	1.4454440000	-0.2290280000
H	4.9882270000	1.2054820000	0.9711370000
H	5.6804300000	-0.0215880000	-0.0909260000
H	4.9598060000	1.4324190000	-0.7848620000
H	5.2953000000	-1.9929350000	-0.8112760000
H	4.0332160000	-2.7380770000	-1.7939800000
H	4.2407780000	-3.2236100000	-0.1073780000
H	3.1853560000	2.5869150000	0.0211110000
H	2.4917500000	2.2697990000	1.6326070000
H	1.4218320000	2.5455120000	0.2275830000
H	-1.0716020000	-0.5819240000	-1.7771570000
H	-2.8323820000	-2.2867620000	-2.0464470000
H	-3.3020060000	-2.4721010000	2.2045060000
H	-1.5226940000	-0.7756070000	2.4741010000
C	-2.5331050000	4.1074630000	0.3059100000
C	-2.0817910000	2.8400540000	-0.4228020000
H	-2.1154770000	4.1317860000	1.3161370000
H	-3.6232860000	4.1679980000	0.3806260000
H	-2.1733900000	4.9897270000	-0.2332460000
C	-2.6781510000	2.7903820000	-1.8319680000

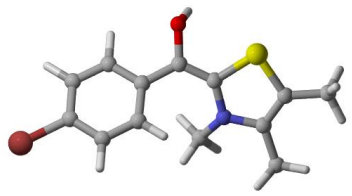
H	-2.3648840000	1.8743520000	-2.3397330000
H	-2.3181300000	3.6450230000	-2.4140340000
H	-3.7721020000	2.8194570000	-1.8127450000
O	-0.6902260000	2.7587990000	-0.4558330000
H	-2.5001930000	1.9759560000	0.1344210000
H	-0.3590030000	2.0104070000	1.5881890000
C	-4.3037220000	-3.5152280000	-0.1123360000
H	-4.4875520000	-4.0606260000	0.8141570000
H	-4.0601390000	-4.2352740000	-0.8957680000
H	-5.2356980000	-3.0205070000	-0.3996040000

thermodynamic data

Zero-point correction= 0.386455 (Hartree/Particle)
Thermal correction to Energy= 0.410409
Thermal correction to Enthalpy= 0.411353
Thermal correction to Gibbs Free Energy= 0.331024
Sum of electronic and zero-point Energies= -1265.670210
Sum of electronic and thermal Energies= -1265.646256
Sum of electronic and thermal Enthalpies= -1265.645312
Sum of electronic and thermal Free Energies= -1265.725641

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.536	87.706	169.067

M062X/6-311+G**/PCM	**Breslowintermediat *p*-Br**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	2.8433380000	1.2433990000	0.5278000000
C	3.1463060000	0.0334110000	-0.0852320000
C	2.1489010000	-0.7580170000	-0.6412660000
C	0.8284680000	-0.3363710000	-0.5624010000
C	0.4820690000	0.8620970000	0.0826940000
C	1.5189850000	1.6520920000	0.6035980000
C	-0.8977140000	1.3359790000	0.1362070000
C	-2.0302060000	0.5875110000	0.0792230000
O	-1.0496900000	2.7207290000	0.0677780000
S	-3.5868880000	1.3240500000	-0.3312880000
C	-4.3778570000	-0.2605660000	-0.2715270000

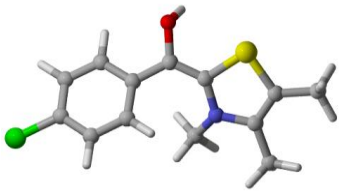
C	-3.5109900000	-1.2227930000	0.0791010000
N	-2.2001330000	-0.7646620000	0.3272910000
C	-5.8297260000	-0.3515500000	-0.6124210000
C	-3.7894070000	-2.6871990000	0.2146020000
C	-1.3268770000	-1.4810440000	1.2542370000
Br	4.9607770000	-0.5397990000	-0.1771040000
H	3.6305890000	1.8591390000	0.9440990000
H	2.3982540000	-1.6824580000	-1.1468640000
H	0.0567850000	-0.9305460000	-1.0381850000
H	1.2803540000	2.5972700000	1.0752240000
H	-1.5105170000	3.0363820000	0.8529740000
H	-6.4184080000	0.3090590000	0.0294980000
H	-6.0157520000	-0.0586480000	-1.6488220000
H	-6.1976000000	-1.3671680000	-0.4722500000
H	-4.7283220000	-2.9418080000	-0.2724370000
H	-2.9920880000	-3.2682860000	-0.2541560000
H	-3.8586060000	-2.9935020000	1.2611120000
H	-1.9315490000	-2.0834000000	1.9303050000
H	-0.6168930000	-2.1301730000	0.7374510000
H	-0.7665470000	-0.7525830000	1.8403540000

thermodynamic data

Zero-point correction= 0.242941 (Hartree/Particle)
Thermal correction to Energy= 0.260577
Thermal correction to Enthalpy= 0.261521
Thermal correction to Gibbs Free Energy= 0.196309
Sum of electronic and zero-point Energies= -3605.779114
Sum of electronic and thermal Energies= -3605.761478
Sum of electronic and thermal Enthalpies= -3605.760534
Sum of electronic and thermal Free Energies= -3605.825747

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.515	65.136	137.252

M062X/6-311+G**/PCM	**Breslowintermediat *p*-Cl**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	3.5563220000	0.9700310000	0.4966920000

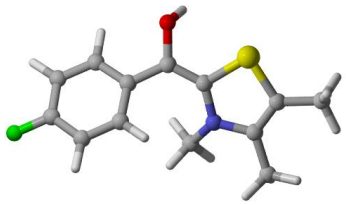
C	3.7940400000	-0.2323870000	-0.1574310000
C	2.7557530000	-0.9544400000	-0.7310060000
C	1.4588290000	-0.4692180000	-0.6319720000
C	1.1777550000	0.7247200000	0.0513640000
C	2.2553670000	1.4433140000	0.5926180000
C	-0.1762950000	1.2670930000	0.1266840000
C	-1.3457850000	0.5784030000	0.0740930000
O	-0.2561910000	2.6588020000	0.0802580000
S	-2.8681270000	1.4005200000	-0.3010760000
C	-3.7410440000	-0.1406000000	-0.2422570000
C	-2.9200620000	-1.1511460000	0.0820000000
N	-1.5825060000	-0.7669770000	0.3081750000
C	-5.2013920000	-0.1499500000	-0.5579500000
C	-3.2760610000	-2.5993200000	0.2112130000
C	-0.7257390000	-1.5410950000	1.2029080000
Cl	5.4335720000	-0.8369330000	-0.2782680000
H	4.3791290000	1.5267000000	0.9279290000
H	2.9613320000	-1.8737720000	-1.2650840000
H	0.6548490000	-1.0079070000	-1.1206230000
H	2.0663200000	2.3836170000	1.0953810000
H	-0.7098900000	2.9838470000	0.8657890000
H	-5.7426380000	0.5340670000	0.1010280000
H	-5.3889280000	0.1643250000	-1.5878220000
H	-5.6209650000	-1.1460540000	-0.4221090000
H	-4.2350410000	-2.7979350000	-0.2628230000
H	-2.5191200000	-3.2202860000	-0.2728450000
H	-3.3470340000	-2.9089360000	1.2567280000
H	-1.3437100000	-2.1434090000	1.8666060000
H	-0.0433760000	-2.1975140000	0.6587690000
H	-0.1346870000	-0.8512100000	1.8058240000

thermodynamic data

Zero-point correction= 0.243799 (Hartree/Particle)
Thermal correction to Energy= 0.261135
Thermal correction to Enthalpy= 0.262079
Thermal correction to Gibbs Free Energy= 0.198355
Sum of electronic and zero-point Energies= -1491.806476
Sum of electronic and thermal Energies= -1491.789139
Sum of electronic and thermal Enthalpies= -1491.788195
Sum of electronic and thermal Free Energies= -1491.851919

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.865	64.632	134.119

M062X/6-311+G**/PCM	**Breslowintermediat *p*-F**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	3.9560080000	0.6838680000	0.4646290000
C	4.1122650000	-0.5028630000	-0.2295620000
C	3.0496380000	-1.1537340000	-0.8294350000
C	1.7813550000	-0.5980530000	-0.7149100000
C	1.5687500000	0.5849010000	0.0093060000
C	2.6818030000	1.2243920000	0.5765330000
C	0.2424600000	1.1965340000	0.1066370000
C	-0.9595950000	0.5699110000	0.0687140000
O	0.2375490000	2.5910840000	0.0784680000
S	-2.4475780000	1.4755570000	-0.2580030000
C	-3.3963440000	-0.0212620000	-0.2043360000
C	-2.6211340000	-1.0775850000	0.0832750000
N	-1.2596710000	-0.7686730000	0.2823990000
C	-4.8621930000	0.0510000000	-0.4842460000
C	-3.0505150000	-2.5072750000	0.1961890000
C	-0.4249890000	-1.5991680000	1.1464740000
F	5.3502090000	-1.0382340000	-0.3367260000
H	4.8181170000	1.1672460000	0.9073640000
H	3.2213290000	-2.0653090000	-1.3883780000
H	0.9465990000	-1.0745840000	-1.2163750000
H	2.5412840000	2.1561630000	1.1101350000
H	-0.2118920000	2.9292680000	0.8609310000
H	-5.3515140000	0.7441080000	0.2053120000
H	-5.0577170000	0.4018910000	-1.5007760000
H	-5.3287400000	-0.9260140000	-0.3631720000
H	-4.0278820000	-2.6476400000	-0.2610560000
H	-2.3368690000	-3.1585330000	-0.3131870000
H	-3.1172800000	-2.8310620000	1.2377320000
H	-1.0587570000	-2.2009740000	1.7952970000
H	0.2311770000	-2.2611590000	0.5772870000
H	0.1937650000	-0.9501810000	1.7673290000

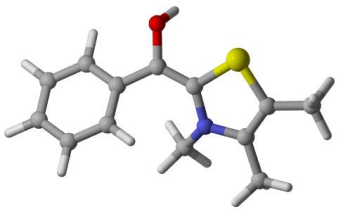
thermodynamic data

Zero-point correction= 0.245542 (Hartree/Particle)
Thermal correction to Energy= 0.262359
Thermal correction to Enthalpy= 0.263303
Thermal correction to Gibbs Free Energy= 0.201382

Sum of electronic and zero-point Energies= -1131.445108
Sum of electronic and thermal Energies= -1131.428290
Sum of electronic and thermal Enthalpies= -1131.427346
Sum of electronic and thermal Free Energies= -1131.489267

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.633	63.634	130.324

M062X/6-311+G**/PCM	**Breslowintermediat *p*-H**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-4.3387940000	-0.2913330000	0.3611410000
C	-4.4283310000	0.8977940000	-0.3605610000
C	-3.2792370000	1.4314530000	-0.9396450000
C	-2.0539730000	0.7940270000	-0.7866810000
C	-1.9447920000	-0.3860590000	-0.0341310000
C	-3.1150310000	-0.9296670000	0.5192020000
C	-0.6682860000	-1.0881790000	0.1035290000
C	0.5756470000	-0.5472050000	0.0726710000
O	-0.7582100000	-2.4804750000	0.1033800000
S	2.0045260000	-1.5563430000	-0.2177930000
C	3.0501980000	-0.1259580000	-0.1767060000
C	2.3444430000	0.9847920000	0.0841380000
N	0.9634940000	0.7704810000	0.2706290000
C	4.5112100000	-0.3008230000	-0.4365070000
C	2.8680680000	2.3840040000	0.1806830000
C	0.1746960000	1.6709950000	1.1068870000
H	-5.2289190000	-0.7237060000	0.8039550000
H	-5.3840320000	1.3934520000	-0.4824910000
H	-3.3386180000	2.3400860000	-1.5280810000
H	-1.1730900000	1.1947280000	-1.2762070000
H	-3.0533560000	-1.8576540000	1.0751030000
H	-0.3524170000	-2.8319910000	0.9035000000
H	4.9478150000	-1.0038870000	0.2779150000
H	4.6932560000	-0.6930540000	-1.4403470000
H	5.0388190000	0.6470990000	-0.3382070000
H	3.8579700000	2.4513860000	-0.2657290000
H	2.2061270000	3.0736260000	-0.3477530000
H	2.9440810000	2.7191850000	1.2179830000

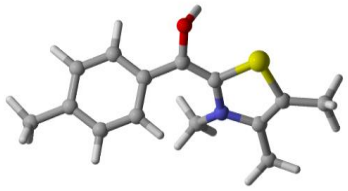
H	0.8402150000	2.2516620000	1.7427090000
H	-0.4403410000	2.3532760000	0.5165360000
H	-0.4836160000	1.0746570000	1.7402390000

thermodynamic data

Zero-point correction= 0.253612 (Hartree/Particle)
Thermal correction to Energy= 0.269626
Thermal correction to Enthalpy= 0.270570
Thermal correction to Gibbs Free Energy= 0.210618
Sum of electronic and zero-point Energies= -1032.194792
Sum of electronic and thermal Energies= -1032.178777
Sum of electronic and thermal Enthalpies= -1032.177833
Sum of electronic and thermal Free Energies= -1032.237786

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	169.193	60.728	126.181

M062X/6-311+G**/PCM	**Breslowintermediat *p*-Me**

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.9232970000	-0.7294540000	0.4610370000
C	-4.1506200000	0.4655500000	-0.2234620000
C	-3.0502430000	1.0989140000	-0.8093490000
C	-1.7717890000	0.5702820000	-0.7017310000
C	-1.5390010000	-0.6142740000	0.0151630000
C	-2.6455020000	-1.2649660000	0.5766630000
C	-0.2045350000	-1.2102200000	0.1052250000
C	0.9898390000	-0.5703750000	0.0673680000
O	-0.1813470000	-2.6050940000	0.0734540000
S	2.4893200000	-1.4585120000	-0.2616620000
C	3.4196730000	0.0504830000	-0.2097310000
C	2.6321430000	1.0968930000	0.0809260000
N	1.2750050000	0.7727080000	0.2826160000
C	4.8850630000	-0.0031240000	-0.4961910000
C	3.0446230000	2.5317310000	0.1932260000
C	0.4369600000	1.5874950000	1.1586840000
C	-5.5308070000	1.0594080000	-0.3365530000
H	-4.7611430000	-1.2513290000	0.9126650000
H	-3.2023280000	2.0140500000	-1.3736170000

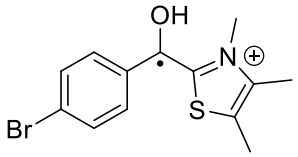
H	-0.9432900000	1.0615480000	-1.2009850000
H	-2.4964380000	-2.1992580000	1.1049380000
H	0.2832700000	-2.9385150000	0.8489570000
H	5.3861730000	-0.6919380000	0.1892760000
H	5.0805110000	-0.3491670000	-1.5144670000
H	5.3404940000	0.9791110000	-0.3748200000
H	4.0195390000	2.6841530000	-0.2654170000
H	2.3221060000	3.1742190000	-0.3148100000
H	3.1089260000	2.8563550000	1.2346620000
H	1.0678370000	2.1884560000	1.8114300000
H	-0.2279390000	2.2480390000	0.5982420000
H	-0.1739000000	0.9267730000	1.7748230000
H	-6.2872330000	0.3691680000	0.0388340000
H	-5.6044790000	1.9865480000	0.2382420000
H	-5.7705310000	1.2997170000	-1.3749560000

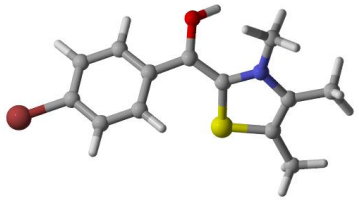
thermodynamic data

Zero-point correction= 0.281339 (Hartree/Particle)
Thermal correction to Energy= 0.299086
Thermal correction to Enthalpy= 0.300030
Thermal correction to Gibbs Free Energy= 0.236214
Sum of electronic and zero-point Energies= -1071.473568
Sum of electronic and thermal Energies= -1071.455822
Sum of electronic and thermal Enthalpies= -1071.454877
Sum of electronic and thermal Free Energies= -1071.518693

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	187.679	66.710	134.312

M062X/6-311+G**/PCM	**Breslowintermediat rad *p*-Br**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.2375400000	-0.6558510000	0.8087650000
C	-3.1840410000	0.0242010000	0.0499450000
C	-2.8316940000	1.1040290000	-0.7544480000
C	-1.5053250000	1.4982150000	-0.8102870000
C	-0.5256990000	0.8116700000	-0.0755300000
C	-0.9115360000	-0.2570350000	0.7474640000
C	0.8562280000	1.2546210000	-0.1620150000

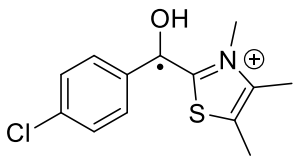
C	1.9605540000	0.3950140000	-0.0312510000
O	1.0106540000	2.5620710000	-0.4277820000
S	1.8905170000	-1.2895490000	-0.4173540000
C	3.6053640000	-1.4490660000	-0.2363950000
C	4.1707860000	-0.2588680000	0.1075570000
N	3.2394850000	0.7603230000	0.2433320000
C	3.6095940000	2.0627590000	0.8185210000
C	4.2506160000	-2.7796200000	-0.4482720000
C	5.6149170000	0.0194700000	0.3624890000
Br	-4.9968990000	-0.5232430000	0.1216080000
H	-2.5333830000	-1.4750960000	1.4505160000
H	-3.5836160000	1.6260010000	-1.3314780000
H	-1.2177260000	2.3342900000	-1.4345820000
H	-0.1855180000	-0.7563050000	1.3770390000
H	1.8449720000	2.7532590000	-0.8744890000
H	4.3613180000	1.8984080000	1.5858610000
H	4.0193490000	2.7205960000	0.0508180000
H	2.7347530000	2.5109020000	1.2803410000
H	5.3255270000	-2.7117320000	-0.2953990000
H	3.8523050000	-3.5142180000	0.2540350000
H	4.0675650000	-3.1425650000	-1.4610890000
H	5.9318100000	0.9229820000	-0.1607900000
H	5.8071180000	0.1529490000	1.4296920000
H	6.2237370000	-0.8092520000	0.0105940000

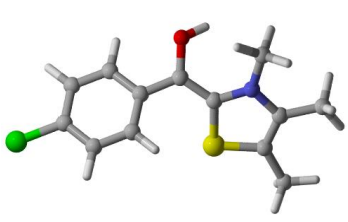
thermodynamic data

Zero-point correction= 0.244286 (Hartree/Particle)
Thermal correction to Energy= 0.260818
Thermal correction to Enthalpy= 0.261763
Thermal correction to Gibbs Free Energy= 0.198632
Sum of electronic and zero-point Energies= -3605.609596
Sum of electronic and thermal Energies= -3605.593063
Sum of electronic and thermal Enthalpies= -3605.592119
Sum of electronic and thermal Free Energies= -3605.655250

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.666	62.294	132.869

M062X/6-311+G**/PCM	**Breslowintermediat rad *p*-Cl**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

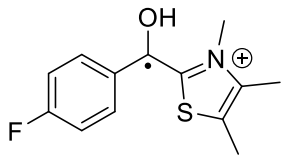
C	-2.8535000000	-0.8642130000	0.8557540000
C	-3.8338780000	-0.2377870000	0.0948850000
C	-3.5383780000	0.8521160000	-0.7177190000
C	-2.2341080000	1.3123590000	-0.7785030000
C	-1.2198640000	0.6814980000	-0.0406760000
C	-1.5497420000	-0.3993150000	0.7904200000
C	0.1378870000	1.1962340000	-0.1344030000
C	1.2843600000	0.3929160000	-0.0226040000
O	0.2153740000	2.5118360000	-0.3907110000
S	1.2803350000	-1.2999870000	-0.3833440000
C	3.0029000000	-1.3836560000	-0.2316040000
C	3.5236570000	-0.1649290000	0.0811720000
N	2.5532820000	0.8166180000	0.2187500000
C	2.8836190000	2.1482430000	0.7484520000
C	3.6999620000	-2.6894430000	-0.4333420000
C	4.9600280000	0.1763680000	0.3011840000
Cl	-5.4716030000	-0.8203220000	0.1740580000
H	-3.1119720000	-1.6924980000	1.5022700000
H	-4.3201680000	1.3291610000	-1.2944090000
H	-1.9895670000	2.1569270000	-1.4095920000
H	-0.7994210000	-0.8559870000	1.4234790000
H	1.0419960000	2.7591720000	-0.8226950000
H	3.2281830000	2.8050870000	-0.0522230000
H	2.0094860000	2.5651420000	1.2402100000
H	3.6748460000	2.0393910000	1.4849830000
H	4.7689120000	-2.5828990000	-0.2617940000
H	3.3166870000	-3.4383370000	0.2620020000
H	3.5470730000	-3.0584430000	-1.4490430000
H	5.1673570000	0.3404580000	1.3612890000
H	5.5941660000	-0.6350420000	-0.0460380000
H	5.2306830000	1.0797770000	-0.2475900000

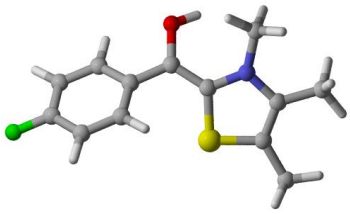
thermodynamic data

Zero-point correction= 0.245338 (Hartree/Particle)
Thermal correction to Energy= 0.262277
Thermal correction to Enthalpy= 0.263222
Thermal correction to Gibbs Free Energy= 0.199424
Sum of electronic and zero-point Energies= -1491.637038
Sum of electronic and thermal Energies= -1491.620099
Sum of electronic and thermal Enthalpies= -1491.619155
Sum of electronic and thermal Free Energies= -1491.682952

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	164.582	63.680	134.273

M062X/6-311+G**/PCM	**Breslowintermediat rad *p*-F**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.1489660000	-1.0653810000	0.9237080000
C	-4.1446310000	-0.5124040000	0.1358510000
C	-3.9243640000	0.5661840000	-0.7059520000
C	-2.6490340000	1.1012330000	-0.7698230000
C	-1.6061790000	0.5513520000	-0.0071300000
C	-1.8754590000	-0.5239350000	0.8530850000
C	-0.2773390000	1.1373660000	-0.1117440000
C	0.9055120000	0.3906240000	-0.0130280000
O	-0.2715060000	2.4548020000	-0.3696550000
S	0.9688320000	-1.3070210000	-0.3487050000
C	2.6961040000	-1.3123870000	-0.2296040000
C	3.1691590000	-0.0671910000	0.0526680000
N	2.1603500000	0.8733870000	0.1973840000
C	2.4374050000	2.2243680000	0.7074600000
C	3.4461300000	-2.5898440000	-0.4236800000
C	4.5944070000	0.3388410000	0.2316810000
F	-5.3774140000	-1.0375790000	0.1976110000
H	-3.3798370000	-1.8889620000	1.5866970000
H	-4.7388940000	0.9655880000	-1.2961990000
H	-2.4474230000	1.9396920000	-1.4237840000
H	-1.1013230000	-0.9159000000	1.5006900000
H	0.5407220000	2.7468090000	-0.8010820000
H	3.2724850000	2.1677480000	1.3999290000
H	2.6980060000	2.8995370000	-0.1096640000
H	1.5666330000	2.5878390000	1.2462650000
H	4.5073850000	-2.4434250000	-0.2340980000
H	3.0809230000	-3.3547200000	0.2639820000
H	3.3231120000	-2.9620200000	-1.4423820000
H	4.8090180000	1.2496840000	-0.3295520000
H	4.8235820000	0.5189260000	1.2846840000
H	5.2541610000	-0.4453340000	-0.1300880000

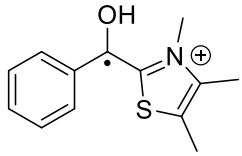
thermodynamic data

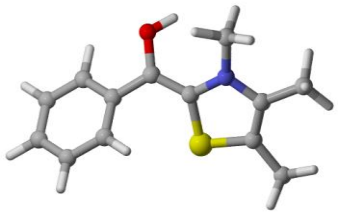
Zero-point correction= 0.246896 (Hartree/Particle)
Thermal correction to Energy= 0.263394
Thermal correction to Enthalpy= 0.264339
Thermal correction to Gibbs Free Energy= 0.201760

Sum of electronic and zero-point Energies= -1131.277341
Sum of electronic and thermal Energies= -1131.260842
Sum of electronic and thermal Enthalpies= -1131.259898
Sum of electronic and thermal Free Energies= -1131.322477

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	165.282	62.587	131.708

M062X/6-311+G**/PCM	**Breslowintermediat rad *p*-H**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	3.3992620000	-1.3572480000	-0.9913250000
C	4.4676800000	-0.9134690000	-0.2160190000
C	4.3021940000	0.1682200000	0.6471870000
C	3.0720440000	0.8005800000	0.7446960000
C	1.9848430000	0.3431680000	-0.0162070000
C	2.1636350000	-0.7329510000	-0.8981540000
C	0.7015260000	1.0215280000	0.1113830000
C	-0.5324980000	0.3623690000	0.0096280000
O	0.7888530000	2.3319680000	0.3887920000
S	-0.7153440000	-1.3302970000	0.3260360000
C	-2.4398720000	-1.2087080000	0.2274990000
C	-2.8241240000	0.0698850000	-0.0388890000
N	-1.7509430000	0.9364300000	-0.1849340000
C	-1.9329780000	2.3084940000	-0.6807560000
C	-3.2802930000	-2.4280080000	0.4248100000
C	-4.2184810000	0.5778490000	-0.2018470000
H	3.5327870000	-2.1798200000	-1.6827860000
H	5.4311360000	-1.4029960000	-0.2921210000
H	5.1341800000	0.5162610000	1.2469750000
H	2.9361170000	1.6378990000	1.4173790000
H	1.3520430000	-1.0537520000	-1.5397650000
H	0.0033990000	2.6722110000	0.8340320000
H	-2.7830320000	2.3212020000	-1.3569770000
H	-2.1263150000	2.9949280000	0.1455360000
H	-1.0470730000	2.6091490000	-1.2334460000
H	-4.3218140000	-2.2172770000	0.1908820000
H	-2.9426790000	-3.2344310000	-0.2281170000
H	-3.2194770000	-2.7781440000	1.4570970000

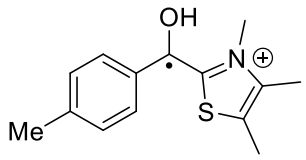
H	-4.3607360000	1.5025580000	0.3595910000
H	-4.4463070000	0.7723410000	-1.2526260000
H	-4.9285730000	-0.1563850000	0.1699290000

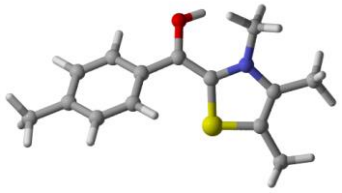
thermodynamic data

Zero-point correction= 0.255251 (Hartree/Particle)
Thermal correction to Energy= 0.270891
Thermal correction to Enthalpy= 0.271835
Thermal correction to Gibbs Free Energy= 0.211052
Sum of electronic and zero-point Energies= -1032.027375
Sum of electronic and thermal Energies= -1032.011736
Sum of electronic and thermal Enthalpies= -1032.010791
Sum of electronic and thermal Free Energies= -1032.071575

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	169.987	59.590	127.929

M062X/6-311+G**/PCM	**Breslowintermediat rad *p*-Me**





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.1465820000	-1.0282420000	0.8947850000
C	-4.1833230000	-0.4824990000	0.1354830000
C	-3.8979600000	0.6136110000	-0.6886990000
C	-2.6216530000	1.1407100000	-0.7619730000
C	-1.5766390000	0.5703780000	-0.0148380000
C	-1.8604620000	-0.5119090000	0.8295150000
C	-0.2435630000	1.1409410000	-0.1189170000
C	0.9339930000	0.3859040000	-0.0133740000
O	-0.2193360000	2.4587230000	-0.3799900000
S	0.9895630000	-1.3120960000	-0.3500460000
C	2.7174760000	-1.3259740000	-0.2279000000
C	3.1958580000	-0.0844720000	0.0587170000
N	2.1911850000	0.8615130000	0.2021370000
C	2.4746920000	2.2086640000	0.7182990000
C	3.4614170000	-2.6068580000	-0.4233770000
C	4.6224800000	0.3145640000	0.2438380000
C	-5.5788800000	-1.0372060000	0.2047310000
H	-3.3520240000	-1.8598570000	1.5593770000

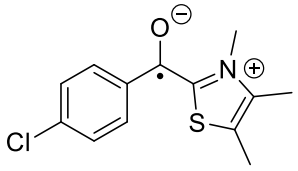
H	-4.6923640000	1.0539590000	-1.2817690000
H	-2.4146070000	1.9846430000	-1.4079270000
H	-1.0895270000	-0.9254220000	1.4682420000
H	0.5978020000	2.7368550000	-0.8109220000
H	3.3008950000	2.1429400000	1.4206560000
H	2.7512250000	2.8832680000	-0.0941590000
H	1.6010020000	2.5796640000	1.2469570000
H	4.5238240000	-2.4653350000	-0.2364260000
H	3.0944510000	-3.3701900000	0.2651170000
H	3.3345860000	-2.9788060000	-1.4417090000
H	4.8434840000	1.2257580000	-0.3143310000
H	4.8488740000	0.4912690000	1.2980230000
H	5.2800480000	-0.4717660000	-0.1172520000
H	-5.6214560000	-1.9233660000	0.8376030000
H	-6.2678970000	-0.2913650000	0.6086390000
H	-5.9360520000	-1.3047610000	-0.7921700000

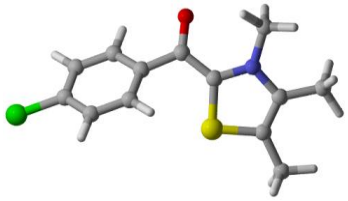
thermodynamic data

Zero-point correction= 0.282473 (Hartree/Particle)
Thermal correction to Energy= 0.300041
Thermal correction to Enthalpy= 0.300985
Thermal correction to Gibbs Free Energy= 0.235899
Sum of electronic and zero-point Energies= -1071.308295
Sum of electronic and thermal Energies= -1071.290727
Sum of electronic and thermal Enthalpies= -1071.289783
Sum of electronic and thermal Free Energies= -1071.354868

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.278	65.828	136.984

M062X/6-311+G**/PCM	**Breslowintermediat radde *p*-Cl**





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.8878870000	-0.7657380000	0.9055630000
C	-3.8175620000	-0.2066020000	0.0402580000
C	-3.4755630000	0.8268700000	-0.8237390000
C	-2.1705690000	1.2989690000	-0.8193850000
C	-1.2046890000	0.7385320000	0.0219210000

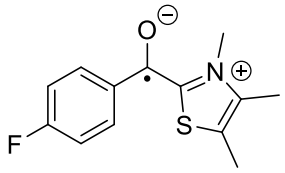
C	-1.5817450000	-0.2881030000	0.8908000000
C	0.1741510000	1.3214720000	-0.0110300000
C	1.2874760000	0.4381860000	0.0736410000
O	0.3099760000	2.5586710000	-0.1698350000
S	1.2120870000	-1.2882850000	-0.1790800000
C	2.9594480000	-1.4042300000	-0.2066530000
C	3.5256110000	-0.1921720000	-0.0089370000
N	2.5978510000	0.8324460000	0.1704730000
C	2.9920120000	2.1954870000	0.5328320000
C	3.5938200000	-2.7422830000	-0.4097170000
C	4.9881260000	0.1157280000	0.0390440000
Cl	-5.4609460000	-0.8063780000	0.0478730000
H	-3.1822270000	-1.5537220000	1.5868900000
H	-4.2191340000	1.2522340000	-1.4858740000
H	-1.8863340000	2.1133440000	-1.4749170000
H	-0.8642610000	-0.7049400000	1.5881860000
H	3.9753380000	2.1616860000	0.9938340000
H	3.0145330000	2.8392230000	-0.3461710000
H	2.2725220000	2.5961410000	1.2406550000
H	4.6794510000	-2.6616020000	-0.4079140000
H	3.3053260000	-3.4323270000	0.3867890000
H	3.2856080000	-3.1815860000	-1.3610620000
H	5.2324360000	0.9448480000	-0.6280070000
H	5.3045020000	0.3865440000	1.0491410000
H	5.5643790000	-0.7520530000	-0.2723330000

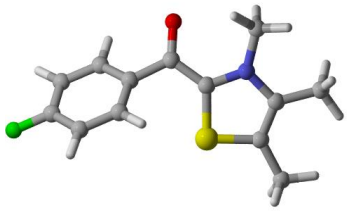
thermodynamic data

Zero-point correction= 0.232438 (Hartree/Particle)
Thermal correction to Energy= 0.249346
Thermal correction to Enthalpy= 0.250290
Thermal correction to Gibbs Free Energy= 0.185705
Sum of electronic and zero-point Energies= -1491.218722
Sum of electronic and thermal Energies= -1491.201814
Sum of electronic and thermal Enthalpies= -1491.200870
Sum of electronic and thermal Free Energies= -1491.265456

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.467	62.282	135.932

M062X/6-311+G**/PCM	**Breslowintermediat radde *p*-F**





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.1958370000	-0.9830520000	0.9290480000
C	-4.1383570000	-0.4807280000	0.0509560000
C	-3.8654920000	0.5559690000	-0.8251640000
C	-2.5885170000	1.1001340000	-0.8203680000
C	-1.5973960000	0.6041970000	0.0326570000
C	-1.9190810000	-0.4313250000	0.9139070000
C	-0.2513110000	1.2597960000	-0.0043330000
C	0.9051910000	0.4335220000	0.0764480000
O	-0.1796700000	2.5021380000	-0.1637950000
S	0.9100110000	-1.2962040000	-0.1688820000
C	2.6607330000	-1.3292320000	-0.2069490000
C	3.1703110000	-0.0912380000	-0.0155620000
N	2.1968210000	0.8893180000	0.1656740000
C	2.5296420000	2.2715650000	0.5148010000
C	3.3564680000	-2.6367890000	-0.4081060000
C	4.6171010000	0.2849310000	0.0237070000
F	-5.3763920000	-1.0173080000	0.0542460000
H	-3.4642000000	-1.7793380000	1.6116950000
H	-4.6394430000	0.9199440000	-1.4891880000
H	-2.3449210000	1.9204520000	-1.4846590000
H	-1.1802350000	-0.7989410000	1.6165460000
H	3.5131390000	2.2864810000	0.9765430000
H	2.5253740000	2.9069920000	-0.3707190000
H	1.7929360000	2.6473200000	1.2182290000
H	4.4369390000	-2.5040550000	-0.4195990000
H	3.1108570000	-3.3341560000	0.3964140000
H	3.0592380000	-3.0976680000	-1.3527210000
H	4.8199030000	1.1200200000	-0.6498320000
H	4.9252740000	0.5764920000	1.0305380000
H	5.2313800000	-0.5573240000	-0.2849740000

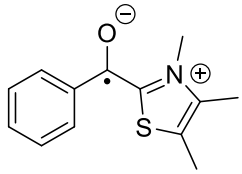
thermodynamic data

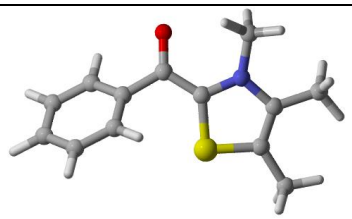
Zero-point correction= 0.234084 (Hartree/Particle)
Thermal correction to Energy= 0.250419
Thermal correction to Enthalpy= 0.251363
Thermal correction to Gibbs Free Energy= 0.188996

Sum of electronic and zero-point Energies= -1130.858287
Sum of electronic and thermal Energies= -1130.841951
Sum of electronic and thermal Enthalpies= -1130.841007
Sum of electronic and thermal Free Energies= -1130.903374

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	157.140	61.255	131.264

M062X/6-311+G**/PCM	**Breslowintermediat radde *p*-H**





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.4583690000	-1.2625150000	0.9788280000
C	-4.4668020000	-0.8815920000	0.0987830000
C	-4.2390730000	0.1514240000	-0.8090040000
C	-3.0077380000	0.7945500000	-0.8381430000
C	-1.9812930000	0.4022410000	0.0264340000
C	-2.2213830000	-0.6256490000	0.9425110000
C	-0.6846010000	1.1500010000	-0.0281920000
C	0.5260530000	0.4064360000	0.0673200000
O	-0.6955410000	2.3918870000	-0.2059030000
S	0.6530840000	-1.3198400000	-0.1741500000
C	2.4024430000	-1.2285370000	-0.2074490000
C	2.8227630000	0.0424950000	-0.0153910000
N	1.7818510000	0.9521820000	0.1614850000
C	2.0118910000	2.3494380000	0.5326020000
C	3.1906430000	-2.4825710000	-0.4085700000
C	4.2391430000	0.5205530000	0.0293300000
H	-3.6360730000	-2.0496060000	1.7022860000
H	-5.4284170000	-1.3804630000	0.1256530000
H	-5.0233890000	0.4557980000	-1.4922270000
H	-2.8247380000	1.6067690000	-1.5320960000
H	-1.4508500000	-0.9117060000	1.6496930000
H	2.9899660000	2.4293940000	0.9996880000
H	1.9642980000	2.9975520000	-0.3422480000
H	1.2473540000	2.6584750000	1.2392190000
H	4.2596530000	-2.2788600000	-0.3766400000
H	2.9637070000	-3.2121380000	0.3725170000
H	2.9596360000	-2.9419910000	-1.3723790000
H	4.3797850000	1.3779430000	-0.6318190000

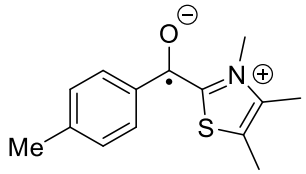
H	4.5269340000	0.8183530000	1.0404250000
H	4.9120910000	-0.2700770000	-0.2932020000

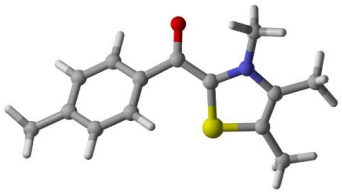
thermodynamic data

Zero-point correction= 0.241756 (Hartree/Particle)
Thermal correction to Energy= 0.257482
Thermal correction to Enthalpy= 0.258426
Thermal correction to Gibbs Free Energy= 0.197273
Sum of electronic and zero-point Energies= -1031.608076
Sum of electronic and thermal Energies= -1031.592350
Sum of electronic and thermal Enthalpies= -1031.591406
Sum of electronic and thermal Free Energies= -1031.652559

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.572	58.506	128.707

M062X/6-311+G**/PCM	**Breslowintermediat radde *p*-Me**





xyz-matrix

33
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.1921750000	-0.9276200000	0.9204110000
C	-4.1747840000	-0.4475680000	0.0556290000
C	-3.8355540000	0.5964240000	-0.8124950000
C	-2.5574390000	1.1336230000	-0.8193030000
C	-1.5663920000	0.6311560000	0.0317030000
C	-1.9036060000	-0.3989370000	0.9105140000
C	-0.2138420000	1.2705660000	-0.0072180000
C	0.9344590000	0.4322690000	0.0791310000
O	-0.1234530000	2.5114660000	-0.1711790000
S	0.9223590000	-1.2985750000	-0.1605510000
C	2.6732150000	-1.3475610000	-0.2055670000
C	3.1949040000	-0.1143300000	-0.0169190000
N	2.2314010000	0.8755830000	0.1661590000
C	2.5780850000	2.2532880000	0.5188910000
C	3.3564140000	-2.6614190000	-0.4086400000
C	4.6453430000	0.2484880000	0.0177950000
C	-5.5649670000	-1.0269650000	0.0471290000
H	-3.4374960000	-1.7204720000	1.6192580000
H	-4.5873720000	0.9907530000	-1.4890580000

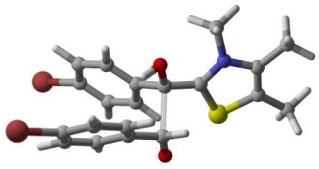
H	-2.3076190000	1.9508150000	-1.4861550000
H	-1.1697570000	-0.7761380000	1.6143750000
H	3.5610610000	2.2570360000	0.9822030000
H	2.5814340000	2.8914610000	-0.3646770000
H	1.8441150000	2.6349560000	1.2220880000
H	4.4382780000	-2.5398980000	-0.4156470000
H	3.1007920000	-3.3589650000	0.3926520000
H	3.0579370000	-3.1164020000	-1.3557800000
H	4.8534630000	1.0826710000	-0.6552810000
H	4.9597500000	0.5361960000	1.0238440000
H	5.2510580000	-0.5988770000	-0.2939630000
H	-5.6929520000	-1.7583050000	0.8456420000
H	-6.3149540000	-0.2430780000	0.1739480000
H	-5.7696340000	-1.5238340000	-0.9046790000

thermodynamic data

Zero-point correction= 0.269821 (Hartree/Particle)
Thermal correction to Energy= 0.287165
Thermal correction to Enthalpy= 0.288110
Thermal correction to Gibbs Free Energy= 0.223460
Sum of electronic and zero-point Energies= -1070.887107
Sum of electronic and thermal Energies= -1070.869762
Sum of electronic and thermal Enthalpies= -1070.868818
Sum of electronic and thermal Free Energies= -1070.933467

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	180.199	64.404	136.066

M062X/6-311+G**/PCM	**TST3 *p*-Br**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	3.7442870000	-0.8893470000	1.0816250000
C	5.0614160000	-0.8844150000	0.6042040000
C	3.4711990000	-1.1930950000	2.4978100000
C	5.1619650000	-0.3397130000	-0.6270150000
S	3.5928420000	0.0951880000	-1.2324490000
C	2.8240100000	-0.4313790000	0.2157520000
C	6.1713090000	-1.4405770000	1.4374780000

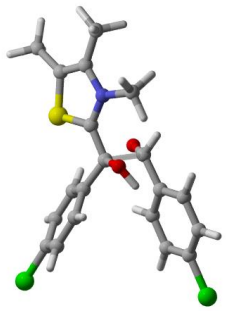
C	6.3766000000	-0.1342140000	-1.4766300000
C	1.3824120000	-0.4802110000	0.3959720000
C	0.6142890000	0.7912690000	0.3677030000
O	1.0488100000	-1.3375590000	1.4542330000
C	0.8039710000	1.7796510000	-0.6096960000
C	-0.0190810000	2.8989480000	-0.6679900000
C	-1.0439910000	3.0424460000	0.2568990000
C	-1.2551610000	2.0870040000	1.2407770000
C	-0.4309740000	0.9696780000	1.2852680000
C	0.8217220000	-1.3833490000	-1.3265910000
O	1.0651010000	-0.6206150000	-2.3021250000
C	-0.6085950000	-1.6774850000	-0.9634710000
C	-0.9579890000	-2.8691990000	-0.3269180000
C	-2.2814430000	-3.1348740000	0.0238410000
C	-3.2511650000	-2.1924950000	-0.2820890000
C	-2.9337320000	-1.0018670000	-0.9313290000
C	-1.6116180000	-0.7528870000	-1.2701330000
H	4.3802370000	-1.0019480000	3.0596550000
H	2.6837110000	-0.5392630000	2.8551440000
H	3.1647840000	-2.2302350000	2.6152290000
H	6.4240680000	-0.7808200000	2.2707890000
H	7.0603260000	-1.5659760000	0.8230860000
H	5.9003280000	-2.4171480000	1.8426910000
H	6.3257320000	0.8255170000	-1.9930660000
H	7.2769550000	-0.1371800000	-0.8638070000
H	6.4674970000	-0.9186690000	-2.2310930000
H	0.2268840000	-1.7893780000	1.2226640000
H	1.5775640000	1.6810660000	-1.3571070000
H	0.1387220000	3.6496320000	-1.4320480000
H	-2.0511460000	2.2073890000	1.9646620000
H	-0.6027810000	0.2256510000	2.0523610000
H	1.4805220000	-2.2539740000	-1.1346710000
H	-0.1955870000	-3.6153850000	-0.1212150000
H	-2.5483940000	-4.0624430000	0.5134640000
H	-3.7096350000	-0.2834710000	-1.1646580000
H	-1.3384380000	0.1642910000	-1.7801240000
Br	-5.0660270000	-2.5458780000	0.1751910000
Br	-2.1636580000	4.5827560000	0.1884080000

thermodynamic data

Zero-point correction= 0.345915 (Hartree/Particle)
Thermal correction to Energy= 0.371155
Thermal correction to Enthalpy= 0.372099
Thermal correction to Gibbs Free Energy= 0.288026
Sum of electronic and zero-point Energies= -6524.761244
Sum of electronic and thermal Energies= -6524.736003
Sum of electronic and thermal Enthalpies= -6524.735059
Sum of electronic and thermal Free Energies= -6524.819133

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	232.903	94.930	176.948

M062X/6-311+G**/PCM	**TST3 *p*-Cl**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	3.1504690000	-1.0874680000	0.6109770000
C	4.4357050000	-0.7068240000	0.1893470000
C	2.9779310000	-2.4090240000	1.2390910000
C	4.4537280000	0.5049470000	-0.4053250000
S	2.8557260000	1.1851080000	-0.4226920000
C	2.1884520000	-0.1812590000	0.3717490000
C	5.5897910000	-1.6262840000	0.4214750000
C	5.5881710000	1.2665280000	-1.0122560000
C	0.7596640000	-0.3246440000	0.5721600000
C	-0.0724400000	0.9194530000	0.4995260000
O	0.4863890000	-1.0897660000	1.7169240000
C	-0.1420640000	1.7034540000	-0.6609980000
C	-0.9892970000	2.8024230000	-0.7343160000
C	-1.7851770000	3.1208180000	0.3567700000
C	-1.7473530000	2.3604960000	1.5161100000
C	-0.8932860000	1.2655150000	1.5793080000
C	0.3515980000	-1.3951310000	-1.0066330000
O	0.7108020000	-0.8142370000	-2.0797530000
C	-1.1210390000	-1.6370790000	-0.7662130000
C	-1.5624060000	-2.6675230000	0.0654330000
C	-2.9209690000	-2.8602750000	0.3131950000
C	-3.8341730000	-2.0131590000	-0.2947690000
C	-3.4255730000	-0.9977360000	-1.1543540000
C	-2.0696770000	-0.8204540000	-1.3881550000
H	3.3357740000	-3.1703570000	0.5478020000
H	3.5629230000	-2.4432610000	2.1577650000
H	1.9349670000	-2.5702910000	1.4675340000
H	5.7177840000	-1.8371940000	1.4850450000
H	6.5059390000	-1.1697430000	0.0554800000
H	5.4522820000	-2.5751980000	-0.1005060000
H	5.7000990000	2.2430660000	-0.5376610000
H	6.5236090000	0.7229260000	-0.8945850000
H	5.4186430000	1.4259860000	-2.0788720000

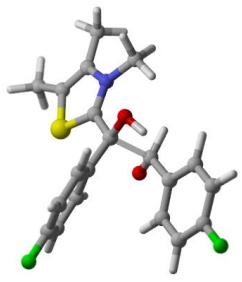
H	-0.4121260000	-1.4367850000	1.6351000000
H	0.4279420000	1.4182550000	-1.5350430000
H	-1.0402650000	3.3961410000	-1.6385460000
Cl	-2.8591100000	4.5002250000	0.2665040000
H	-2.3733030000	2.6201640000	2.3605890000
H	-0.8650880000	0.6781360000	2.4877490000
H	0.9460240000	-2.2571170000	-0.6392110000
H	-0.8426110000	-3.3503340000	0.5084890000
H	-3.2617070000	-3.6613060000	0.9568360000
Cl	-5.5441570000	-2.2394370000	0.0063510000
H	-4.1619680000	-0.3625780000	-1.6310070000
H	-1.7253300000	-0.0467890000	-2.0635120000

thermodynamic data

Zero-point correction= 0.347365 (Hartree/Particle)
Thermal correction to Energy= 0.372332
Thermal correction to Enthalpy= 0.373276
Thermal correction to Gibbs Free Energy= 0.289613
Sum of electronic and zero-point Energies= -2296.818974
Sum of electronic and thermal Energies= -2296.794007
Sum of electronic and thermal Enthalpies= -2296.793063
Sum of electronic and thermal Free Energies= -2296.876726

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.642	93.888	176.084

M062X/6-311+G**/PCM	**TST3 *p*-F**



xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	2.7543950000	-1.0517770000	0.5923550000
C	4.0472030000	-0.6922690000	0.1747950000
C	2.5586190000	-2.3476230000	1.2656350000
C	4.0862320000	0.5166830000	-0.4242420000
S	2.4995910000	1.2238940000	-0.4485980000
C	1.8093930000	-0.1266610000	0.3537710000
C	5.1884780000	-1.6279550000	0.4077290000

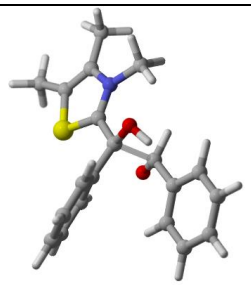
C	5.2336330000	1.2528700000	-1.0383070000
C	0.3809770000	-0.2405940000	0.5626420000
C	-0.4198350000	1.0278480000	0.5234480000
O	0.1012470000	-1.0199270000	1.6965660000
C	-0.4861640000	1.8313490000	-0.6239200000
C	-1.2951870000	2.9614080000	-0.6626740000
C	-2.0485800000	3.2766220000	0.4523930000
C	-2.0236580000	2.5070570000	1.5995290000
C	-1.2058650000	1.3824120000	1.6264820000
C	-0.0697260000	-1.2729280000	-1.0264880000
O	0.2862020000	-0.6802920000	-2.0954110000
C	-1.5440130000	-1.4914470000	-0.7706700000
C	-1.9946100000	-2.5342620000	0.0409100000
C	-3.3539600000	-2.7086990000	0.3011710000
C	-4.2443360000	-1.8269020000	-0.2790310000
C	-3.8407740000	-0.7975030000	-1.1154110000
C	-2.4840090000	-0.6401020000	-1.3601840000
H	3.1011080000	-3.1070010000	0.7076840000
H	2.9463940000	-2.2885430000	2.2831380000
H	1.5071320000	-2.5906250000	1.2946240000
H	5.2436610000	-1.9302870000	1.4550060000
H	6.1242440000	-1.1396300000	0.1474630000
H	5.0953010000	-2.5282300000	-0.2038690000
H	5.3319100000	2.2506150000	-0.6070340000
H	6.1671620000	0.7183160000	-0.8730020000
H	5.0899660000	1.3621330000	-2.1151980000
H	-0.8034300000	-1.3497220000	1.6120790000
H	0.0572810000	1.5390450000	-1.5124080000
H	-1.3535220000	3.5822410000	-1.5481700000
F	-2.8391780000	4.3728860000	0.4187970000
H	-2.6296480000	2.7862460000	2.4525930000
H	-1.1784990000	0.7772630000	2.5231430000
H	0.5122250000	-2.1551710000	-0.6880910000
H	-1.2815040000	-3.2397720000	0.4583510000
H	-3.7179380000	-3.5144040000	0.9262210000
F	-5.5646530000	-1.9823450000	-0.0362560000
H	-4.5825690000	-0.1450290000	-1.5597400000
H	-2.1315430000	0.1437320000	-2.0192810000

thermodynamic data

Zero-point correction= 0.350232 (Hartree/Particle)
Thermal correction to Energy= 0.374185
Thermal correction to Enthalpy= 0.375129
Thermal correction to Gibbs Free Energy= 0.296077
Sum of electronic and zero-point Energies= -1576.098003
Sum of electronic and thermal Energies= -1576.074050
Sum of electronic and thermal Enthalpies= -1576.073106
Sum of electronic and thermal Free Energies= -1576.152158

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.804	92.077	166.378

M062X/6-311+G**/PCM	**TST3 *p*-H**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	2.3537490000	-1.0173030000	0.5624740000
C	3.6471520000	-0.6799900000	0.1289100000
C	2.1244300000	-2.3624970000	1.1179600000
C	3.7120240000	0.5544550000	-0.4126540000
S	2.1485320000	1.3108540000	-0.3656740000
C	1.4305110000	-0.0576600000	0.3813670000
C	4.7614910000	-1.6598020000	0.3014370000
C	4.8723440000	1.2897180000	-1.0030610000
C	-0.0010290000	-0.1444230000	0.5925800000
C	-0.7687180000	1.1451880000	0.5887420000
O	-0.2992260000	-0.9458190000	1.7069030000
C	-0.8215420000	1.9737190000	-0.5414750000
C	-1.5925040000	3.1313770000	-0.5370150000
C	-2.3353130000	3.4835540000	0.5864600000
C	-2.3026050000	2.6599200000	1.7073380000
C	-1.5297210000	1.5026670000	1.7087980000
C	-0.4654580000	-1.1389170000	-1.0101020000
O	-0.0792220000	-0.5508260000	-2.0723140000
C	-1.9473660000	-1.3250300000	-0.7709170000
C	-2.4240930000	-2.3698800000	0.0245960000
C	-3.7907740000	-2.5166580000	0.2646690000
C	-4.6940640000	-1.6247880000	-0.3030180000
C	-4.2275140000	-0.5959640000	-1.1229780000
C	-2.8664790000	-0.4502950000	-1.3581860000
H	2.7949740000	-2.5136100000	1.9629810000
H	1.0991160000	-2.4470470000	1.4471160000
H	2.3376470000	-3.1010120000	0.3457330000
H	4.9375400000	-1.8747190000	1.3575610000
H	5.6791370000	-1.2529730000	-0.1159740000
H	4.5453920000	-2.6010450000	-0.2071810000
H	5.7683640000	0.6720200000	-0.9866230000
H	4.6679450000	1.5638520000	-2.0398350000
H	5.0791000000	2.2050490000	-0.4452770000
H	-1.2102730000	-1.2547390000	1.6096430000

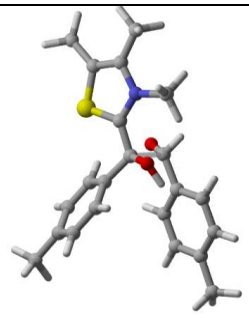
H	-0.2979700000	1.6779850000	-1.4411340000
H	-1.6216310000	3.7538410000	-1.4242580000
H	-2.9363090000	4.3853440000	0.5864380000
H	-2.8785520000	2.9183160000	2.5887630000
H	-1.5119370000	0.8752800000	2.5908390000
H	0.0870360000	-2.0401070000	-0.6713600000
H	-1.7236050000	-3.0914740000	0.4377880000
H	-4.1458310000	-3.3331600000	0.8827970000
H	-5.7565230000	-1.7365950000	-0.1207840000
H	-4.9317360000	0.0906130000	-1.5796070000
H	-2.4916930000	0.3366590000	-2.0015870000

thermodynamic data

Zero-point correction= 0.366956 (Hartree/Particle)
Thermal correction to Energy= 0.389257
Thermal correction to Enthalpy= 0.390202
Thermal correction to Gibbs Free Energy= 0.314631
Sum of electronic and zero-point Energies= -1377.595899
Sum of electronic and thermal Energies= -1377.573597
Sum of electronic and thermal Enthalpies= -1377.572653
Sum of electronic and thermal Free Energies= -1377.648224

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	244.263	86.071	159.053

M062X/6-311+G**/PCM	**TST3 *p*-Me**

xyz-matrix

51
XYZ file generated by gabedit : coordinates in Angstrom

N	2.7761930000	-1.0540640000	0.5989450000
C	4.0700570000	-0.6936250000	0.1855870000
C	2.5809530000	-2.3475950000	1.2765580000
C	4.1090780000	0.5132250000	-0.4175090000
S	2.5207680000	1.2168540000	-0.4524310000
C	1.8298950000	-0.1320790000	0.3523140000
C	5.2118310000	-1.6266690000	0.4268260000
C	5.2579610000	1.2489680000	-1.0295160000

C	0.3994200000	-0.2482310000	0.5504280000
C	-0.3988410000	1.0233640000	0.5113800000
O	0.1145190000	-1.0282430000	1.6836290000
C	-0.4632000000	1.8330200000	-0.6315720000
C	-1.2648000000	2.9677740000	-0.6542960000
C	-2.0407410000	3.3361530000	0.4470260000
C	-1.9822560000	2.5242450000	1.5788990000
C	-1.1792350000	1.3878300000	1.6131980000
C	-0.0375940000	-1.2813170000	-1.0213550000
O	0.3223610000	-0.6984340000	-2.0980420000
C	-1.5115250000	-1.5125310000	-0.7723220000
C	-1.9587030000	-2.5631070000	0.0303720000
C	-3.3200320000	-2.7477800000	0.2754610000
C	-4.2688550000	-1.8930060000	-0.2826560000
C	-3.8169680000	-0.8596220000	-1.1127730000
C	-2.4640210000	-0.6724920000	-1.3568570000
H	2.9751340000	-2.2867100000	2.2915650000
H	1.5287890000	-2.5868210000	1.3121140000
H	3.1186110000	-3.1100390000	0.7178520000
H	5.2650220000	-1.9225700000	1.4760820000
H	6.1477420000	-1.1391520000	0.1654580000
H	5.1209110000	-2.5309590000	-0.1791480000
H	5.3486880000	2.2509560000	-0.6064670000
H	6.1927310000	0.7202430000	-0.8525610000
H	5.1220140000	1.3482570000	-2.1084320000
H	-0.7894350000	-1.3584160000	1.5889290000
H	0.0773300000	1.5403400000	-1.5220990000
H	-1.2966930000	3.5743760000	-1.5543600000
H	-2.5707380000	2.7844670000	2.4532660000
H	-1.1553610000	0.7830830000	2.5109920000
H	0.5454290000	-2.1626610000	-0.6793030000
H	-1.2398900000	-3.2647200000	0.4467640000
H	-3.6454170000	-3.5758010000	0.8971490000
H	-4.5431030000	-0.1976420000	-1.5751200000
H	-2.1220750000	0.1229320000	-2.0083540000
C	-5.7383680000	-2.0660880000	0.0019270000
H	-6.3404950000	-1.8106440000	-0.8717850000
H	-6.0517200000	-1.4117410000	0.8203680000
H	-5.9658390000	-3.0929470000	0.2917430000
C	-2.9293420000	4.5519800000	0.3970950000
H	-2.4294780000	5.3839510000	-0.1025850000
H	-3.2152410000	4.8722800000	1.3998530000
H	-3.8458690000	4.3376230000	-0.1596240000

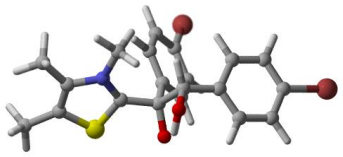
thermodynamic data

Zero-point correction= 0.421625 (Hartree/Particle)
Thermal correction to Energy= 0.447628
Thermal correction to Enthalpy= 0.448572
Thermal correction to Gibbs Free Energy= 0.364070
Sum of electronic and zero-point Energies= -1456.154635
Sum of electronic and thermal Energies= -1456.128632
Sum of electronic and thermal Enthalpies= -1456.127688

Sum of electronic and thermal Free Energies= -1456.212190

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	280.891	98.318	177.850

M062X/6-311+G**/PCM	**Zwitterion2 *p*-Br**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

C	2.9565160000	-2.5910020000	-0.6517870000
C	3.6893680000	-1.7046120000	0.1264520000
C	3.0795000000	-0.8987520000	1.0783190000
C	1.7011940000	-0.9865200000	1.2403090000
C	0.9362650000	-1.8576870000	0.4646400000
C	1.5777120000	-2.6608450000	-0.4752000000
C	-0.5675590000	-1.8851350000	0.6273650000
C	-1.2518330000	-0.9488790000	-0.4403510000
C	-0.6792140000	0.4748520000	-0.3067990000
C	-2.7939170000	-0.8374440000	-0.1875040000
O	-1.1082300000	-1.4984730000	-1.6525770000
S	-3.6881250000	-0.4907230000	-1.5910520000
C	-5.1651500000	-0.3989550000	-0.6999960000
C	-4.9473590000	-0.6749380000	0.6080740000
N	-3.5906560000	-0.9269260000	0.8728870000
C	0.2767540000	0.8834820000	-1.2325650000
C	0.9000020000	2.1218860000	-1.1175270000
C	0.5474810000	2.9544910000	-0.0626030000
C	-0.4156700000	2.5814030000	0.8646700000
C	-1.0253190000	1.3373860000	0.7315290000
C	-6.4711000000	-0.0850230000	-1.3650490000
C	-5.9847940000	-0.7247070000	1.6811630000
Br	5.5789610000	-1.6028100000	-0.1079270000
Br	1.3940370000	4.6524640000	0.1153870000
H	3.4508760000	-3.2159090000	-1.3846230000
H	3.6665010000	-0.2198180000	1.6834390000
H	1.2157190000	-0.3548990000	1.9779110000
H	0.9976980000	-3.3463570000	-1.0798880000
H	-0.7881090000	-1.5765560000	1.6485930000
H	0.5279420000	0.2058670000	-2.0395020000
H	1.6484940000	2.4335980000	-1.8354270000
H	-0.6893140000	3.2466780000	1.6733880000

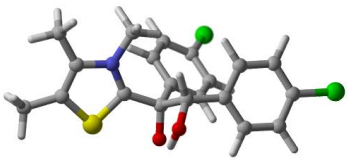
H	-1.7836620000	1.0601320000	1.4562780000
H	-7.1951290000	-0.8823360000	-1.1900590000
H	-6.8841410000	0.8479270000	-0.9766700000
H	-6.3427800000	0.0254700000	-2.4413140000
H	-6.0843450000	-1.7272100000	2.1027120000
H	-5.7604160000	-0.0259640000	2.4895700000
H	-6.9453530000	-0.4438350000	1.2522350000
C	-3.1491520000	-1.3542440000	2.2127000000
H	-4.0148200000	-1.3984440000	2.8631180000
H	-2.4402380000	-0.6398560000	2.6249160000
H	-2.7023180000	-2.3432310000	2.1328350000
O	-1.1175250000	-3.1674890000	0.4153840000
H	-1.2632410000	-3.1839570000	-0.5495220000

thermodynamic data

Zero-point correction= 0.348170 (Hartree/Particle)
Thermal correction to Energy= 0.373448
Thermal correction to Enthalpy= 0.374392
Thermal correction to Gibbs Free Energy= 0.288921
Sum of electronic and zero-point Energies= -6524.779010
Sum of electronic and thermal Energies= -6524.753732
Sum of electronic and thermal Enthalpies= -6524.752788
Sum of electronic and thermal Free Energies= -6524.838259

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.342	94.809	179.890

M062X/6-311+G**/PCM	**Zwitterion2 *p*-Cl**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

C	3.4547040000	-2.3560680000	-0.6763170000
C	4.0851710000	-1.6879010000	0.3647080000
C	3.3600430000	-1.0747070000	1.3778550000
C	1.9720090000	-1.1218850000	1.3268520000
C	1.3102290000	-1.7665930000	0.2816870000
C	2.0644270000	-2.3944640000	-0.7075830000
C	-0.1965040000	-1.7369630000	0.2037610000
C	-0.7537020000	-0.4838420000	-0.6622560000
C	0.0095140000	0.8375330000	-0.4627270000

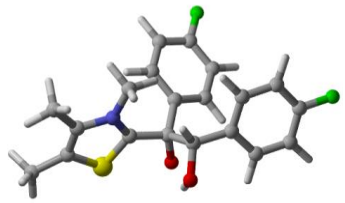
C	-2.2290910000	-0.3336740000	-0.2253800000
O	-0.7528990000	-0.8682680000	-1.9542150000
S	-3.3905210000	-0.5182640000	-1.4452070000
C	-4.6864770000	-0.3235640000	-0.3135290000
C	-4.2002900000	-0.1407770000	0.9387150000
N	-2.8002850000	-0.1484910000	0.9593060000
C	1.2690730000	0.9444040000	-1.0666240000
C	2.0210240000	2.1048840000	-0.9761510000
C	1.4973540000	3.1957220000	-0.2899920000
C	0.2365320000	3.1453620000	0.2754910000
C	-0.5007830000	1.9643240000	0.1786590000
C	-6.1201410000	-0.3585570000	-0.7460250000
C	-4.9758920000	0.0613350000	2.1973980000
Cl	5.8353400000	-1.6312140000	0.4101090000
Cl	2.4413660000	4.6644650000	-0.1657770000
H	4.0412660000	-2.8377540000	-1.4485870000
H	3.8717300000	-0.5706710000	2.1880900000
H	1.4012320000	-0.6369480000	2.1132120000
H	1.5595590000	-2.9119900000	-1.5140500000
H	-0.5919690000	-1.7256800000	1.2208050000
H	1.6546050000	0.1037750000	-1.6284470000
H	2.9977700000	2.1702530000	-1.4394130000
H	-0.1763860000	4.0123690000	0.7753030000
H	-1.4995520000	1.9701490000	0.5971060000
H	-6.7143260000	-0.9605220000	-0.0575280000
H	-6.5392710000	0.6492780000	-0.7737150000
H	-6.2159480000	-0.7924770000	-1.7409380000
H	-4.6797340000	-0.6542150000	2.9669480000
H	-4.8351560000	1.0696420000	2.5939040000
H	-6.0363540000	-0.0742150000	1.9932210000
C	-2.0802960000	0.0281570000	2.2297160000
H	-2.4918990000	0.8946610000	2.7449130000
H	-1.0279030000	0.2010030000	2.0341370000
H	-2.2093560000	-0.8629680000	2.8436350000
O	-0.7169940000	-2.8569220000	-0.4613890000
H	-0.8242790000	-2.4921540000	-1.3787750000

thermodynamic data

Zero-point correction= 0.348806 (Hartree/Particle)
Thermal correction to Energy= 0.373508
Thermal correction to Enthalpy= 0.374452
Thermal correction to Gibbs Free Energy= 0.291117
Sum of electronic and zero-point Energies= -2296.837778
Sum of electronic and thermal Energies= -2296.813076
Sum of electronic and thermal Enthalpies= -2296.812132
Sum of electronic and thermal Free Energies= -2296.895467

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.380	93.679	175.394

M062X/6-311+G**/PCM	**Zwitterion2 *p*-F**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

C	3.9221190000	-2.1025990000	-0.5626350000
C	4.4972430000	-1.3801080000	0.4666680000
C	3.7486250000	-0.7591680000	1.4504810000
C	2.3639690000	-0.8595250000	1.3804680000
C	1.7426490000	-1.5620880000	0.3472150000
C	2.5338790000	-2.1919770000	-0.6117830000
C	0.2362040000	-1.5919070000	0.2496330000
C	-0.3606140000	-0.3805810000	-0.6457290000
C	0.3430610000	0.9768640000	-0.4654480000
C	-1.8457770000	-0.2771590000	-0.2277680000
O	-0.3321110000	-0.7912500000	-1.9304700000
S	-2.9865890000	-0.5180030000	-1.4575020000
C	-4.3011880000	-0.3350570000	-0.3460960000
C	-3.8360050000	-0.1144480000	0.9077920000
N	-2.4371120000	-0.0842580000	0.9459890000
C	1.6091780000	1.1229870000	-1.0490410000
C	2.3050760000	2.3199350000	-0.9830450000
C	1.7098650000	3.3940250000	-0.3407420000
C	0.4493570000	3.3139540000	0.2093850000
C	-0.2297160000	2.0965220000	0.1356220000
C	-5.7302720000	-0.4202530000	-0.7881500000
C	-4.6365550000	0.0939930000	2.1496080000
F	5.8449790000	-1.2877020000	0.5229120000
F	2.3806640000	4.5650850000	-0.2745550000
H	4.5515680000	-2.5819650000	-1.3021360000
H	4.2445980000	-0.2167500000	2.2457470000
H	1.7627800000	-0.3714750000	2.1415410000
H	2.0589440000	-2.7533700000	-1.4067240000
H	-0.1721240000	-1.5762910000	1.2616940000
H	2.0439480000	0.2835800000	-1.5754650000
H	3.2860350000	2.4325960000	-1.4284080000
H	0.0014120000	4.1841820000	0.6721040000
H	-1.2346510000	2.0662690000	0.5376300000
H	-6.2774080000	-1.1438200000	-0.1819160000
H	-6.2203550000	0.5506130000	-0.6923680000
H	-5.7974920000	-0.7326580000	-1.8296210000
H	-4.3300450000	-0.5918780000	2.9417160000
H	-4.5338170000	1.1161950000	2.5217200000

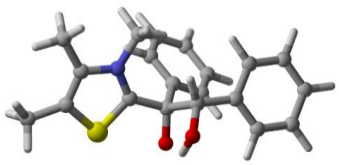
H	-5.6888070000	-0.0818100000	1.9325590000
O	-0.2327210000	-2.7450020000	-0.3983960000
H	-0.3450980000	-2.4005270000	-1.3236170000
C	-1.7377510000	0.1385410000	2.2205410000
H	-2.1904530000	0.9929360000	2.7210240000
H	-0.6918310000	0.3533660000	2.0315700000
H	-1.8342070000	-0.7494700000	2.8449160000

thermodynamic data

Zero-point correction= 0.351764 (Hartree/Particle)
Thermal correction to Energy= 0.375624
Thermal correction to Enthalpy= 0.376568
Thermal correction to Gibbs Free Energy= 0.296636
Sum of electronic and zero-point Energies= -1576.116891
Sum of electronic and thermal Energies= -1576.093032
Sum of electronic and thermal Enthalpies= -1576.092088
Sum of electronic and thermal Free Energies= -1576.172019

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	235.707	91.831	168.230

M062X/6-311+G**/PCM	**Zwitterion2 *p*-H**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

C	4.3666290000	-1.8200760000	-0.3518000000
C	4.9300310000	-1.0289180000	0.6463800000
C	4.1034640000	-0.3960790000	1.5718930000
C	2.7233160000	-0.5437640000	1.4852780000
C	2.1504150000	-1.3167450000	0.4745950000
C	2.9845960000	-1.9675160000	-0.4333620000
C	0.6486610000	-1.4034890000	0.3490220000
C	0.0253580000	-0.2674230000	-0.6283880000
C	0.6725310000	1.1269840000	-0.5272030000
C	-1.4673340000	-0.1990920000	-0.2310180000
O	0.0830640000	-0.7574000000	-1.8848530000
S	-2.5851460000	-0.5837710000	-1.4451900000
C	-3.9179300000	-0.3813960000	-0.3549140000
C	-3.4737510000	-0.0445400000	0.8810050000
N	-2.0759710000	0.0515320000	0.9215650000

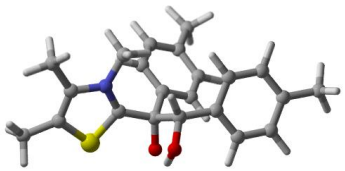
C	1.9551220000	1.2859740000	-1.0695780000
C	2.5878550000	2.5204460000	-1.0676170000
C	1.9448240000	3.6416030000	-0.5428250000
C	0.6575380000	3.5100940000	-0.0422540000
C	0.0277440000	2.2641660000	-0.0398150000
C	-5.3299240000	-0.5578690000	-0.8198500000
C	-4.2774980000	0.2330160000	2.1077840000
H	5.0054530000	-2.3247260000	-1.0676840000
H	6.0059930000	-0.9147390000	0.7093260000
H	4.5341640000	0.2110490000	2.3597880000
H	2.0846950000	-0.0418380000	2.2068820000
H	2.5447870000	-2.5843630000	-1.2077880000
H	0.2186860000	-1.3422050000	1.3506190000
H	2.4499800000	0.4284410000	-1.5061470000
H	3.5838670000	2.6121990000	-1.4860630000
H	2.4374100000	4.6068390000	-0.5441740000
H	0.1288500000	4.3755140000	0.3401330000
H	-0.9898600000	2.2164060000	0.3288320000
H	-5.9711450000	-0.8616290000	0.0067720000
H	-5.7194690000	0.3746210000	-1.2336840000
H	-5.3920470000	-1.3235790000	-1.5933720000
H	-3.9430850000	-0.3754270000	2.9502340000
H	-4.2071170000	1.2851270000	2.3943450000
H	-5.3247780000	0.0080610000	1.9181200000
C	-1.3922070000	0.4053720000	2.1742260000
H	-1.8691740000	1.2885550000	2.5962210000
H	-0.3519300000	0.6315590000	1.9686450000
H	-1.4678530000	-0.4263630000	2.8744180000
O	0.2292440000	-2.6067600000	-0.2398540000
H	0.1215840000	-2.3150810000	-1.1850360000

thermodynamic data

Zero-point correction= 0.368536 (Hartree/Particle)
Thermal correction to Energy= 0.390555
Thermal correction to Enthalpy= 0.391499
Thermal correction to Gibbs Free Energy= 0.317082
Sum of electronic and zero-point Energies= -1377.614606
Sum of electronic and thermal Energies= -1377.592586
Sum of electronic and thermal Enthalpies= -1377.591642
Sum of electronic and thermal Free Energies= -1377.666059

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	245.077	85.821	156.623

M062X/6-311+G**/PCM	**Zwitterion2 *p*-Me**

xyz-matrix

51
XYZ file generated by gabedit : coordinates in Angstrom

C	3.8937770000	-2.1179410000	-0.5868560000
C	4.5251010000	-1.4500730000	0.4649430000
C	3.7219110000	-0.8618370000	1.4444980000
C	2.3353940000	-0.9333000000	1.3683170000
C	1.7097640000	-1.5894130000	0.3084420000
C	2.5062850000	-2.1928930000	-0.6624510000
C	0.2044390000	-1.6036380000	0.2024300000
C	-0.3915180000	-0.3744860000	-0.6705060000
C	0.3127120000	0.9801960000	-0.4765680000
C	-1.8709680000	-0.2770460000	-0.2320470000
O	-0.3815400000	-0.7672100000	-1.9627680000
S	-3.0309460000	-0.5195150000	-1.4435230000
C	-4.3300420000	-0.3496980000	-0.3061830000
C	-3.8442280000	-0.1309110000	0.9403340000
N	-2.4422890000	-0.0931870000	0.9517480000
C	1.5907700000	1.1356790000	-1.0333030000
C	2.2686570000	2.3404510000	-0.9511730000
C	1.6961290000	3.4566500000	-0.3277800000
C	0.4123950000	3.3186320000	0.1856780000
C	-0.2704180000	2.1018970000	0.1076490000
C	-5.7565840000	-0.4344980000	-0.7510170000
C	-4.6043570000	0.0741270000	2.2088090000
C	6.0283400000	-1.4017770000	0.5621600000
C	2.4500020000	4.7578080000	-0.2412610000
H	4.4980590000	-2.5862930000	-1.3576950000
H	4.1891150000	-0.3428860000	2.2756280000
H	1.7338740000	-0.4609470000	2.1402480000
H	2.0333160000	-2.7158020000	-1.4853770000
H	-0.2071120000	-1.6023860000	1.2136260000
H	2.0454480000	0.2976940000	-1.5458890000
H	3.2596750000	2.4259590000	-1.3871540000
H	-0.0760700000	4.1708650000	0.6468700000
H	-1.2823820000	2.0707910000	0.4941640000
H	-6.4019730000	-0.7184090000	0.0791560000
H	-6.0983750000	0.5272050000	-1.1392610000
H	-5.8736620000	-1.1788290000	-1.5391480000
H	-4.2641380000	-0.6086760000	2.9896150000
H	-4.4919930000	1.0973650000	2.5750180000
H	-5.6631710000	-0.1053090000	2.0365380000

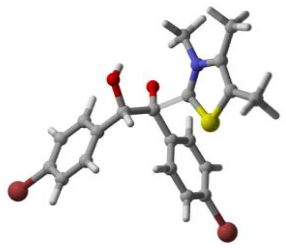
H	6.4872880000	-1.4221510000	-0.4275940000
H	6.3607740000	-0.5010400000	1.0805460000
H	6.4067640000	-2.2634690000	1.1196150000
H	3.3579510000	4.6410980000	0.3558750000
H	2.7550990000	5.0980500000	-1.2336050000
H	1.8401670000	5.5376740000	0.2160200000
O	-0.2726430000	-2.7434690000	-0.4660280000
H	-0.3874400000	-2.3777250000	-1.3834730000
C	-1.7155700000	0.1327890000	2.2103790000
H	-2.1566560000	0.9886980000	2.7184670000
H	-0.6744990000	0.3476260000	1.9958500000
H	-1.7973920000	-0.7534150000	2.8394910000

thermodynamic data

Zero-point correction= 0.422992 (Hartree/Particle)
Thermal correction to Energy= 0.447081
Thermal correction to Enthalpy= 0.448025
Thermal correction to Gibbs Free Energy= 0.368919
Sum of electronic and zero-point Energies= -1456.173564
Sum of electronic and thermal Energies= -1456.149475
Sum of electronic and thermal Enthalpies= -1456.148531
Sum of electronic and thermal Free Energies= -1456.227637

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	280.548	94.051	166.494

M062X/6-311+G**/PCM	**TST5 *p*-Br**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	3.5836300000	-2.0357110000	0.4960000000
C	4.8284240000	-2.0015030000	-0.1625990000
C	3.3256380000	-3.0063360000	1.5668390000
C	4.8592530000	-1.0476590000	-1.1211500000
S	3.3191280000	-0.2274760000	-1.1525850000
C	2.6470690000	-1.1796600000	0.1026640000
C	5.9095400000	-2.9504880000	0.2415370000
C	5.9672570000	-0.6647260000	-2.0499970000

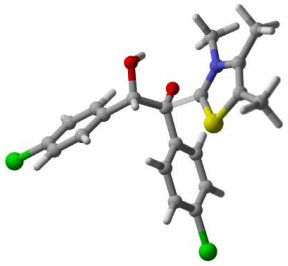
C	0.5781010000	-0.9769010000	0.9187900000
C	0.5181860000	0.5102690000	0.6758980000
O	0.5992400000	-1.4140350000	2.0769350000
C	0.3462250000	1.0577130000	-0.5960900000
C	0.3003940000	2.4352740000	-0.7763660000
C	0.4269710000	3.2609750000	0.3335670000
C	0.5889340000	2.7413070000	1.6117500000
C	0.6295310000	1.3615590000	1.7729880000
C	-0.0464350000	-1.9150460000	-0.1422120000
O	0.2558880000	-3.2435000000	0.2225820000
C	-1.5479410000	-1.6782120000	-0.1974720000
C	-2.1553150000	-1.2496870000	-1.3748740000
C	-3.5296530000	-1.0336340000	-1.4372760000
C	-4.2914470000	-1.2559730000	-0.2996820000
C	-3.7138800000	-1.6902540000	0.8881670000
C	-2.3409550000	-1.8982390000	0.9303210000
H	4.1620950000	-3.0078440000	2.2640950000
H	2.4185600000	-2.7029530000	2.0808610000
H	3.2025530000	-4.0016820000	1.1387880000
H	5.5507040000	-3.9817190000	0.2258460000
H	6.2698940000	-2.7328700000	1.2498100000
H	6.7517330000	-2.8749100000	-0.4428680000
H	6.8711710000	-1.2304550000	-1.8273540000
H	5.6895060000	-0.8581110000	-3.0880680000
H	6.2015720000	0.3972360000	-1.9568720000
H	0.2582050000	0.4203370000	-1.4681360000
H	0.1700540000	2.8579830000	-1.7643410000
Br	0.3782750000	5.1481760000	0.0952850000
H	0.6785010000	3.4013330000	2.4650860000
H	0.7513020000	0.9301570000	2.7590050000
H	0.3813850000	-1.7371550000	-1.1283750000
H	0.3459530000	-3.2300100000	1.1880720000
H	-1.5572030000	-1.0856470000	-2.2653840000
H	-3.9950810000	-0.7025020000	-2.3567630000
Br	-6.1718760000	-0.9633040000	-0.3646650000
H	-4.3249110000	-1.8619840000	1.7650700000
H	-1.8818210000	-2.2325510000	1.8542530000

thermodynamic data

Zero-point correction= 0.346214 (Hartree/Particle)
Thermal correction to Energy= 0.371793
Thermal correction to Enthalpy= 0.372737
Thermal correction to Gibbs Free Energy= 0.285723
Sum of electronic and zero-point Energies= -6524.767855
Sum of electronic and thermal Energies= -6524.742276
Sum of electronic and thermal Enthalpies= -6524.741332
Sum of electronic and thermal Free Energies= -6524.828347

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.304	94.711	183.138

M062X/6-311+G**/PCM	**TST5 *p*-Cl**



xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	3.2139920000	-1.3942220000	0.5116910000
C	4.4529400000	-1.2411630000	-0.1413200000
C	3.0388900000	-2.3993920000	1.5672330000
C	4.4043790000	-0.2696250000	-1.0812820000
S	2.7997320000	0.4168310000	-1.1033370000
C	2.2092930000	-0.6133070000	0.1308940000
C	5.6099190000	-2.1016730000	0.2503770000
C	5.4780600000	0.2279940000	-1.9958770000
C	0.1330540000	-0.6069190000	0.9184250000
C	-0.0696540000	0.8691320000	0.6827940000
O	0.1780080000	-1.0472810000	2.0760560000
C	-0.2917280000	1.4028800000	-0.5873710000
C	-0.4734280000	2.7696980000	-0.7611630000
C	-0.4330850000	3.5986200000	0.3523660000
C	-0.2240310000	3.0915750000	1.6281870000
C	-0.0459790000	1.7225720000	1.7839160000
C	-0.3934720000	-1.5901580000	-0.1546270000
O	0.0049140000	-2.8915660000	0.2178190000
C	-1.9069960000	-1.4769940000	-0.2539090000
C	-2.5111900000	-1.1993130000	-1.4774500000
C	-3.8955500000	-1.1096360000	-1.5908750000
C	-4.6709510000	-1.3028960000	-0.4577910000
C	-4.0967730000	-1.5854080000	0.7758560000
C	-2.7135380000	-1.6703490000	0.8695880000
H	3.8551730000	-2.3188680000	2.2837190000
H	2.0934500000	-2.2007580000	2.0627120000
H	3.0324840000	-3.3975640000	1.1285770000
H	5.3453650000	-3.1600840000	0.2020540000
H	5.9388850000	-1.8811370000	1.2686880000
H	6.4491890000	-1.9320230000	-0.4205460000
H	6.4099630000	-0.3103560000	-1.8279880000
H	5.1909620000	0.0957460000	-3.0407560000
H	5.6665230000	1.2904510000	-1.8306050000
H	-0.3183120000	0.7637560000	-1.4621840000
H	-0.6426810000	3.1866770000	-1.7457620000
Cl	-0.6556140000	5.3198760000	0.1419930000

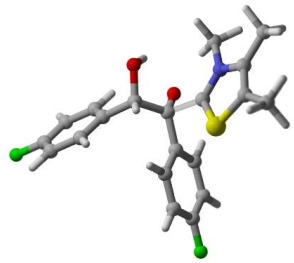
H	-0.2037960000	3.7565700000	2.4822970000
H	0.1140300000	1.3004210000	2.7684410000
H	0.0431310000	-1.3793510000	-1.1307090000
H	0.0683370000	-2.8708820000	1.1854600000
H	-1.8997360000	-1.0566920000	-2.3626040000
H	-4.3635180000	-0.8983960000	-2.5438900000
Cl	-6.4124740000	-1.1939890000	-0.5843260000
H	-4.7231900000	-1.7343470000	1.6463020000
H	-2.2567580000	-1.8860380000	1.8291910000

thermodynamic data

Zero-point correction= 0.346820 (Hartree/Particle)
Thermal correction to Energy= 0.372214
Thermal correction to Enthalpy= 0.373158
Thermal correction to Gibbs Free Energy= 0.285393
Sum of electronic and zero-point Energies= -2296.823892
Sum of electronic and thermal Energies= -2296.798497
Sum of electronic and thermal Enthalpies= -2296.797553
Sum of electronic and thermal Free Energies= -2296.885319

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.568	94.027	184.719

M062X/6-311+G**/PCM	**TST5 *p*-F**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	2.9137160000	-1.1761490000	0.5151960000
C	4.1665150000	-0.9641580000	-0.0930960000
C	2.7402950000	-2.2158540000	1.5371240000
C	4.1141040000	0.0285840000	-1.0102960000
S	2.4890240000	0.6627220000	-1.0663310000
C	1.8957770000	-0.4189170000	0.1223790000
C	5.3397370000	-1.7938840000	0.3161260000
C	5.1985430000	0.5860500000	-1.8763200000
C	-0.1774960000	-0.4583910000	0.8672360000
C	-0.4040220000	1.0194100000	0.6666320000
O	-0.1448470000	-0.9274360000	2.0161980000

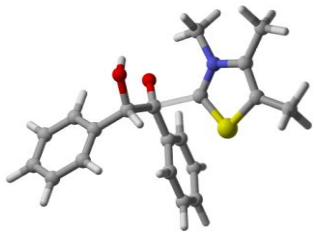
C	-0.6212090000	1.5799350000	-0.5934290000
C	-0.8216010000	2.9478270000	-0.7376120000
C	-0.8030160000	3.7358390000	0.3995810000
C	-0.6006900000	3.2160590000	1.6655670000
C	-0.4037250000	1.8459720000	1.7891770000
C	-0.6834690000	-1.4207600000	-0.2349510000
O	-0.2750810000	-2.7270930000	0.1115850000
C	-2.1963500000	-1.3193190000	-0.3525160000
C	-2.7860260000	-1.0321270000	-1.5816460000
C	-4.1695680000	-0.9487870000	-1.7132970000
C	-4.9440260000	-1.1601770000	-0.5891390000
C	-4.3988080000	-1.4530770000	0.6492370000
C	-3.0159500000	-1.5303300000	0.7591430000
H	3.5257260000	-2.1223500000	2.2859170000
H	1.7699360000	-2.0674690000	2.0009810000
H	2.7914310000	-3.2009060000	1.0723540000
H	5.1169450000	-2.8592060000	0.2270660000
H	5.6227370000	-1.5924500000	1.3520800000
H	6.1963280000	-1.5725660000	-0.3168520000
H	5.3534690000	1.6467050000	-1.6697280000
H	6.1397680000	0.0665960000	-1.7010020000
H	4.9441270000	0.4830320000	-2.9328730000
H	-0.6298780000	0.9593330000	-1.4817600000
H	-0.9890530000	3.4009950000	-1.7065730000
F	-0.9952070000	5.0647650000	0.2677440000
H	-0.6014210000	3.8736760000	2.5258060000
H	-0.2460170000	1.4004720000	2.7636910000
H	-0.2364510000	-1.1828890000	-1.2002860000
H	-0.2283890000	-2.7281270000	1.0804470000
H	-2.1620900000	-0.8739720000	-2.4552880000
H	-4.6417830000	-0.7295240000	-2.6625960000
F	-6.2873480000	-1.0796210000	-0.7021240000
H	-5.0493850000	-1.6125450000	1.5000520000
H	-2.5680660000	-1.7527260000	1.7212480000

thermodynamic data

Zero-point correction= 0.350685 (Hartree/Particle)
Thermal correction to Energy= 0.374513
Thermal correction to Enthalpy= 0.375457
Thermal correction to Gibbs Free Energy= 0.296246
Sum of electronic and zero-point Energies= -1576.102896
Sum of electronic and thermal Energies= -1576.079069
Sum of electronic and thermal Enthalpies= -1576.078125
Sum of electronic and thermal Free Energies= -1576.157336

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	235.010	91.502	166.714

M062X/6-311+G**/PCM	**TST5 *p*-H**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	2.5682820000	-1.0174690000	0.5178650000
C	3.8351020000	-0.7822440000	-0.0516010000
C	2.3696480000	-2.1024510000	1.4868660000
C	3.8052240000	0.2501780000	-0.9249220000
S	2.1835130000	0.8918760000	-0.9900530000
C	1.5614690000	-0.2403250000	0.1360010000
C	4.9978080000	-1.6310550000	0.3485790000
C	4.9103620000	0.8414480000	-1.7409920000
C	-0.5176970000	-0.3190760000	0.8154520000
C	-0.7404510000	1.1693970000	0.6924750000
O	-0.5197800000	-0.8538340000	1.9375050000
C	-0.9245920000	1.7985360000	-0.5403260000
C	-1.1199300000	3.1743380000	-0.6056820000
C	-1.1353810000	3.9339390000	0.5614550000
C	-0.9608220000	3.3097740000	1.7941640000
C	-0.7676550000	1.9337220000	1.8580880000
C	-0.9941900000	-1.2172910000	-0.3529020000
O	-0.5863880000	-2.5406210000	-0.0721650000
C	-2.5048730000	-1.1187940000	-0.5001350000
C	-3.0686420000	-0.7499080000	-1.7199660000
C	-4.4515970000	-0.6747380000	-1.8704260000
C	-5.2844520000	-0.9706780000	-0.7963500000
C	-4.7286310000	-1.3437800000	0.4261030000
C	-3.3480020000	-1.4169460000	0.5733440000
H	3.1413130000	-2.0479750000	2.2536110000
H	1.3909690000	-1.9699800000	1.9378990000
H	2.4259370000	-3.0650760000	0.9776750000
H	4.7749750000	-2.6913850000	0.2129620000
H	5.2600270000	-1.4711000000	1.3971530000
H	5.8676620000	-1.3869650000	-0.2574420000
H	5.8446540000	0.3072140000	-1.5730820000
H	4.6764320000	0.7922180000	-2.8061270000
H	5.0679310000	1.8897140000	-1.4800180000
H	-0.9109220000	1.2252920000	-1.4602170000
H	-1.2605770000	3.6525690000	-1.5679950000
H	-1.2868290000	5.0057790000	0.5104200000
H	-0.9769140000	3.8959000000	2.7057930000

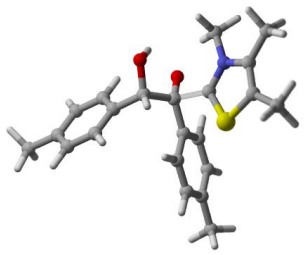
H	-0.6331550000	1.4329030000	2.8093100000
H	-0.5258490000	-0.9221830000	-1.2920200000
H	-0.5674030000	-2.5966560000	0.8960990000
H	-2.4227110000	-0.5232100000	-2.5627190000
H	-4.8757610000	-0.3884700000	-2.8258440000
H	-6.3607060000	-0.9138440000	-0.9102100000
H	-5.3729390000	-1.5772500000	1.2658930000
H	-2.9171690000	-1.7038590000	1.5265830000

thermodynamic data

Zero-point correction= 0.366799 (Hartree/Particle)
Thermal correction to Energy= 0.389356
Thermal correction to Enthalpy= 0.390300
Thermal correction to Gibbs Free Energy= 0.312615
Sum of electronic and zero-point Energies= -1377.601384
Sum of electronic and thermal Energies= -1377.578827
Sum of electronic and thermal Enthalpies= -1377.577883
Sum of electronic and thermal Free Energies= -1377.655568

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	244.324	86.101	163.501

M062X/6-311+G**/PCM	**TST5 *p*-Me**

xyz-matrix

51
XYZ file generated by gabedit : coordinates in Angstrom

N	2.9206640000	-1.2008010000	0.5079200000
C	4.1723840000	-0.9843770000	-0.1011180000
C	2.7499420000	-2.2465120000	1.5243990000
C	4.1172640000	0.0127190000	-1.0133620000
S	2.4919310000	0.6462820000	-1.0648400000
C	1.9023480000	-0.4424220000	0.1191330000
C	5.3472970000	-1.8143450000	0.3027850000
C	5.2002180000	0.5756400000	-1.8778170000
C	-0.1374300000	-0.4771080000	0.8603030000
C	-0.3702440000	1.0012940000	0.6669660000
O	-0.1049260000	-0.9531490000	2.0106290000
C	-0.6046730000	1.5683720000	-0.5865000000

C	-0.8070830000	2.9380130000	-0.7146730000
C	-0.7826670000	3.7775990000	0.4012360000
C	-0.5611160000	3.2003320000	1.6538220000
C	-0.3591110000	1.8315920000	1.7861840000
C	-0.6612700000	-1.4341870000	-0.2398860000
O	-0.2500580000	-2.7434900000	0.1009060000
C	-2.1741400000	-1.3331580000	-0.3455000000
C	-2.7770280000	-1.0533580000	-1.5683480000
C	-4.1640320000	-0.9806290000	-1.6813430000
C	-4.9837820000	-1.1846060000	-0.5728630000
C	-4.3738030000	-1.4719420000	0.6528110000
C	-2.9919160000	-1.5442780000	0.7680750000
H	3.5392670000	-2.1584410000	2.2697250000
H	1.7816730000	-2.0990160000	1.9928490000
H	2.7980050000	-3.2285100000	1.0528990000
H	5.1257390000	-2.8795890000	0.2098160000
H	5.6319840000	-1.6167610000	1.3390200000
H	6.2024270000	-1.5893320000	-0.3308740000
H	6.1423010000	0.0565090000	-1.7061680000
H	4.9447730000	0.4776330000	-2.9346140000
H	5.3541430000	1.6354680000	-1.6662140000
H	-0.6295850000	0.9493740000	-1.4764570000
H	-0.9892900000	3.3620840000	-1.6968990000
H	-0.5511180000	3.8321450000	2.5363930000
H	-0.1928910000	1.3880250000	2.7607930000
H	-0.2224720000	-1.1961190000	-1.2091930000
H	-0.2034760000	-2.7434280000	1.0699480000
H	-2.1597080000	-0.8957810000	-2.4478360000
H	-4.6130650000	-0.7679850000	-2.6461750000
H	-4.9939900000	-1.6414940000	1.5275840000
H	-2.5396600000	-1.7648810000	1.7291420000
C	-6.4833840000	-1.0837210000	-0.6787270000
H	-6.9709100000	-1.8916280000	-0.1296370000
H	-6.8086340000	-1.1274390000	-1.7188440000
H	-6.8370980000	-0.1394420000	-0.2557760000
C	-0.9679390000	5.2653400000	0.2556740000
H	-0.0019980000	5.7596350000	0.1182330000
H	-1.4337710000	5.6925860000	1.1448700000
H	-1.5873400000	5.5030530000	-0.6103720000

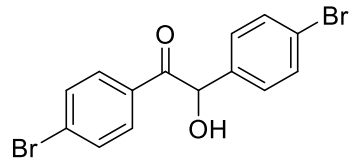
thermodynamic data

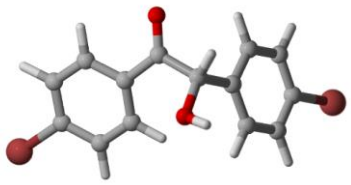
Zero-point correction= 0.421706 (Hartree/Particle)
Thermal correction to Energy= 0.447420
Thermal correction to Enthalpy= 0.448364
Thermal correction to Gibbs Free Energy= 0.365275
Sum of electronic and zero-point Energies= -1456.160396
Sum of electronic and thermal Energies= -1456.134682
Sum of electronic and thermal Enthalpies= -1456.133738
Sum of electronic and thermal Free Energies= -1456.216826

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	280.760	97.753	174.875

M062X/6-311+G**/PCM	***p*-Br-Benzoin**





xyz-matrix

28
XYZ file generated by gabedit : coordinates in Angstrom

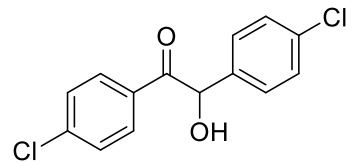
C	-2.5585070000	-0.6175260000	0.7169200000
C	-3.6669910000	-0.4509110000	-0.1032030000
C	-3.7605240000	0.6067920000	-1.0020520000
C	-2.7103250000	1.5092840000	-1.0780820000
C	-1.5889410000	1.3708500000	-0.2558230000
C	-1.5226430000	0.3058470000	0.6447310000
C	-0.4853890000	2.3641850000	-0.4144860000
C	0.5940940000	2.5051160000	0.6662880000
O	-0.4053430000	3.0573920000	-1.4044330000
C	1.6847690000	1.4632530000	0.4383820000
O	-0.0104860000	2.4179890000	1.9376450000
C	2.3899260000	1.4577480000	-0.7662090000
C	3.3937320000	0.5252010000	-0.9968370000
C	3.6869080000	-0.4046290000	-0.0061530000
C	3.0034070000	-0.4147880000	1.2008430000
C	1.9986950000	0.5245180000	1.4160170000
Br	-5.0942170000	-1.6976110000	0.0128060000
Br	5.0586260000	-1.6882690000	-0.3061260000
H	-2.5049380000	-1.4509830000	1.4048950000
H	-4.6350450000	0.7195480000	-1.6295230000
H	-2.7553630000	2.3370060000	-1.7753210000
H	-0.6662190000	0.1849010000	1.2929970000
H	1.0222690000	3.4989780000	0.5065220000
H	0.5581260000	2.8516150000	2.5818910000
H	2.1575190000	2.1900620000	-1.5324230000
H	3.9406180000	0.5245710000	-1.9307480000
H	3.2452770000	-1.1432800000	1.9637710000
H	1.4608080000	0.5206960000	2.3564140000

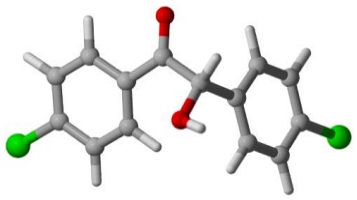
thermodynamic data

Zero-point correction= 0.204786 (Hartree/Particle)
Thermal correction to Energy= 0.220933
Thermal correction to Enthalpy= 0.221878
Thermal correction to Gibbs Free Energy= 0.156975
Sum of electronic and zero-point Energies= -5838.004816
Sum of electronic and thermal Energies= -5837.988668
Sum of electronic and thermal Enthalpies= -5837.987724
Sum of electronic and thermal Free Energies= -5838.052626

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.638	60.150	136.600

M062X/6-311+G**/PCM	***p*-Cl-Benzoin**





xyz-matrix

28
XYZ file generated by gabedit : coordinates in Angstrom

C	-2.5139540000	-1.0494920000	0.7686200000
C	-3.6123140000	-0.9250940000	-0.0715050000
C	-3.7246360000	0.1222900000	-0.9798430000
C	-2.7034580000	1.0567320000	-1.0470210000
C	-1.5885570000	0.9576450000	-0.2092860000
C	-1.5044340000	-0.0976200000	0.7018980000
C	-0.5101220000	1.9781450000	-0.3654550000
C	0.6126980000	2.0884880000	0.6744190000
O	-0.4773000000	2.7116570000	-1.3291550000
C	1.6742850000	1.0310300000	0.3891210000
O	0.0582690000	1.9955970000	1.9688140000
C	2.3025400000	1.0104090000	-0.8571960000
C	3.2748450000	0.0620890000	-1.1456640000
C	3.6174830000	-0.8666610000	-0.1708180000
C	3.0129590000	-0.8614330000	1.0770540000
C	2.0366620000	0.0925130000	1.3502550000
Cl	-4.8845550000	-2.1152550000	0.0110320000
Cl	4.8390930000	-2.0657190000	-0.5276090000
H	-2.4508430000	-1.8759880000	1.4643920000
H	-4.5933650000	0.1964910000	-1.6211670000
H	-2.7625080000	1.8767050000	-1.7521810000
H	-0.6546210000	-0.1869970000	1.3636870000

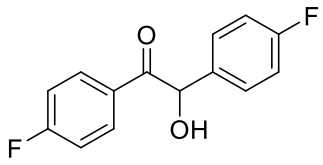
H	1.0503920000	3.0772570000	0.5101010000
H	0.6421570000	2.4425920000	2.5896100000
H	2.0328860000	1.7419940000	-1.6117540000
H	3.7621920000	0.0432320000	-2.1120290000
H	3.2971640000	-1.5913640000	1.8244790000
H	1.5576650000	0.1003530000	2.3219510000

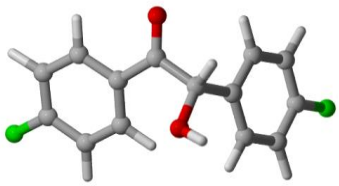
thermodynamic data

Zero-point correction= 0.205846 (Hartree/Particle)
Thermal correction to Energy= 0.221530
Thermal correction to Enthalpy= 0.222474
Thermal correction to Gibbs Free Energy= 0.159051
Sum of electronic and zero-point Energies= -1610.060555
Sum of electronic and thermal Energies= -1610.044871
Sum of electronic and thermal Enthalpies= -1610.043927
Sum of electronic and thermal Free Energies= -1610.107350

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.012	59.318	133.485

M062X/6-311+G**/PCM		***p*-F-Benzoin**





xyz-matrix

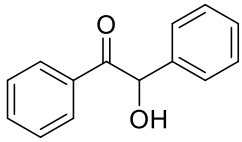
28
XYZ file generated by gabedit : coordinates in Angstrom

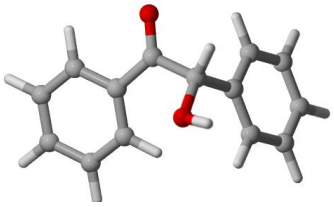
C	-2.5669630000	-1.4471580000	0.6166750000
C	-3.6753470000	-1.1763580000	-0.1661100000
C	-3.7955680000	-0.0272000000	-0.9309050000
C	-2.7499690000	0.8816160000	-0.9079130000
C	-1.6159770000	0.6483180000	-0.1227630000
C	-1.5338850000	-0.5194340000	0.6415110000
C	-0.5225580000	1.6606320000	-0.1768320000
C	0.6130460000	1.6447460000	0.8540920000
O	-0.4858370000	2.4978760000	-1.0529060000
C	1.6912070000	0.6647370000	0.4034400000
O	0.0864240000	1.3568360000	2.1308010000
C	2.3325550000	0.8736990000	-0.8194990000
C	3.3271750000	0.0092870000	-1.2570450000
C	3.6678160000	-1.0612470000	-0.4479490000
C	3.0578770000	-1.2971450000	0.7688120000
C	2.0593290000	-0.4230500000	1.1906550000

F	-4.6814590000	-2.0675420000	-0.1841590000
F	4.6360280000	-1.9041920000	-0.8634380000
H	-2.5249280000	-2.3622600000	1.1931020000
H	-4.6866970000	0.1374970000	-1.5228780000
H	-2.8022260000	1.7876910000	-1.4987200000
H	-0.6670300000	-0.7117930000	1.2576510000
H	1.0274100000	2.6568180000	0.8253690000
H	0.7051910000	1.6707090000	2.7982040000
H	2.0543070000	1.7222330000	-1.4354570000
H	3.8344490000	0.1566100000	-2.2020470000
H	3.3593260000	-2.1461020000	1.3694370000
H	1.5719510000	-0.5921510000	2.1435310000

thermodynamic data

M062X/6-311+G**/PCM	***p*-H-Benzoin**





xyz-matrix

28
XYZ file generated by gabedit : coordinates in Angstrom

C	2.4864920000	1.8810010000	0.2032520000
C	3.6513920000	1.5032150000	-0.4578150000
C	3.8063560000	0.1930100000	-0.9081560000
C	2.7944090000	-0.7329080000	-0.6995680000
C	1.6245680000	-0.3616410000	-0.0282480000
C	1.4756860000	0.9517950000	0.4254430000
C	0.5626170000	-1.3983080000	0.1369450000
C	-0.6293800000	-1.1588160000	1.0726730000
O	0.5953770000	-2.4352990000	-0.4905530000
C	-1.6868970000	-0.3372250000	0.3421000000
O	-0.1759270000	-0.5676650000	2.2715690000
C	-2.2395040000	-0.8401210000	-0.8379890000
C	-3.2117980000	-0.1198540000	-1.5212210000
C	-3.6450260000	1.1099040000	-1.0296090000
C	-3.0998810000	1.6111920000	0.1475230000
C	-2.1212940000	0.8920360000	0.8311320000
H	2.3652200000	2.8997890000	0.5506340000
H	4.4391770000	2.2292070000	-0.6220110000
H	4.7130800000	-0.1017880000	-1.4224010000
H	2.8961640000	-1.7528600000	-1.0500700000
H	0.5786960000	1.2503860000	0.9496140000

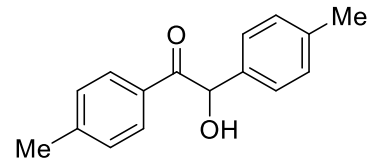
H	-1.0363050000	-2.1562920000	1.2646090000
H	-0.8397460000	-0.7104000000	2.9540840000
H	-1.9063050000	-1.7999330000	-1.2196770000
H	-3.6335740000	-0.5192850000	-2.4360280000
H	-4.4050310000	1.6708740000	-1.5603290000
H	-3.4346370000	2.5653130000	0.5376500000
H	-1.6987860000	1.2890290000	1.7470230000

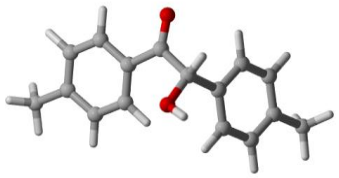
thermodynamic data

Zero-point correction= 0.225776 (Hartree/Particle)
Thermal correction to Energy= 0.239023
Thermal correction to Enthalpy= 0.239967
Thermal correction to Gibbs Free Energy= 0.184188
Sum of electronic and zero-point Energies= -690.839355
Sum of electronic and thermal Energies= -690.826108
Sum of electronic and thermal Enthalpies= -690.825164
Sum of electronic and thermal Free Energies= -690.880943

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	149.989	51.600	117.398

M062X/6-311+G**/PCM	***p*-Me-Benzoin**





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	2.5908880000	1.3994820000	0.6091220000
C	3.7356890000	1.1722220000	-0.1548940000
C	3.8022100000	0.0043660000	-0.9252120000
C	2.7565420000	-0.9024190000	-0.9289300000
C	1.6164380000	-0.6749360000	-0.1488030000
C	1.5429550000	0.4851950000	0.6243820000
C	0.5186710000	-1.6791810000	-0.2153910000
C	-0.6068680000	-1.6833840000	0.8265550000
O	0.4691240000	-2.4996630000	-1.1084480000
C	-1.6912710000	-0.6964800000	0.4095700000
O	-0.0664270000	-1.4274600000	2.1054430000
C	-2.3577880000	-0.8872280000	-0.8039210000
C	-3.3630460000	-0.0172130000	-1.1998180000
C	-3.7367660000	1.0665580000	-0.3972910000
C	-3.0689620000	1.2461350000	0.8118680000

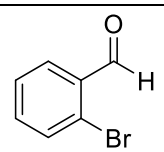
C	-2.0539990000	0.3784530000	1.2135480000
C	4.8834680000	2.1450560000	-0.1500080000
C	-4.8267370000	2.0078870000	-0.8392340000
H	2.5202170000	2.3021930000	1.2060480000
H	4.6853660000	-0.1885080000	-1.5254120000
H	2.8079320000	-1.8014830000	-1.5314500000
H	0.6721760000	0.6798400000	1.2353030000
H	-1.0217590000	-2.6951110000	0.7798630000
H	-0.7110920000	-1.6961000000	2.7679890000
H	-2.0884080000	-1.7264840000	-1.4373250000
H	-3.8715280000	-0.1818020000	-2.1444860000
H	-3.3438580000	2.0761280000	1.4542960000
H	-1.5512120000	0.5413170000	2.1601710000
H	4.6372330000	3.0451500000	0.4133000000
H	5.7678160000	1.6893670000	0.3025660000
H	5.1507720000	2.4340890000	-1.1687070000
H	-4.5109760000	2.5842450000	-1.7125940000
H	-5.7274590000	1.4573140000	-1.1190020000
H	-5.0853370000	2.7097520000	-0.0457760000

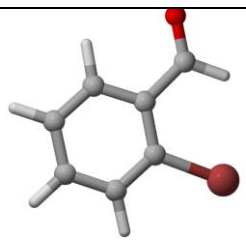
thermodynamic data

Zero-point correction= 0.280360 (Hartree/Particle)
Thermal correction to Energy= 0.297260
Thermal correction to Enthalpy= 0.298204
Thermal correction to Gibbs Free Energy= 0.233456
Sum of electronic and zero-point Energies= -769.399464
Sum of electronic and thermal Energies= -769.382564
Sum of electronic and thermal Enthalpies= -769.381620
Sum of electronic and thermal Free Energies= -769.446368

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.534	63.732	136.275

B3LYP/6-31G*	***o*-Br-Benzaldehyd**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

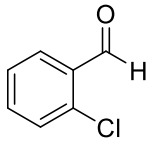
C	-0.3267280000	-1.8006910000	0.0000030000
C	-1.6851500000	-2.1181070000	0.0000030000
C	-2.6492750000	-1.1054500000	-0.0000010000
C	-2.2458880000	0.2235480000	-0.0000040000
C	-0.8842300000	0.5711440000	-0.0000050000
C	0.0632430000	-0.4630570000	0.0000000000
C	-0.5317070000	2.0167170000	-0.0000120000
O	-1.3622830000	2.9055460000	0.0000100000
Br	1.9468480000	-0.0963900000	0.0000000000
H	0.4257150000	-2.5814700000	0.0000060000
H	-1.9866360000	-3.1619570000	0.0000050000
H	-3.7058750000	-1.3561600000	-0.0000010000
H	-2.9652540000	1.0369240000	-0.0000080000
H	0.5490590000	2.2472980000	0.0000160000

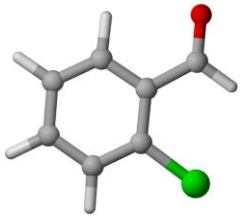
thermodynamic data

Zero-point correction= 0.100238 (Hartree/Particle)
Thermal correction to Energy= 0.107920
Thermal correction to Enthalpy= 0.108864
Thermal correction to Gibbs Free Energy= 0.066517
Sum of electronic and zero-point Energies= -2916.574938
Sum of electronic and thermal Energies= -2916.567257
Sum of electronic and thermal Enthalpies= -2916.566313
Sum of electronic and thermal Free Energies= -2916.608660

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.721	28.035	89.127

B3LYP/6-31G*	***o*-Cl-Benzaldehyd**





xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	-1.2239900000	-1.3614470000	0.0000040000
C	-2.3667280000	-0.5620610000	0.0000040000
C	-2.2569070000	0.8319340000	-0.0000010000
C	-0.9983830000	1.4191250000	-0.0000060000

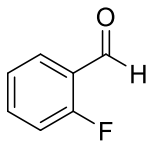
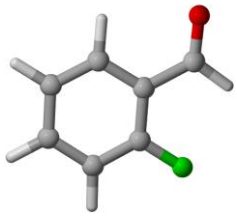
C	0.1700380000	0.6385130000	-0.0000060000
C	0.0332800000	-0.7588890000	0.0000000000
C	1.4820340000	1.3395900000	-0.0000100000
O	1.5876320000	2.5518640000	0.0000110000
Cl	1.4443280000	-1.8152650000	-0.0000010000
H	-1.3008110000	-2.4434390000	0.0000070000
H	-3.3452350000	-1.0341920000	0.0000090000
H	-3.1490310000	1.4510170000	-0.0000030000
H	-0.8735350000	2.4976570000	-0.0000100000
H	2.3779220000	0.6929710000	0.0000190000

thermodynamic data

Zero-point correction= 0.100635 (Hartree/Particle)
Thermal correction to Energy= 0.108120
Thermal correction to Enthalpy= 0.109064
Thermal correction to Gibbs Free Energy= 0.067914
Sum of electronic and zero-point Energies= -805.064570
Sum of electronic and thermal Energies= -805.057085
Sum of electronic and thermal Enthalpies= -805.056141
Sum of electronic and thermal Free Energies= -805.097291

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	67.846	27.735	86.608

B3LYP/6-31G*	***o*-F-Benzaldehyd**

xyz-matrix

14
XYZ file generated by gabedit : coordinates in Angstrom

C	1.7503660000	0.7625300000	0.0000000000
C	2.2347150000	-0.5455060000	-0.0000020000
C	1.3524050000	-1.6334470000	0.0000000000
C	-0.0190420000	-1.4092110000	0.0000010000
C	-0.5345890000	-0.1024960000	0.0000010000
C	0.3753720000	0.9602790000	0.0000010000
C	-1.9980660000	0.1258940000	0.0000040000
O	-2.8173880000	-0.7748110000	-0.0000030000
F	-0.0932450000	2.2261720000	0.0000000000
H	2.4123880000	1.6219870000	0.0000000000

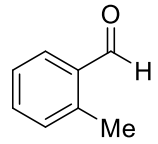
H	3.3077590000	-0.7152180000	-0.0000030000
H	1.7400970000	-2.6476240000	0.0000010000
H	-0.7306190000	-2.2292950000	0.0000020000
H	-2.3182740000	1.1848310000	-0.0000030000

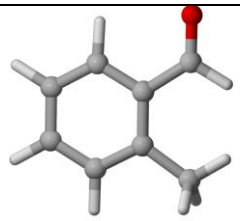
thermodynamic data

Zero-point correction= 0.102146 (Hartree/Particle)
Thermal correction to Energy= 0.109251
Thermal correction to Enthalpy= 0.110195
Thermal correction to Gibbs Free Energy= 0.070372
Sum of electronic and zero-point Energies= -444.703010
Sum of electronic and thermal Energies= -444.695904
Sum of electronic and thermal Enthalpies= -444.694960
Sum of electronic and thermal Free Energies= -444.734784

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.556	26.797	83.816

B3LYP/6-31G*	***o*-Me-Benzaldehyd**





xyz-matrix

17
XYZ file generated by gabedit : coordinates in Angstrom

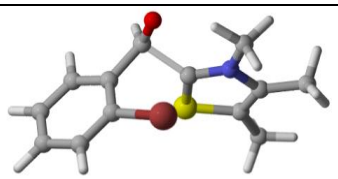
C	1.7704310000	0.6295110000	0.0000000000
C	2.2010430000	-0.6937870000	0.0000080000
C	1.2672330000	-1.7363950000	0.0000010000
C	-0.0850920000	-1.4314330000	-0.0000070000
C	-0.5299610000	-0.0955260000	-0.0000080000
C	0.4069210000	0.9618290000	-0.0000090000
C	-1.9987990000	0.1166610000	0.0000050000
O	-2.8166910000	-0.7869930000	0.0000040000
C	0.0435630000	2.4333860000	0.0000010000
H	2.5055660000	1.4316330000	-0.0000040000
H	3.2656120000	-0.9134550000	0.0000120000
H	1.5977240000	-2.7712700000	0.0000020000
H	-0.8409580000	-2.2106400000	-0.0000100000
H	-2.3493690000	1.1664500000	0.0000050000
H	-1.0295760000	2.6260500000	-0.0003140000
H	0.4659770000	2.9307830000	0.8814840000
H	0.4665110000	2.9309140000	-0.8811520000

thermodynamic data

Zero-point correction= 0.137863 (Hartree/Particle)
Thermal correction to Energy= 0.145160
Thermal correction to Enthalpy= 0.146104
Thermal correction to Gibbs Free Energy= 0.105905
Sum of electronic and zero-point Energies= -384.748857
Sum of electronic and thermal Energies= -384.741560
Sum of electronic and thermal Enthalpies= -384.740616
Sum of electronic and thermal Free Energies= -384.780814

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.089	27.901	84.605

B3LYP/6-31G*	**TST1 *o*-Br**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9145530000	0.3016500000	0.6563850000
S	1.3684600000	1.7843160000	-0.0932530000
N	1.9426970000	-0.5431650000	0.5794530000
C	3.1096900000	-0.0812570000	-0.0713790000
C	2.9753610000	1.1999760000	-0.5058720000
C	4.2940980000	-0.9884330000	-0.2082580000
C	3.9551090000	2.0712560000	-1.2317330000
C	1.8230080000	-1.9256740000	1.0827420000
C	-1.7232820000	0.5660220000	0.8057070000
C	-2.3840820000	1.7626230000	1.1075810000
C	-3.4386740000	2.2375240000	0.3264510000
C	-3.8530920000	1.5084660000	-0.7872650000
C	-3.2086240000	0.3135230000	-1.1151390000
C	-2.1612610000	-0.1404300000	-0.3182950000
C	-0.6308890000	0.0682220000	1.7565170000
O	-0.7147520000	-1.0916520000	2.2360380000
H	-0.3303400000	0.9131130000	2.4265880000
H	5.0800520000	-0.5049860000	-0.7917280000
H	4.7189030000	-1.2524620000	0.7678370000
H	4.0279950000	-1.9234100000	-0.7146700000
H	3.5377720000	2.4372490000	-2.1769110000

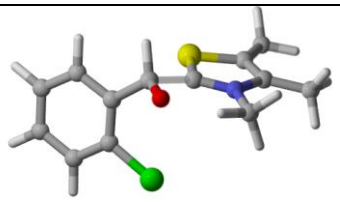
H	4.8734640000	1.5248880000	-1.4636680000
H	4.2311440000	2.9471560000	-0.6325500000
H	0.9053650000	-1.9748880000	1.6768980000
H	2.6989490000	-2.1666800000	1.6892670000
H	1.7579030000	-2.6116540000	0.2333350000
H	-2.0642260000	2.3199220000	1.9862660000
H	-3.9359610000	3.1671430000	0.5899060000
H	-4.6739800000	1.8620550000	-1.4054100000
Br	-1.2892020000	-1.7671720000	-0.8468100000
H	-3.5126620000	-0.2609060000	-1.9838760000

thermodynamic data

Zero-point correction= 0.241347 (Hartree/Particle)
Thermal correction to Energy= 0.258289
Thermal correction to Enthalpy= 0.259233
Thermal correction to Gibbs Free Energy= 0.194902
Sum of electronic and zero-point Energies= -3603.372273
Sum of electronic and thermal Energies= -3603.355331
Sum of electronic and thermal Enthalpies= -3603.354387
Sum of electronic and thermal Free Energies= -3603.418719

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.079	62.363	135.397

B3LYP/6-31G*	**TST1 *o*-Cl**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.7465110000	-0.0201230000	0.5781250000
S	1.1081010000	1.6219540000	0.2036670000
N	1.8322130000	-0.7564570000	0.3435080000
C	2.9773600000	-0.0812480000	-0.1385230000
C	2.7609170000	1.2542400000	-0.2722970000
C	4.2266770000	-0.8533490000	-0.4340440000
C	3.6899850000	2.3307760000	-0.7456290000
C	1.8144580000	-2.2208560000	0.5369220000
C	-1.9086600000	0.0270700000	0.6643000000
C	-2.6544950000	1.0756150000	1.2167300000
C	-3.7293680000	1.6553620000	0.5421030000
C	-4.0815850000	1.1840660000	-0.7214870000

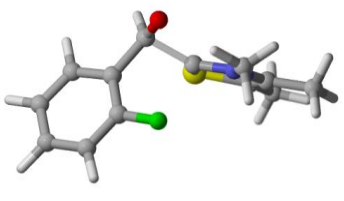
C	-3.3546930000	0.1428530000	-1.3012110000
C	-2.2859990000	-0.4225130000	-0.6076480000
C	-0.8006860000	-0.6036570000	1.5170700000
O	-0.8067770000	-1.8445380000	1.7250830000
H	-0.5875700000	0.0873510000	2.3728480000
H	4.9916860000	-0.1961210000	-0.8518650000
H	4.6418460000	-1.3155720000	0.4696880000
H	4.0422630000	-1.6553800000	-1.1580730000
H	3.2785060000	2.8576280000	-1.6143800000
H	4.6591810000	1.9163400000	-1.0366490000
H	3.8686140000	3.0768470000	0.0377340000
H	0.8684340000	-2.4708820000	1.0275650000
H	2.6654040000	-2.5126630000	1.1573760000
H	1.8828020000	-2.7136160000	-0.4370030000
H	-2.3842970000	1.4289420000	2.2101370000
H	-4.2902580000	2.4638130000	1.0032160000
H	-4.9178270000	1.6199530000	-1.2613080000
Cl	-1.3889520000	-1.7096790000	-1.4177780000
H	-3.6100120000	-0.2312570000	-2.2874280000

thermodynamic data

Zero-point correction= 0.241614 (Hartree/Particle)
Thermal correction to Energy= 0.258423
Thermal correction to Enthalpy= 0.259367
Thermal correction to Gibbs Free Energy= 0.195445
Sum of electronic and zero-point Energies= -1491.859662
Sum of electronic and thermal Energies= -1491.842853
Sum of electronic and thermal Enthalpies= -1491.841909
Sum of electronic and thermal Free Energies= -1491.905831

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.163	62.083	134.534

B3LYP/6-31G*	**TST1 *o*-F**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.6488710000	-0.0489220000	-0.5420120000
S	1.2873850000	-1.6411080000	-0.3760270000

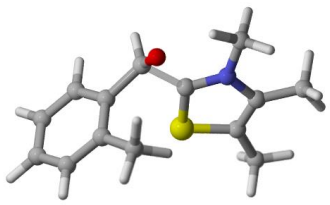
N	1.5839810000	0.8208630000	-0.1592990000
C	2.8177110000	0.2901610000	0.2827630000
C	2.8364840000	-1.0682890000	0.2287160000
C	3.9080200000	1.2135340000	0.7340260000
C	3.9309720000	-2.0252130000	0.5925390000
C	1.3114640000	2.2726710000	-0.1540720000
C	-2.0190400000	-0.0281810000	-0.5417120000
C	-2.9004690000	-1.0592120000	-0.8801440000
C	-3.9629800000	-1.4205530000	-0.0473350000
C	-4.1617440000	-0.7407400000	1.1540220000
C	-3.2950080000	0.2922580000	1.5211540000
C	-2.2529900000	0.6275780000	0.6682830000
C	-0.9297480000	0.4055700000	-1.5230280000
O	-0.8843460000	1.5983030000	-1.9234960000
H	-0.7708010000	-0.4176050000	-2.2634270000
H	4.7570380000	0.6432450000	1.1160600000
H	4.2724560000	1.8430770000	-0.0867210000
H	3.5658880000	1.8808750000	1.5334400000
H	4.2603800000	-2.6042670000	-0.2783420000
H	3.5991410000	-2.7387340000	1.3557460000
H	4.8025380000	-1.4964880000	0.9883540000
H	0.4004480000	2.4331180000	-0.7375880000
H	2.1561440000	2.7973030000	-0.6055570000
H	1.1720180000	2.6092780000	0.8764420000
H	-2.7495560000	-1.5793180000	-1.8242200000
H	-4.6349220000	-2.2228500000	-0.3394700000
H	-4.9851750000	-1.0098800000	1.8098510000
H	-3.4133340000	0.8358730000	2.4533090000
F	-1.4036420000	1.6097410000	1.0624910000

thermodynamic data

Zero-point correction= 0.243274 (Hartree/Particle)
Thermal correction to Energy= 0.259641
Thermal correction to Enthalpy= 0.260585
Thermal correction to Gibbs Free Energy= 0.198217
Sum of electronic and zero-point Energies= -1131.498425
Sum of electronic and thermal Energies= -1131.482058
Sum of electronic and thermal Enthalpies= -1131.481114
Sum of electronic and thermal Free Energies= -1131.543482

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.927	61.141	131.265

B3LYP/6-31G*	**TST1 *o*-Me**

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	0.6943230000	0.3562850000	-0.4811390000
S	0.7236120000	-1.3455330000	-0.2388970000
N	1.9239430000	0.8376450000	-0.2843470000
C	2.9310440000	-0.0942350000	0.0495640000
C	2.4453330000	-1.3632360000	0.1180760000
C	4.3353100000	0.3746290000	0.2813120000
C	3.1569480000	-2.6401150000	0.4501570000
C	2.2046560000	2.2787340000	-0.4450100000
C	-1.9415800000	0.4832070000	-0.3954420000
C	-2.5333140000	-0.2172580000	-1.4525830000
C	-3.6015140000	-1.0910170000	-1.2462260000
C	-4.0956040000	-1.2637620000	0.0448780000
C	-3.5131410000	-0.5673790000	1.1057300000
C	-2.4368560000	0.3088710000	0.9169930000
C	-0.8012980000	1.4500020000	-0.7277370000
O	-0.6577140000	2.5255510000	-0.0658990000
H	-0.6965880000	1.4925030000	-1.8413180000
H	5.0008790000	-0.4768940000	0.4362690000
H	4.7162520000	0.9456090000	-0.5732560000
H	4.4083910000	1.0181490000	1.1665200000
H	3.0334110000	-3.3836050000	-0.3457390000
H	2.7706120000	-3.0824900000	1.3760920000
H	4.2291680000	-2.4723130000	0.5846840000
H	1.2366430000	2.7957620000	-0.4148660000
H	2.7221490000	2.4467010000	-1.3944310000
H	2.8370280000	2.6172110000	0.3783810000
H	-2.1515990000	-0.0605290000	-2.4604870000
H	-4.0464970000	-1.6204720000	-2.0850120000
H	-4.9325970000	-1.9326600000	0.2296490000
H	-3.9036570000	-0.7039700000	2.1122990000
C	-1.8415100000	1.0264260000	2.1058410000
H	-2.3954930000	0.7828130000	3.0192220000
H	-1.8358830000	2.1059220000	1.9444800000
H	-0.7926840000	0.7419440000	2.2610040000

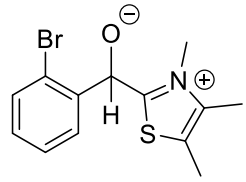
thermodynamic data

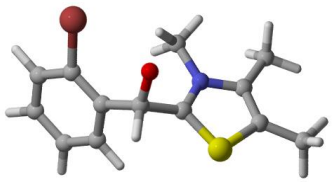
Zero-point correction= 0.279281 (Hartree/Particle)
Thermal correction to Energy= 0.296444
Thermal correction to Enthalpy= 0.297388
Thermal correction to Gibbs Free Energy= 0.232895
Sum of electronic and zero-point Energies= -1071.546677

Sum of electronic and thermal Energies= -1071.529515
Sum of electronic and thermal Enthalpies= -1071.528570
Sum of electronic and thermal Free Energies= -1071.593063

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.021	63.912	135.737

B3LYP/6-31G*	**Zwitterion1 *o*-Br**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	1.9276170000	2.9920810000	-0.6641320000
C	3.1128230000	2.3805390000	-1.0807410000
C	3.3386340000	1.0427110000	-0.7730220000
C	2.3839610000	0.3124710000	-0.0545690000
C	1.1883320000	0.8957760000	0.3698520000
C	0.9948680000	2.2510170000	0.0529330000
C	0.0788660000	0.2059080000	1.2230200000
C	-1.2944600000	0.2650900000	0.5202840000
O	0.1366710000	-1.0860180000	1.4980980000
S	-2.7140220000	0.8329610000	1.3196160000
C	-3.7642010000	0.1145860000	0.1033240000
C	-3.0120880000	-0.4901950000	-0.8539800000
N	-1.6312180000	-0.3840730000	-0.6098390000
C	-5.2528820000	0.2248510000	0.2311650000
C	-3.5039800000	-1.2108280000	-2.0729590000
C	-0.5998930000	-1.0704520000	-1.4030100000
H	3.8599110000	2.9398860000	-1.6372890000
H	1.7376970000	4.0379770000	-0.8904440000
H	4.2542040000	0.5493390000	-1.0820590000
Br	2.8337030000	-1.5263890000	0.2805570000
H	0.0776560000	2.7305420000	0.3935250000
H	-0.0298520000	0.8897910000	2.1086360000
H	-5.7569000000	-0.2456610000	-0.6169690000
H	-5.6113830000	-0.2658750000	1.1440220000
H	-5.5766360000	1.2718860000	0.2707350000
H	-3.2809110000	-2.2838640000	-2.0314080000
H	-4.5862070000	-1.1037370000	-2.1643450000
H	-3.0518940000	-0.8102150000	-2.9874970000
H	-1.0727470000	-1.8105130000	-2.0460590000

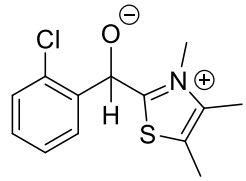
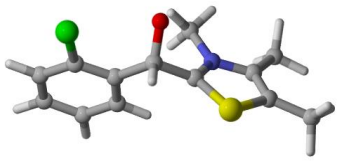
H	-0.0475160000	-0.3514350000	-2.0124900000
H	0.0689030000	-1.5565710000	-0.6866220000

thermodynamic data

Zero-point correction= 0.242422 (Hartree/Particle)
Thermal correction to Energy= 0.259695
Thermal correction to Enthalpy= 0.260639
Thermal correction to Gibbs Free Energy= 0.195681
Sum of electronic and zero-point Energies= -3603.369122
Sum of electronic and thermal Energies= -3603.351849
Sum of electronic and thermal Enthalpies= -3603.350905
Sum of electronic and thermal Free Energies= -3603.415863

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.961	63.582	136.716

B3LYP/6-31G*	**Zwitterion1 *o*-Cl**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	2.3269410000	-2.3235620000	-1.0157130000
C	3.6582710000	-1.9980830000	-0.7646120000
C	3.9765470000	-0.7291900000	-0.2814650000
C	2.9623460000	0.1976470000	-0.0385410000
C	1.6100180000	-0.1070520000	-0.2562830000
C	1.3272830000	-1.3823150000	-0.7641050000
C	0.5141820000	0.9485300000	0.0425910000
C	-0.9186280000	0.4042050000	-0.1468880000
O	0.4606050000	1.4502760000	1.2743860000
S	-2.0355650000	1.1064810000	-1.2571030000
C	-3.3937510000	0.2540750000	-0.5353800000
C	-2.9535900000	-0.5250970000	0.4891310000
N	-1.5662960000	-0.4292770000	0.6883140000
C	-4.7832430000	0.4626010000	-1.0560070000
C	-3.7738220000	-1.4180430000	1.3704730000
C	-0.8549670000	-1.0435800000	1.8233760000
H	4.4498220000	-2.7189370000	-0.9501000000
H	2.0641970000	-3.3032190000	-1.4063180000
H	5.0083160000	-0.4475340000	-0.0972950000
Cl	3.4535990000	1.7984330000	0.5069680000

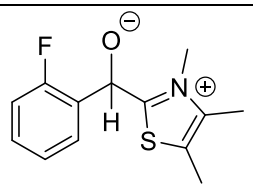
H	0.2937910000	-1.6460500000	-0.9774050000
H	0.6250280000	1.7113310000	-0.7743570000
H	-5.5002280000	-0.1717250000	-0.5283740000
H	-5.1038690000	1.5035280000	-0.9281800000
H	-4.8523070000	0.2250420000	-2.1241960000
H	-3.8139700000	-1.0482320000	2.4021520000
H	-4.7992710000	-1.4755700000	1.0013520000
H	-3.3704360000	-2.4365530000	1.3970220000
H	-1.5608400000	-1.2234220000	2.6335960000
H	-0.3881720000	-1.9835620000	1.5191600000
H	-0.1005130000	-0.3002360000	2.1153890000

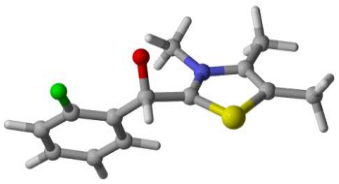
thermodynamic data

Zero-point correction= 0.242838 (Hartree/Particle)
Thermal correction to Energy= 0.259816
Thermal correction to Enthalpy= 0.260761
Thermal correction to Gibbs Free Energy= 0.196816
Sum of electronic and zero-point Energies= -1491.857496
Sum of electronic and thermal Energies= -1491.840518
Sum of electronic and thermal Enthalpies= -1491.839573
Sum of electronic and thermal Free Energies= -1491.903518

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.037	63.111	134.582

B3LYP/6-31G*	**Zwitterion1 *o*-F**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	2.7994080000	1.6947120000	1.3592610000
C	4.0622770000	1.3557110000	0.8745260000
C	4.2132710000	0.2229040000	0.0736320000
C	3.0961080000	-0.5446180000	-0.2372810000
C	1.8099640000	-0.2273330000	0.2126950000
C	1.6947630000	0.9045350000	1.0284660000
C	0.6269160000	-1.1390080000	-0.1856960000
C	-0.7457010000	-0.4992660000	0.0909210000
O	0.4971530000	-1.4683290000	-1.4716570000
S	-1.9509960000	-1.2728450000	1.0519610000

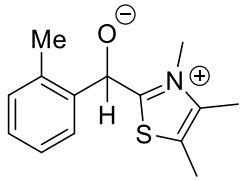
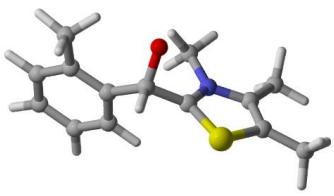
C	-3.2054540000	-0.1821780000	0.4756200000
C	-2.6673470000	0.7202740000	-0.3877930000
N	-1.2892090000	0.5315710000	-0.5848010000
C	-4.6213080000	-0.3450550000	0.9379130000
C	-3.3784310000	1.8302470000	-1.1015520000
C	-0.4955710000	1.2518240000	-1.5954230000
H	4.9294200000	1.9622210000	1.1210620000
H	2.6713470000	2.5690930000	1.9917380000
H	5.1815610000	-0.0829530000	-0.3101710000
F	3.2862110000	-1.6541980000	-0.9767960000
H	0.7159240000	1.1741140000	1.4202790000
H	0.6771680000	-2.0090720000	0.5226610000
H	-5.2652830000	0.4298850000	0.5140510000
H	-5.0290590000	-1.3171900000	0.6355160000
H	-4.6982530000	-0.2807930000	2.0299210000
H	-3.4260290000	1.6562010000	-2.1833270000
H	-4.4033110000	1.9190020000	-0.7370780000
H	-2.8820470000	2.7938420000	-0.9403370000
H	-1.1648470000	1.6770880000	-2.3423890000
H	0.0931720000	2.0440590000	-1.1270290000
H	0.1541540000	0.4869580000	-2.0399760000

thermodynamic data

Zero-point correction= 0.244486 (Hartree/Particle)
Thermal correction to Energy= 0.261038
Thermal correction to Enthalpy= 0.261982
Thermal correction to Gibbs Free Energy= 0.199420
Sum of electronic and zero-point Energies= -1131.495317
Sum of electronic and thermal Energies= -1131.478765
Sum of electronic and thermal Enthalpies= -1131.477821
Sum of electronic and thermal Free Energies= -1131.540383

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.804	62.153	131.672

B3LYP/6-31G*		**Zwitterion1 *o*-Me**

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

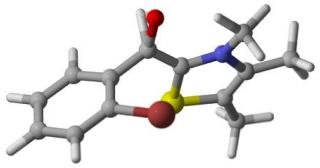
C	2.7149790000	-1.8414220000	-1.2832370000
C	3.9760430000	-1.5419900000	-0.7724300000
C	4.1554990000	-0.3708130000	-0.0363100000
C	3.1019660000	0.5184400000	0.2168020000
C	1.8176210000	0.1972790000	-0.2763850000
C	1.6531600000	-0.9709110000	-1.0316180000
C	0.6282440000	1.1551880000	-0.0342670000
C	-0.7419650000	0.4941450000	-0.1718620000
O	0.4623920000	1.7005340000	1.1849120000
S	-1.9804240000	1.1376950000	-1.1860030000
C	-3.2073110000	0.1151470000	-0.4456540000
C	-2.6354060000	-0.6759520000	0.5002690000
N	-1.2533200000	-0.4582950000	0.6324050000
C	-4.6368610000	0.2128310000	-0.8831450000
C	-3.3143690000	-1.6997170000	1.3595750000
C	-0.4253840000	-1.0502310000	1.6962150000
H	4.8157300000	-2.2099680000	-0.9475130000
H	2.5545020000	-2.7432320000	-1.8691500000
H	5.1430100000	-0.1302660000	0.3528490000
H	0.6707560000	-1.2093630000	-1.4362090000
H	0.6750110000	1.9002510000	-0.8733380000
H	-5.2607890000	-0.5115520000	-0.3531810000
H	-5.0463520000	1.2108380000	-0.6853550000
H	-4.7434050000	0.0199990000	-1.9574490000
H	-3.3249620000	-1.4050690000	2.4160030000
H	-4.3510460000	-1.8311570000	1.0446360000
H	-2.8185060000	-2.6745920000	1.2901370000
H	-1.0719540000	-1.4162930000	2.4926810000
H	0.1809580000	-1.8680710000	1.3004090000
H	0.2086890000	-0.2324710000	2.0554620000
C	3.3786270000	1.8036090000	0.9651040000
H	2.5680450000	2.0271310000	1.6615500000
H	3.4346360000	2.6518540000	0.2678990000
H	4.3375120000	1.7490240000	1.4921490000

thermodynamic data

Zero-point correction= 0.280363 (Hartree/Particle)
Thermal correction to Energy= 0.297851
Thermal correction to Enthalpy= 0.298795
Thermal correction to Gibbs Free Energy= 0.234426
Sum of electronic and zero-point Energies= -1071.546824
Sum of electronic and thermal Energies= -1071.529336
Sum of electronic and thermal Enthalpies= -1071.528391
Sum of electronic and thermal Free Energies= -1071.592761

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.905	65.250	135.477

B3LYP/6-31G*	**TST2 *o*-Br**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9447740000	0.1688560000	0.6086580000
S	1.2521150000	1.6159200000	-0.3464390000
N	2.0722960000	-0.6083520000	0.6459240000
C	3.1923870000	-0.0490020000	-0.0013750000
C	2.9433990000	1.1459180000	-0.5848400000
C	4.4904170000	-0.7986980000	0.0149690000
C	3.8514160000	2.0550100000	-1.3531980000
C	2.0304170000	-2.0283860000	1.0230660000
C	-1.5013370000	0.6042010000	0.7451250000
C	-1.9968340000	1.8338130000	1.1975820000
C	-3.1744050000	2.3760000000	0.6801150000
C	-3.8840180000	1.6847940000	-0.3013780000
C	-3.4132220000	0.4565390000	-0.7715010000
C	-2.2334330000	-0.0625530000	-0.2483390000
C	-0.2661530000	-0.0246070000	1.3198180000
O	-0.4998430000	-1.1997710000	2.1141710000
H	-0.1466830000	0.0271610000	2.5016930000
H	4.3957210000	-1.7856810000	-0.4531640000
H	5.2582470000	-0.2449900000	-0.5281160000
H	4.8522860000	-0.9542410000	1.0388340000
H	3.4528760000	2.2603110000	-2.3547350000
H	4.8428200000	1.6109590000	-1.4766470000
H	3.9793250000	3.0210370000	-0.8484960000
H	1.9755380000	-2.6545520000	0.1247950000
H	1.1314350000	-2.1771010000	1.6266850000
H	2.9274190000	-2.2850280000	1.5916610000
H	-1.4468690000	2.3635760000	1.9712160000
H	-3.5389090000	3.3308320000	1.0484480000
H	-4.8053420000	2.0948190000	-0.7058890000
H	-3.9529260000	-0.0903020000	-1.5372490000
Br	-1.5819010000	-1.7338910000	-0.9103730000

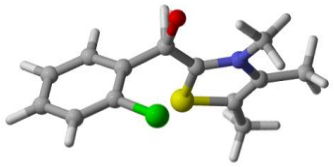
thermodynamic data

Zero-point correction= 0.238465 (Hartree/Particle)
Thermal correction to Energy= 0.255623
Thermal correction to Enthalpy= 0.256567
Thermal correction to Gibbs Free Energy= 0.192059
Sum of electronic and zero-point Energies= -3603.321062
Sum of electronic and thermal Energies= -3603.303904
Sum of electronic and thermal Enthalpies= -3603.302960

Sum of electronic and thermal Free Energies= -3603.367468

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.406	63.579	135.769

B3LYP/6-31G*	**TST2 *o*-Cl**



xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

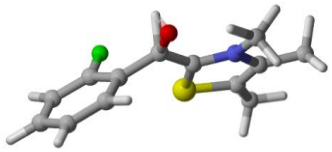
C	0.7568040000	-0.1748570000	0.4452890000
S	0.9302970000	1.4745910000	-0.1474110000
N	1.9704890000	-0.8110580000	0.3946110000
C	3.0423050000	-0.0005640000	-0.0290600000
C	2.6760790000	1.2603980000	-0.3551130000
C	4.4209920000	-0.5872570000	-0.0778720000
C	3.5005280000	2.4132360000	-0.8372140000
C	2.1099670000	-2.2688630000	0.5200060000
C	-1.7240510000	0.0374350000	0.5905550000
C	-2.2738930000	1.0747850000	1.3569600000
C	-3.4775250000	1.6857100000	1.0052120000
C	-4.1640810000	1.2568890000	-0.1301800000
C	-3.6425050000	0.2263480000	-0.9138310000
C	-2.4348660000	-0.3664460000	-0.5515350000
C	-0.4548460000	-0.6492720000	1.0088180000
O	-0.6072880000	-2.0007720000	1.4736860000
H	-0.3643100000	-0.8768500000	2.1681110000
H	4.4694320000	-1.4558590000	-0.7451600000
H	5.1379690000	0.1513580000	-0.4405000000
H	4.7541250000	-0.9169520000	0.9139860000
H	3.1275320000	2.7956040000	-1.7957260000
H	4.5436220000	2.1195560000	-0.9820470000
H	3.4852290000	3.2479310000	-0.1248700000
H	2.2692290000	-2.7191610000	-0.4666260000
H	1.1809440000	-2.6469520000	0.9534710000
H	2.9608100000	-2.5046350000	1.1650300000
H	-1.7405290000	1.3974040000	2.2475310000
H	-3.8795750000	2.4862960000	1.6196270000
H	-5.1061300000	1.7192290000	-0.4117220000
H	-4.1632940000	-0.1167020000	-1.8017450000
Cl	-1.7943750000	-1.6491400000	-1.5696920000

thermodynamic data

Zero-point correction= 0.238853 (Hartree/Particle)
Thermal correction to Energy= 0.255854
Thermal correction to Enthalpy= 0.256798
Thermal correction to Gibbs Free Energy= 0.193105
Sum of electronic and zero-point Energies= -1491.809492
Sum of electronic and thermal Energies= -1491.792492
Sum of electronic and thermal Enthalpies= -1491.791548
Sum of electronic and thermal Free Energies= -1491.855240

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	160.551	63.308	134.052

B3LYP/6-31G*	**TST2 *o*-F**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.6551900000	0.4281850000	0.1394060000
S	-0.7761600000	-1.3010170000	-0.1565370000
N	-1.9119320000	0.9820900000	0.0857690000
C	-2.9559950000	0.0624690000	-0.1320760000
C	-2.5323110000	-1.2127390000	-0.2900830000
C	-4.3707780000	0.5577770000	-0.1676900000
C	-3.3112030000	-2.4697170000	-0.5265110000
C	-2.1709910000	2.4297160000	0.0569930000
C	1.8721960000	0.4496580000	0.0804940000
C	2.7030410000	1.1340930000	-0.8220660000
C	3.9396930000	0.6205230000	-1.2030760000
C	4.3939490000	-0.5876010000	-0.6647040000
C	3.6067270000	-1.2720810000	0.2597460000
C	2.3759600000	-0.7353220000	0.6197180000
C	0.5678300000	1.0748570000	0.4816440000
O	0.6261990000	2.5097710000	0.6176780000
H	0.5517910000	1.5601790000	1.5648160000
H	-4.5216600000	1.3076770000	-0.9530500000
H	-5.0572220000	-0.2682630000	-0.3612410000
H	-4.6631330000	1.0169330000	0.7845300000
H	-2.9833900000	-2.9749790000	-1.4435920000
H	-4.3791440000	-2.2595050000	-0.6286210000
H	-3.1889930000	-3.1812410000	0.2998360000
H	-2.5052250000	2.7309770000	-0.9423830000
H	-1.2331640000	2.9309670000	0.3027240000

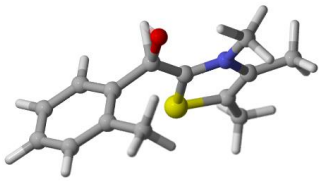
H	-2.9484470000	2.6802280000	0.7845690000
H	2.3546880000	2.0902220000	-1.1989560000
H	4.5558270000	1.1660440000	-1.9125010000
H	5.3609960000	-0.9905490000	-0.9523420000
H	3.9320900000	-2.1996990000	0.7197920000
F	1.6377680000	-1.4027150000	1.5453810000

thermodynamic data

Zero-point correction= 0.240247 (Hartree/Particle)
Thermal correction to Energy= 0.256856
Thermal correction to Enthalpy= 0.257800
Thermal correction to Gibbs Free Energy= 0.194788
Sum of electronic and zero-point Energies= -1131.449031
Sum of electronic and thermal Energies= -1131.432422
Sum of electronic and thermal Enthalpies= -1131.431478
Sum of electronic and thermal Free Energies= -1131.494490

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.179	62.379	132.620

B3LYP/6-31G*	**TST2 *o*-Me**

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.6567620000	0.3115500000	0.3006760000
S	-0.7854780000	-1.4052790000	-0.0748450000
N	-1.8999540000	0.8896830000	0.2191440000
C	-2.9506200000	-0.0058550000	-0.0623890000
C	-2.5432480000	-1.2830670000	-0.2437670000
C	-4.3534650000	0.5187450000	-0.1312400000
C	-3.3354040000	-2.5169030000	-0.5468130000
C	-2.1148560000	2.3430650000	0.2340810000
C	1.8399210000	0.1684280000	0.3959950000
C	2.3145770000	-0.8504300000	1.2315980000
C	3.5154530000	-1.5075090000	0.9587710000
C	4.2626820000	-1.1316400000	-0.1558960000
C	3.7998140000	-0.1111000000	-0.9894640000
C	2.5915570000	0.5468800000	-0.7387280000
C	0.5637830000	0.8928150000	0.7291470000
O	0.6838430000	2.3138330000	0.9629480000

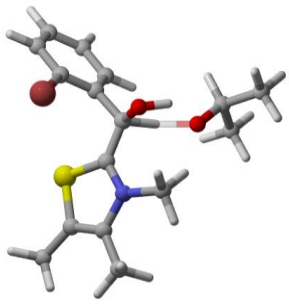
H	0.5003340000	1.3177290000	1.8379150000
H	-4.4581210000	1.3007210000	-0.8926050000
H	-5.0490080000	-0.2841450000	-0.3814440000
H	-4.6718590000	0.9493730000	0.8261420000
H	-2.9846890000	-2.9995460000	-1.4677500000
H	-4.3954500000	-2.2840120000	-0.6786910000
H	-3.2548110000	-3.2567410000	0.2597530000
H	-2.3840370000	2.6968030000	-0.7680680000
H	-1.1772220000	2.8052070000	0.5506980000
H	-2.9217120000	2.5924000000	0.9293910000
H	1.7362400000	-1.1228570000	2.1116950000
H	3.8686190000	-2.2941100000	1.6203800000
H	5.2059620000	-1.6251160000	-0.3760440000
H	4.3876800000	0.1822070000	-1.8568430000
C	2.0902630000	1.6321210000	-1.6597390000
H	2.8694060000	1.9532810000	-2.3585000000
H	1.7469440000	2.4923480000	-1.0746990000
H	1.2361450000	1.2798600000	-2.2547910000

thermodynamic data

Zero-point correction= 0.276345 (Hartree/Particle)
Thermal correction to Energy= 0.293700
Thermal correction to Enthalpy= 0.294644
Thermal correction to Gibbs Free Energy= 0.230937
Sum of electronic and zero-point Energies= -1071.497386
Sum of electronic and thermal Energies= -1071.480031
Sum of electronic and thermal Enthalpies= -1071.479087
Sum of electronic and thermal Free Energies= -1071.542794

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	184.299	65.334	134.083

B3LYP/6-31G*	**TST2 mit Isopropanol *o*-Br**



xyz-matrix

43
XYZ file generated by gabedit : coordinates in Angstrom

C	0.0677880000	0.9549200000	0.0513060000

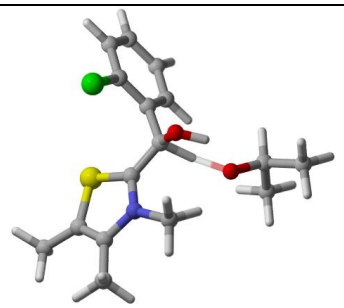
S	-1.0177220000	1.4007630000	1.3291540000
N	0.6417600000	2.0547720000	-0.4826570000
C	0.2222560000	3.2732300000	0.0863390000
C	-0.6705050000	3.1073270000	1.0960930000
C	0.7560510000	4.5730240000	-0.4363410000
C	-1.3465390000	4.1258490000	1.9628830000
C	1.7126430000	1.9656720000	-1.4990950000
C	-0.4869980000	-1.4615390000	0.3729120000
C	0.0100460000	-2.2606350000	1.4135690000
C	-0.7616710000	-3.2609780000	2.0037280000
C	-2.0622270000	-3.4867270000	1.5539370000
C	-2.5873750000	-2.7084330000	0.5217680000
C	-1.8021540000	-1.7114290000	-0.0535230000
C	0.4072210000	-0.4229120000	-0.2664460000
O	0.6027930000	-0.6464770000	-1.6575570000
H	1.5995240000	-0.5601270000	0.0871090000
H	0.5893990000	4.6721680000	-1.5149750000
H	0.2540530000	5.4089030000	0.0537530000
H	1.8316360000	4.6806070000	-0.2517600000
H	-1.0434250000	5.1396750000	1.6901550000
H	-1.0951890000	3.9781400000	3.0201660000
H	-2.4378900000	4.0684660000	1.8725920000
H	2.1762700000	2.9456040000	-1.5949050000
H	1.2883690000	1.6534570000	-2.4528900000
H	2.4540560000	1.2255530000	-1.1696740000
H	1.0284290000	-2.0903300000	1.7516420000
H	-0.3455180000	-3.8647940000	2.8050760000
Br	-2.5816860000	-0.6606440000	-1.4501600000
C	4.8427870000	-1.9599760000	-0.9980880000
C	3.8181530000	-1.5798600000	0.0822010000
H	4.3306010000	-2.3720100000	-1.8749230000
H	5.5658230000	-2.7035310000	-0.6374340000
H	5.3946940000	-1.0674230000	-1.3188630000
C	4.5157450000	-1.0174260000	1.3323060000
H	3.7760230000	-0.7626260000	2.1014750000
H	5.0577900000	-0.0989650000	1.0739480000
H	5.2291700000	-1.7304920000	1.7665580000
O	2.9091160000	-0.6554250000	-0.4375010000
H	3.3013600000	-2.5153960000	0.3834880000
H	1.5597730000	-0.9088120000	-1.6666950000
H	-2.6732990000	-4.2663750000	2.0004790000
H	-3.5980080000	-2.8701950000	0.1625940000

thermodynamic data

Zero-point correction= 0.349759 (Hartree/Particle)
Thermal correction to Energy= 0.373006
Thermal correction to Enthalpy= 0.373950
Thermal correction to Gibbs Free Energy= 0.294450
Sum of electronic and zero-point Energies= -3797.623890
Sum of electronic and thermal Energies= -3797.600643
Sum of electronic and thermal Enthalpies= -3797.599699
Sum of electronic and thermal Free Energies= -3797.679199

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.065	85.284	167.322

B3LYP/6-31G*	**TST2 mit Isopropanol *o*-Cl**

xyz-matrix

43
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9276760000	-0.0153020000	-0.1217940000
S	-1.5785460000	-1.1406470000	1.0272890000
N	-1.8894960000	0.8341830000	-0.5436360000
C	-3.1636720000	0.6036670000	0.0109920000
C	-3.1784750000	-0.4246920000	0.8977340000
C	-4.3292450000	1.4526700000	-0.3992950000
C	-4.3086240000	-0.9849440000	1.7068420000
C	-1.5887800000	1.9866070000	-1.4213210000
C	1.3341100000	-1.0730210000	0.0686190000
C	2.1780920000	-0.8751760000	1.1724170000
C	3.0095280000	-1.8847430000	1.6548720000
C	3.0180580000	-3.1296360000	1.0268390000
C	2.1923730000	-3.3602840000	-0.0732950000
C	1.3618320000	-2.3412740000	-0.5393530000
C	0.4905830000	0.0782820000	-0.4341820000
O	0.7481740000	0.4098780000	-1.7918730000
H	0.8581590000	1.1565550000	0.0687960000
H	-4.4674240000	1.4474600000	-1.4864400000
H	-5.2473490000	1.0734460000	0.0524660000
H	-4.2114910000	2.4953890000	-0.0809890000
H	-5.2399630000	-0.4494470000	1.5070530000
H	-4.1056520000	-0.9067960000	2.7817790000
H	-4.4778880000	-2.0442990000	1.4796360000
H	-2.4569880000	2.6424780000	-1.4348030000
H	-1.3667510000	1.6325380000	-2.4275110000
H	-0.7155070000	2.5188310000	-1.0201320000
H	2.1804130000	0.1018380000	1.6476120000
H	3.6525680000	-1.6958120000	2.5096620000
Cl	0.3292970000	-2.7000880000	-1.9190270000

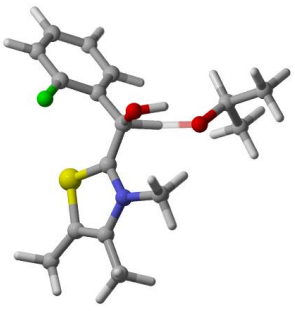
C	2.8206250000	4.2407220000	-0.5978450000
C	2.2893990000	3.1305870000	0.3224050000
H	3.1147170000	3.8187900000	-1.5654840000
H	3.6890350000	4.7544400000	-0.1646770000
H	2.0336300000	4.9836130000	-0.7793330000
C	1.8856220000	3.6967340000	1.6945010000
H	1.5244480000	2.8936680000	2.3492860000
H	1.0690070000	4.4197350000	1.5733070000
H	2.7214170000	4.1990020000	2.1995890000
O	1.2092780000	2.4909140000	-0.2891580000
H	3.1260120000	2.4200340000	0.4904430000
H	1.1900900000	1.2920160000	-1.6825910000
H	3.6654720000	-3.9247540000	1.3863670000
H	2.1870680000	-4.3236840000	-0.5723160000

thermodynamic data

Zero-point correction= 0.350298 (Hartree/Particle)
Thermal correction to Energy= 0.373285
Thermal correction to Enthalpy= 0.374230
Thermal correction to Gibbs Free Energy= 0.296472
Sum of electronic and zero-point Energies= -1686.111953
Sum of electronic and thermal Energies= -1686.088966
Sum of electronic and thermal Enthalpies= -1686.088022
Sum of electronic and thermal Free Energies= -1686.165780

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.240	84.916	163.655

B3LYP/6-31G*	**TST2 mit Isopropanol *o*-F**

xyz-matrix

43
XYZ file generated by gabedit : coordinates in Angstrom

C	-0.9181410000	-0.0412040000	-0.2089040000
S	-1.6742120000	-1.2156630000	0.8202440000
N	-1.8046390000	0.9164960000	-0.5583490000
C	-3.1020670000	0.7358060000	-0.0411960000

C	-3.2120180000	-0.3671930000	0.7433860000
C	-4.1903210000	1.7099440000	-0.3797920000
C	-4.3953340000	-0.9077990000	1.4871710000
C	-1.4026840000	2.1137240000	-1.3280130000
C	1.2425140000	-1.2954430000	-0.1169440000
C	2.1914540000	-1.3028810000	0.9137220000
C	2.9162280000	-2.4545510000	1.2268330000
C	2.7061710000	-3.6271230000	0.4996680000
C	1.7687820000	-3.6515270000	-0.5349370000
C	1.0607440000	-2.4919220000	-0.8213600000
C	0.5039550000	-0.0386630000	-0.5099690000
O	0.7828650000	0.3619990000	-1.8487400000
H	0.9660380000	0.9694780000	0.0638830000
H	-4.3082720000	1.8202310000	-1.4637080000
H	-5.1434000000	1.3633300000	0.0231220000
H	-3.9972630000	2.7046740000	0.0394690000
H	-4.2036170000	-0.9460760000	2.5663320000
H	-4.6442780000	-1.9246430000	1.1606380000
H	-5.2783430000	-0.2833260000	1.3308540000
H	-2.2056950000	2.8457310000	-1.2662880000
H	-1.2214040000	1.8385180000	-2.3668820000
H	-0.4814610000	2.5242410000	-0.8927760000
H	2.3631610000	-0.3840350000	1.4676080000
H	3.6475120000	-2.4330290000	2.0295620000
F	0.1409540000	-2.5274620000	-1.8102530000
C	3.2204710000	3.8721500000	-0.3773350000
C	2.5677180000	2.7651760000	0.4652490000
H	3.4839080000	3.4849920000	-1.3680860000
H	4.1299700000	4.2677860000	0.0939270000
H	2.5139190000	4.7001680000	-0.5160720000
C	2.2075110000	3.2788340000	1.8697500000
H	1.7588940000	2.4758230000	2.4678170000
H	1.4704980000	4.0881720000	1.7921210000
H	3.0841680000	3.6588640000	2.4111330000
O	1.4355730000	2.2815390000	-0.1935140000
H	3.3251910000	1.9627060000	0.5903750000
H	1.3045720000	1.1891910000	-1.6868210000
H	3.2698040000	-4.5260970000	0.7334590000
H	1.5799760000	-4.5466680000	-1.1187770000

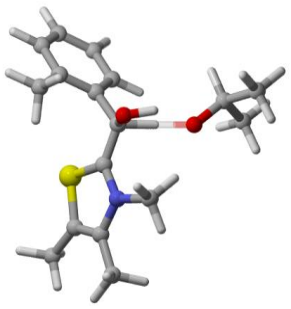
thermodynamic data

Zero-point correction= 0.351803 (Hartree/Particle)
Thermal correction to Energy= 0.374419
Thermal correction to Enthalpy= 0.375363
Thermal correction to Gibbs Free Energy= 0.298550
Sum of electronic and zero-point Energies= -1325.750627
Sum of electronic and thermal Energies= -1325.728012
Sum of electronic and thermal Enthalpies= -1325.727067
Sum of electronic and thermal Free Energies= -1325.803880

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	234.951	84.015	161.666

B3LYP/6-31G*	**TST2 mit Isopropanol *o*-Me**

xyz-matrix

46
XYZ file generated by gabedit : coordinates in Angstrom

C	0.9298920000	-0.0646100000	0.2193790000
S	1.6668570000	-1.2867990000	-0.7707680000
N	1.8364420000	0.8847970000	0.5448470000
C	3.1321110000	0.6606730000	0.0403300000
C	3.2222040000	-0.4683330000	-0.7090420000
C	4.2386640000	1.6231850000	0.3519460000
C	4.3970170000	-1.0537670000	-1.4323460000
C	1.4587800000	2.1111260000	1.2796500000
C	-1.2535490000	-1.2788190000	0.1089380000
C	-1.9141180000	-1.2839360000	-1.1274990000
C	-2.6374860000	-2.3943120000	-1.5627230000
C	-2.7141590000	-3.5203450000	-0.7457490000
C	-2.0638100000	-3.5249410000	0.4891750000
C	-1.3269290000	-2.4227200000	0.9394220000
C	-0.4938620000	-0.0330910000	0.5161850000
O	-0.7675530000	0.4145200000	1.8414150000
H	-0.9268680000	0.9734610000	-0.0777700000
H	4.3561110000	1.7657050000	1.4321980000
H	5.1856160000	1.2451720000	-0.0369160000
H	4.0665700000	2.6078990000	-0.0989440000
H	4.6224010000	-2.0669350000	-1.0783460000
H	5.2930440000	-0.4449530000	-1.2885630000
H	4.2088590000	-1.1167710000	-2.5110010000
H	2.2717750000	2.8290480000	1.1885150000
H	1.2830800000	1.8727920000	2.3287780000
H	0.5396360000	2.5224200000	0.8404910000
H	-1.8631630000	-0.3946130000	-1.7509590000
H	-3.1431080000	-2.3730270000	-2.5244030000
C	-3.1335340000	3.9231850000	0.3677880000
C	-2.5113460000	2.7987840000	-0.4749880000
H	-3.3861720000	3.5495970000	1.3666400000
H	-4.0453350000	4.3270490000	-0.0918880000

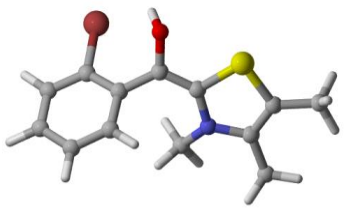
H	-2.4134970000	4.7426860000	0.4867180000
C	-2.1674560000	3.2940830000	-1.8896780000
H	-1.7417290000	2.4786530000	-2.4876270000
H	-1.4171580000	4.0929450000	-1.8324920000
H	-3.0476280000	3.6819540000	-2.4195590000
O	-1.3731160000	2.3066540000	0.1690490000
H	-3.2788640000	2.0044640000	-0.5785420000
H	-1.2672360000	1.2516490000	1.6489240000
H	-3.2784400000	-4.3933230000	-1.0638830000
H	-2.1263620000	-4.4068960000	1.1229650000
C	-0.6455940000	-2.4775040000	2.2870180000
H	-0.7083810000	-3.4839150000	2.7134230000
H	-1.0980830000	-1.7657560000	2.9831890000
H	0.4145260000	-2.2054400000	2.2168700000

thermodynamic data

Zero-point correction= 0.387871 (Hartree/Particle)
Thermal correction to Energy= 0.411256
Thermal correction to Enthalpy= 0.412200
Thermal correction to Gibbs Free Energy= 0.333952
Sum of electronic and zero-point Energies= -1265.798774
Sum of electronic and thermal Energies= -1265.775389
Sum of electronic and thermal Enthalpies= -1265.774444
Sum of electronic and thermal Free Energies= -1265.852693

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	258.067	86.918	164.688

B3LYP/6-31G*	**Breslowintermediat *o*-Br**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.5373120000	1.1010140000	-0.0368240000
C	-3.3644100000	2.3898160000	-0.5443320000
C	-2.1231470000	2.7663900000	-1.0592320000
C	-1.0698500000	1.8547880000	-1.0796190000
C	-1.2013200000	0.5469310000	-0.5681240000
C	-2.4666870000	0.2135880000	-0.0478040000
C	-0.0894930000	-0.4161190000	-0.6583660000

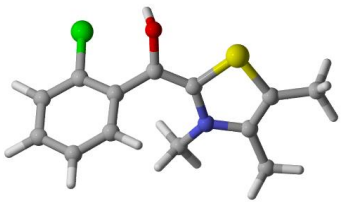
C	1.2172750000	-0.2099290000	-0.3333720000
O	-0.3367240000	-1.5955970000	-1.3731350000
S	2.4549140000	-1.3661040000	-0.8706290000
C	3.7282230000	-0.3979210000	-0.0936640000
C	3.2160300000	0.6856510000	0.5271550000
N	1.8100000000	0.8032650000	0.4214520000
C	5.1499340000	-0.8483380000	-0.2232610000
C	3.9820140000	1.7434330000	1.2658320000
C	1.0159480000	1.5754220000	1.3707870000
Br	-2.7410730000	-1.5161280000	0.7521610000
H	-4.4903150000	0.7905360000	0.3778980000
H	-4.1964640000	3.0879200000	-0.5350980000
H	-1.9809710000	3.7629440000	-1.4684330000
H	-0.1194340000	2.1339660000	-1.5254200000
H	-0.8484740000	-2.1966070000	-0.8027460000
H	5.2888980000	-1.8498040000	0.2049380000
H	5.4642550000	-0.9002910000	-1.2738740000
H	5.8337370000	-0.1712080000	0.2960790000
H	5.0535970000	1.6289210000	1.0917720000
H	3.6949540000	2.7482860000	0.9328290000
H	3.8236640000	1.6982110000	2.3514040000
H	1.6536740000	1.9345380000	2.1786340000
H	0.5261980000	2.4346990000	0.9003950000
H	0.2361640000	0.9336040000	1.7959170000

thermodynamic data

Zero-point correction= 0.242607 (Hartree/Particle)
Thermal correction to Energy= 0.260283
Thermal correction to Enthalpy= 0.261227
Thermal correction to Gibbs Free Energy= 0.196077
Sum of electronic and zero-point Energies= -3603.402458
Sum of electronic and thermal Energies= -3603.384782
Sum of electronic and thermal Enthalpies= -3603.383838
Sum of electronic and thermal Free Energies= -3603.448988

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.330	65.128	137.120

B3LYP/6-31G*	**Breslowintermediat *o*-Cl**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

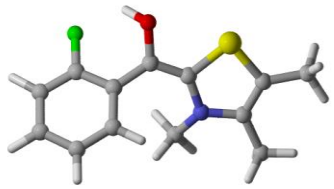
C	-3.9719970000	0.4803860000	0.1318130000
C	-3.9465800000	1.6930990000	-0.5582050000
C	-2.7630230000	2.1150800000	-1.1651600000
C	-1.6206620000	1.3219150000	-1.0911680000
C	-1.6015230000	0.0960090000	-0.3927380000
C	-2.8155100000	-0.2895850000	0.2123210000
C	-0.3963450000	-0.7479740000	-0.3826200000
C	0.8958530000	-0.3561330000	-0.1909400000
O	-0.5460990000	-2.0571370000	-0.8622320000
S	2.2214050000	-1.4589530000	-0.6199770000
C	3.4224910000	-0.2511960000	-0.1101150000
C	2.8295840000	0.8662050000	0.3612060000
N	1.4153660000	0.8216530000	0.3456410000
C	4.8756250000	-0.5741180000	-0.2688920000
C	3.5150020000	2.1055670000	0.8563840000
C	0.5961990000	1.6723890000	1.2012330000
Cl	-2.8960870000	-1.7759530000	1.1713520000
H	-4.8784630000	0.1364000000	0.6189170000
H	-4.8475270000	2.2965550000	-0.6199890000
H	-2.7350610000	3.0497780000	-1.7186360000
H	-0.7156680000	1.6261020000	-1.6092410000
H	-0.8243660000	-2.6280230000	-0.1258330000
H	5.1343210000	-0.7729880000	-1.3170740000
H	5.5088050000	0.2460110000	0.0806750000
H	5.1475480000	-1.4691340000	0.3060660000
H	4.5815810000	2.0675490000	0.6271200000
H	3.1034820000	3.0048300000	0.3820640000
H	3.4215410000	2.2336380000	1.9428800000
H	1.2359120000	2.2328260000	1.8828290000
H	-0.0109010000	2.3791340000	0.6256820000
H	-0.0836550000	1.0474260000	1.7908460000

thermodynamic data

Zero-point correction= 0.242876 (Hartree/Particle)
Thermal correction to Energy= 0.260421
Thermal correction to Enthalpy= 0.261365
Thermal correction to Gibbs Free Energy= 0.197182
Sum of electronic and zero-point Energies= -1491.890928
Sum of electronic and thermal Energies= -1491.873383
Sum of electronic and thermal Enthalpies= -1491.872439
Sum of electronic and thermal Free Energies= -1491.936622

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.417	64.946	135.084

B3LYP/6-31G*	**Breslowintermediat *o*-F**

xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

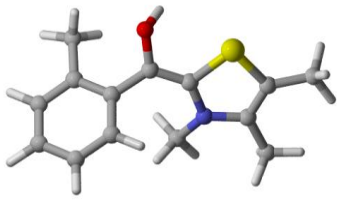
C	-4.1823030000	0.0557160000	0.2738050000
C	-4.2458480000	1.2611880000	-0.4297360000
C	-3.0906610000	1.7702170000	-1.0267340000
C	-1.8817910000	1.0829720000	-0.9245010000
C	-1.7725970000	-0.1238370000	-0.2024670000
C	-2.9654080000	-0.5962840000	0.3701140000
C	-0.5337770000	-0.9048130000	-0.1153190000
C	0.7455800000	-0.4434340000	-0.0384910000
O	-0.6366680000	-2.2827370000	-0.3347520000
S	2.1060040000	-1.5511540000	-0.3301250000
C	3.2599680000	-0.2124400000	-0.1310850000
C	2.6334510000	0.9438790000	0.1700400000
N	1.2230100000	0.8390060000	0.2558570000
C	4.7173420000	-0.4889710000	-0.3333230000
C	3.2737900000	2.2847350000	0.3815890000
C	0.4479870000	1.7210910000	1.1258490000
F	-2.9232010000	-1.7641110000	1.0820160000
H	-5.0539220000	-0.3785200000	0.7529070000
H	-5.1913410000	1.7884260000	-0.5144960000
H	-3.1349910000	2.6941520000	-1.5967470000
H	-1.0015690000	1.4567140000	-1.4387140000
H	-1.3055100000	-2.6293600000	0.2778650000
H	4.9234810000	-0.8585610000	-1.3462930000
H	5.3211350000	0.4090500000	-0.1758890000
H	5.0748650000	-1.2542330000	0.3681650000
H	4.3168750000	2.2648300000	0.0597470000
H	2.7599370000	3.0628950000	-0.1956480000
H	3.2663940000	2.5967620000	1.4342610000
H	1.1213410000	2.3632440000	1.6940520000
H	-0.2491700000	2.3530620000	0.5658790000
H	-0.1369140000	1.1157470000	1.8273350000

thermodynamic data

Zero-point correction= 0.244802 (Hartree/Particle)
Thermal correction to Energy= 0.261769
Thermal correction to Enthalpy= 0.262713
Thermal correction to Gibbs Free Energy= 0.200261
Sum of electronic and zero-point Energies= -1131.528969
Sum of electronic and thermal Energies= -1131.512002
Sum of electronic and thermal Enthalpies= -1131.511058
Sum of electronic and thermal Free Energies= -1131.573510

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.263	63.840	131.441

B3LYP/6-31G*	**Breslowintermediat *o*-Me**

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	-4.1345900000	0.1661400000	0.3333510000
C	-4.2156000000	1.2803500000	-0.5051680000
C	-3.0904940000	1.6790270000	-1.2245140000
C	-1.9047730000	0.9562730000	-1.1025160000
C	-1.8044880000	-0.1592380000	-0.2494050000
C	-2.9526110000	-0.5651190000	0.4805980000
C	-0.5393460000	-0.9086670000	-0.1829720000
C	0.7320630000	-0.4203290000	-0.1254000000
O	-0.6692760000	-2.2864660000	-0.4164010000
S	2.1142250000	-1.4847170000	-0.5023000000
C	3.2600020000	-0.1794630000	-0.1154180000
C	2.6122620000	0.9446640000	0.2601740000
N	1.2057990000	0.8347770000	0.2769600000
C	4.7241590000	-0.4436590000	-0.2778140000
C	3.2473080000	2.2549380000	0.6238910000
C	0.3555590000	1.7237890000	1.0580650000
C	-2.9131370000	-1.7376490000	1.4311980000
H	-5.0112640000	-0.1397060000	0.9005840000
H	-5.1508320000	1.8266340000	-0.5951630000
H	-3.1379470000	2.5342000000	-1.8939260000
H	-1.0384450000	1.2340610000	-1.6970490000
H	-0.1443650000	-2.7661260000	0.2476680000
H	4.9771440000	-0.7105250000	-1.3124450000
H	5.3207630000	0.4310960000	-0.0048090000
H	5.0501010000	-1.2766150000	0.3592440000
H	4.3133290000	2.2395260000	0.3902800000
H	2.7948480000	3.0837160000	0.0661410000
H	3.1520710000	2.4849400000	1.6930890000
H	0.9710510000	2.4485520000	1.5899770000
H	-0.3615910000	2.2605400000	0.4290650000
H	-0.2160560000	1.1378610000	1.7883320000
H	-2.0425000000	-1.6773680000	2.0972410000

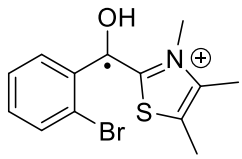
H	-3.8135590000	-1.7654810000	2.0533150000
H	-2.8346040000	-2.6878950000	0.8933310000

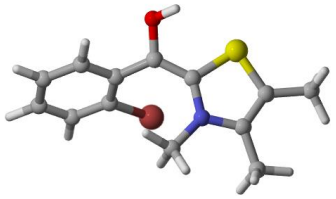
thermodynamic data

Zero-point correction= 0.280763 (Hartree/Particle)
Thermal correction to Energy= 0.298559
Thermal correction to Enthalpy= 0.299503
Thermal correction to Gibbs Free Energy= 0.235418
Sum of electronic and zero-point Energies= -1071.574935
Sum of electronic and thermal Energies= -1071.557138
Sum of electronic and thermal Enthalpies= -1071.556194
Sum of electronic and thermal Free Energies= -1071.620279

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	187.349	66.767	134.878

B3LYP/6-31G*	**Breslowintermediat rad *o*-Br**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	3.3602770000	-0.9147230000	-0.0727000000
C	4.3114690000	-0.0570710000	-0.6282450000
C	3.9829010000	1.2717590000	-0.9094880000
C	2.7000410000	1.7343180000	-0.6495120000
C	1.7050210000	0.8797590000	-0.1214940000
C	2.0747030000	-0.4492130000	0.1850210000
C	0.3904890000	1.4550360000	0.1534010000
O	0.4602080000	2.6650990000	0.7581130000
Br	0.8674900000	-1.6498820000	1.0533980000
C	-0.8805260000	0.8844180000	-0.0531300000
S	-2.2429170000	1.3505670000	0.9356210000
C	-3.2971690000	0.2462160000	0.0860640000
C	-2.6063220000	-0.4305740000	-0.8840010000
N	-1.2696070000	-0.0457310000	-0.9766370000
C	-4.7396910000	0.1545070000	0.4784440000
C	-3.1523650000	-1.4762600000	-1.8082010000
C	-0.3868660000	-0.5510180000	-2.0396140000
H	3.6202550000	-1.9356350000	0.1834160000
H	5.3127670000	-0.4282650000	-0.8239840000

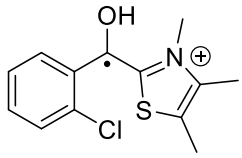
H	4.7252350000	1.9436600000	-1.3278240000
H	2.4386640000	2.7658060000	-0.8604460000
H	-0.3622240000	3.1770450000	0.6515510000
H	-5.2536990000	-0.6188270000	-0.0955760000
H	-4.8482010000	-0.0883080000	1.5413180000
H	-5.2574800000	1.1038360000	0.2986880000
H	-2.5343690000	-2.3801490000	-1.7961130000
H	-4.1605300000	-1.7598840000	-1.5050360000
H	-3.2097600000	-1.1164810000	-2.8426160000
H	-0.9787480000	-0.7343260000	-2.9351750000
H	0.3696580000	0.1994690000	-2.2612890000
H	0.0967860000	-1.4747360000	-1.7134940000

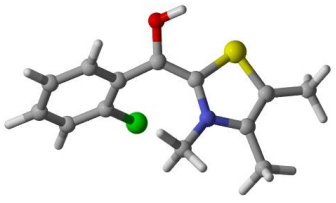
thermodynamic data

Zero-point correction= 0.244291 (Hartree/Particle)
Thermal correction to Energy= 0.261603
Thermal correction to Enthalpy= 0.262547
Thermal correction to Gibbs Free Energy= 0.197439
Sum of electronic and zero-point Energies= -3603.193924
Sum of electronic and thermal Energies= -3603.176613
Sum of electronic and thermal Enthalpies= -3603.175668
Sum of electronic and thermal Free Energies= -3603.240777

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.158	64.211	137.032

B3LYP/6-31G*	**Breslowintermediat rad *o*-Cl**





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.4100460000	1.1507750000	0.5651440000
C	-4.4078740000	0.5572180000	-0.2094180000
C	-4.1401190000	-0.6094010000	-0.9306850000
C	-2.8710980000	-1.1696910000	-0.8870830000
C	-1.8286170000	-0.5711020000	-0.1421160000
C	-2.1363290000	0.5907440000	0.6044070000
C	-0.5330510000	-1.2457310000	-0.1230980000
O	-0.6377620000	-2.5882400000	0.0255160000
Cl	-0.9616400000	1.3244810000	1.6860310000

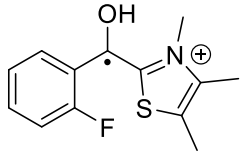
C	0.7546840000	-0.6769090000	-0.1617270000
S	2.1196570000	-1.4902440000	0.5663280000
C	3.1955930000	-0.1893090000	0.1139730000
C	2.5106680000	0.7963040000	-0.5457020000
N	1.1590400000	0.5020090000	-0.7240520000
C	4.6478290000	-0.2741290000	0.4703530000
C	3.0740980000	2.0795330000	-1.0764480000
C	0.2874010000	1.3445540000	-1.5586270000
H	-3.6219990000	2.0327700000	1.1594680000
H	-5.3984050000	1.0009780000	-0.2322790000
H	-4.9190950000	-1.0805760000	-1.5211330000
H	-2.6560120000	-2.0779880000	-1.4395580000
H	0.1627870000	-3.0544550000	-0.2769720000
H	5.1752550000	0.6373330000	0.1824800000
H	4.7857290000	-0.4162390000	1.5479060000
H	5.1297550000	-1.1151020000	-0.0416660000
H	2.4722500000	2.9386170000	-0.7624960000
H	4.0874710000	2.2311390000	-0.7035860000
H	3.1238090000	2.0806490000	-2.1720750000
H	0.8744730000	1.7544610000	-2.3798440000
H	-0.5146320000	0.7332750000	-1.9676070000
H	-0.1380260000	2.1576080000	-0.9660160000

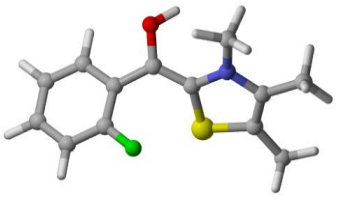
thermodynamic data

Zero-point correction= 0.244579 (Hartree/Particle)
Thermal correction to Energy= 0.261745
Thermal correction to Enthalpy= 0.262689
Thermal correction to Gibbs Free Energy= 0.198572
Sum of electronic and zero-point Energies= -1491.681136
Sum of electronic and thermal Energies= -1491.663970
Sum of electronic and thermal Enthalpies= -1491.663026
Sum of electronic and thermal Free Energies= -1491.727143

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.247	63.994	134.945

B3LYP/6-31G*	**Breslowintermediat rad *o*-F**	





xyz-matrix

31
XYZ file generated by gabedit : coordinates in Angstrom

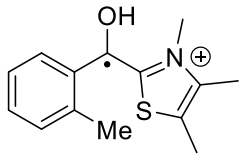
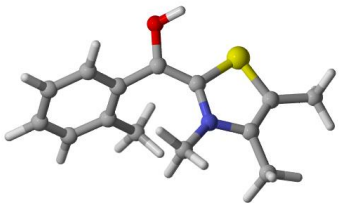
C	3.4472460000	-1.2681960000	-0.8223950000
C	4.4962560000	-0.7388940000	-0.0691910000
C	4.2812070000	0.3623360000	0.7698280000
C	3.0190890000	0.9279210000	0.8637540000
C	1.9246720000	0.3994900000	0.1341730000
C	2.1917590000	-0.6941980000	-0.7180420000
C	0.6290430000	1.0395860000	0.2280610000
O	0.6894880000	2.3796420000	0.4620480000
F	1.1996730000	-1.1844870000	-1.4884610000
C	-0.6218640000	0.3930970000	0.1297040000
S	-0.8799530000	-1.2589490000	0.6160890000
C	-2.6031360000	-1.1126240000	0.3829890000
C	-2.9327390000	0.1448150000	-0.0459290000
N	-1.8214090000	0.9761760000	-0.1998460000
C	-3.4858460000	-2.2964080000	0.6363330000
C	-4.3022950000	0.6598890000	-0.3696480000
C	-1.9359500000	2.2846370000	-0.8730690000
H	3.5906440000	-2.1022330000	-1.5006880000
H	5.4842460000	-1.1822160000	-0.1447810000
H	5.1011680000	0.7736970000	1.3490830000
H	2.8470110000	1.7809440000	1.5100710000
H	-0.0915800000	2.6878410000	0.9523900000
H	-4.5394410000	-2.0303500000	0.5307100000
H	-3.2716330000	-3.1041100000	-0.0731550000
H	-3.3397040000	-2.6929890000	1.6469820000
H	-4.4986600000	1.6183960000	0.1225280000
H	-4.4408460000	0.7994240000	-1.4487070000
H	-5.0619460000	-0.0461320000	-0.0326990000
H	-2.6131810000	2.1868670000	-1.7221130000
H	-2.3347540000	3.0405740000	-0.1890200000
H	-0.9598110000	2.5947880000	-1.2387530000

thermodynamic data

Zero-point correction= 0.245876 (Hartree/Particle)
Thermal correction to Energy= 0.262790
Thermal correction to Enthalpy= 0.263734
Thermal correction to Gibbs Free Energy= 0.200114
Sum of electronic and zero-point Energies= -1131.321046
Sum of electronic and thermal Energies= -1131.304132
Sum of electronic and thermal Enthalpies= -1131.303188
Sum of electronic and thermal Free Energies= -1131.366808

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.903	63.207	133.899

B3LYP/6-31G*	**Breslowintermediat rad *o*-Me**

xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	3.4002300000	1.1216220000	-0.9331640000
C	4.4032710000	0.7430110000	-0.0388540000
C	4.1671220000	-0.2696170000	0.8940090000
C	2.9203460000	-0.8783220000	0.9353760000
C	1.8847470000	-0.4651600000	0.0672540000
C	2.1313800000	0.5342190000	-0.9139810000
C	0.6057220000	-1.1615570000	0.1799060000
O	0.7198370000	-2.5086050000	0.2522560000
C	-0.6822010000	-0.5979650000	0.1550220000
S	-2.0724840000	-1.5119100000	-0.3894860000
C	-3.1310430000	-0.1422620000	-0.1311540000
C	-2.4257620000	0.9329580000	0.3376990000
N	-1.0682430000	0.6657830000	0.5238930000
C	-4.5922790000	-0.2741990000	-0.4318860000
C	-2.9733490000	2.2882880000	0.6697570000
C	-0.1865160000	1.6060240000	1.2372940000
C	1.1272440000	0.9150860000	-1.9807780000
H	3.6165870000	1.8739350000	-1.6866320000
H	5.3757040000	1.2239760000	-0.0873960000
H	4.9493280000	-0.5838490000	1.5776480000
H	2.7226900000	-1.6704530000	1.6501770000
H	-0.0747210000	-2.9259520000	0.6325270000
H	-5.1139600000	0.6699450000	-0.2636010000
H	-4.7598560000	-0.5700800000	-1.4735390000
H	-5.0581980000	-1.0318970000	0.2087180000
H	-2.3735120000	3.0838080000	0.2156040000
H	-3.9928440000	2.3876870000	0.2958230000
H	-3.0026390000	2.4620750000	1.7522760000
H	-0.7648210000	2.1158790000	2.0074930000
H	0.6218680000	1.0500200000	1.7065670000
H	0.2377680000	2.3429520000	0.5509170000
H	0.6132030000	0.0379070000	-2.3869440000
H	0.3553060000	1.6067180000	-1.6205830000
H	1.6333610000	1.4134930000	-2.8115590000

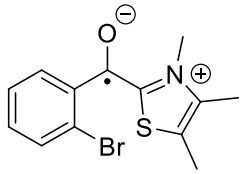
thermodynamic data

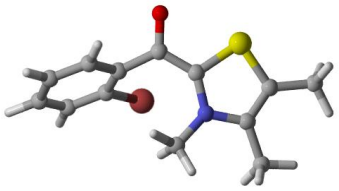
Zero-point correction= 0.282287 (Hartree/Particle)
Thermal correction to Energy= 0.299844
Thermal correction to Enthalpy= 0.300788
Thermal correction to Gibbs Free Energy= 0.236392
Sum of electronic and zero-point Energies= -1071.368357

Sum of electronic and thermal Energies= -1071.350801
Sum of electronic and thermal Enthalpies= -1071.349857
Sum of electronic and thermal Free Energies= -1071.414253

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.155	66.010	135.533

B3LYP/6-31G*	**Breslowintermediat radde *o*-Br**





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.4450560000	-0.7094300000	0.2359830000
C	-4.2558980000	0.2260210000	0.8759670000
C	-3.7795180000	1.5199960000	1.1030000000
C	-2.4933270000	1.8653750000	0.7002320000
C	-1.6382150000	0.9329730000	0.0865000000
C	-2.1559340000	-0.3458870000	-0.1542590000
C	-0.2977630000	1.4268740000	-0.3904820000
O	-0.2788220000	2.4258030000	-1.1529050000
Br	-1.1115360000	-1.6618880000	-1.0859010000
C	0.9462750000	0.8325170000	-0.0262280000
S	2.3605490000	1.3787940000	-0.9059980000
C	3.3759670000	0.2292600000	-0.0321840000
C	2.6572290000	-0.4665340000	0.8874380000
N	1.3013360000	-0.1097120000	0.9210850000
C	4.8345830000	0.1454540000	-0.3621150000
C	3.1693970000	-1.5259540000	1.8182700000
C	0.3830170000	-0.5891730000	1.9508190000
H	-3.8079030000	-1.7096310000	0.0250060000
H	-5.2602410000	-0.0541200000	1.1811800000
H	-4.4126430000	2.2587610000	1.5862910000
H	-2.1212140000	2.8750510000	0.8452640000
H	5.3453480000	-0.5957360000	0.2584080000
H	4.9924750000	-0.1321030000	-1.4119400000
H	5.3334080000	1.1100860000	-0.2034610000
H	2.5779550000	-2.4462210000	1.7455510000
H	4.2026330000	-1.7765970000	1.5724460000
H	3.1533450000	-1.2022730000	2.8670200000
H	0.9483190000	-0.8799590000	2.8365120000
H	-0.3012160000	0.2149650000	2.2246780000

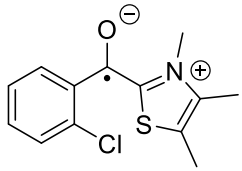
H -0.1986180000 -1.4442450000 1.5935470000

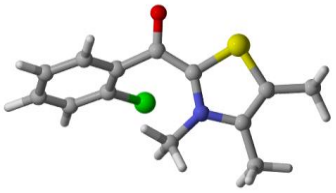
thermodynamic data

Zero-point correction= 0.231583 (Hartree/Particle)
Thermal correction to Energy= 0.248731
Thermal correction to Enthalpy= 0.249676
Thermal correction to Gibbs Free Energy= 0.184880
Sum of electronic and zero-point Energies= -3602.816498
Sum of electronic and thermal Energies= -3602.799349
Sum of electronic and thermal Enthalpies= -3602.798405
Sum of electronic and thermal Free Energies= -3602.863200

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.081	62.904	136.373

B3LYP/6-31G*	**Breslowintermediat radde *o*-Cl**





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	3.5227070000	-1.0195590000	0.4556330000
C	4.3996600000	-0.4447760000	-0.4617810000
C	3.9995230000	0.6707590000	-1.2019090000
C	2.7225590000	1.1939220000	-1.0272720000
C	1.8000900000	0.6120260000	-0.1394860000
C	2.2412310000	-0.4877570000	0.6112490000
C	0.4742160000	1.3071400000	0.0303730000
O	0.4850800000	2.5324410000	0.3102730000
Cl	1.2021090000	-1.2223580000	1.8388590000
C	-0.7866060000	0.6591820000	-0.1196170000
S	-2.2008280000	1.5551210000	0.4021890000
C	-3.2395550000	0.1773980000	0.0272590000
C	-2.5261010000	-0.8505640000	-0.5020860000
N	-1.1559550000	-0.5746520000	-0.6222610000
C	-4.7084980000	0.2728190000	0.3037420000
C	-3.0536900000	-2.1831000000	-0.9463500000
C	-0.2446420000	-1.4362460000	-1.3716920000
H	3.8272910000	-1.8660000000	1.0622750000
H	5.3961870000	-0.8598450000	-0.5839300000
H	4.6843180000	1.1352840000	-1.9057370000

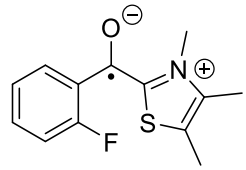
H	2.4076470000	2.0777480000	-1.5735550000
H	-5.2312420000	-0.6438010000	0.0177190000
H	-4.9052320000	0.4515940000	1.3683070000
H	-5.1636790000	1.1013230000	-0.2538320000
H	-2.4890190000	-3.0086190000	-0.4974090000
H	-4.0974260000	-2.2952820000	-0.6479620000
H	-3.0111250000	-2.3061270000	-2.0363570000
H	-0.8024950000	-1.9775140000	-2.1371810000
H	0.5077870000	-0.8196460000	-1.8637150000
H	0.2600560000	-2.1553980000	-0.7189950000

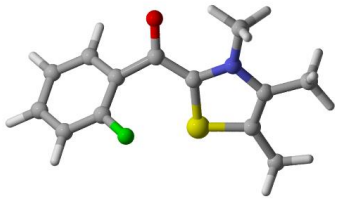
thermodynamic data

Zero-point correction= 0.231755 (Hartree/Particle)
Thermal correction to Energy= 0.248817
Thermal correction to Enthalpy= 0.249762
Thermal correction to Gibbs Free Energy= 0.185559
Sum of electronic and zero-point Energies= -1491.304186
Sum of electronic and thermal Energies= -1491.287123
Sum of electronic and thermal Enthalpies= -1491.286179
Sum of electronic and thermal Free Energies= -1491.350382

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.135	62.709	135.127

B3LYP/6-31G*	**Breslowintermediat radde *o*-F**





xyz-matrix

30
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.5207150000	-1.1545530000	0.7355850000
C	-4.4467410000	-0.7203740000	-0.2112220000
C	-4.1151830000	0.3197240000	-1.0849020000
C	-2.8581860000	0.9127650000	-1.0122250000
C	-1.8901660000	0.4742010000	-0.0927130000
C	-2.2700400000	-0.5483240000	0.7817040000
C	-0.5819570000	1.2165710000	-0.0328680000
O	-0.6193260000	2.4738810000	-0.0597490000
F	-1.4043260000	-0.9655430000	1.7365890000
C	0.6388820000	0.4714650000	-0.0333920000
S	0.7424000000	-1.2497510000	-0.3909400000

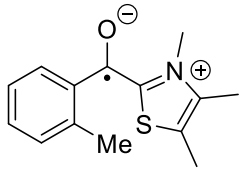
C	2.5032250000	-1.2045540000	-0.3330990000
C	2.9436700000	0.0517920000	-0.0614750000
N	1.9200270000	0.9884610000	0.0965060000
C	3.2747530000	-2.4644860000	-0.5763300000
C	4.3704940000	0.4941490000	0.0745440000
C	2.1915170000	2.3524090000	0.5621000000
H	-3.7512320000	-1.9403170000	1.4478020000
H	-5.4270420000	-1.1864420000	-0.2578390000
H	-4.8383570000	0.6698690000	-1.8158640000
H	-2.5961300000	1.7389760000	-1.6656810000
H	4.3500620000	-2.2992130000	-0.4685580000
H	2.9867790000	-3.2510320000	0.1325840000
H	3.0989630000	-2.8561540000	-1.5864640000
H	4.6364000000	1.2396290000	-0.6849310000
H	4.5653350000	0.9415720000	1.0563050000
H	5.0464010000	-0.3541770000	-0.0440090000
H	2.4950940000	2.3436510000	1.6164570000
H	2.9928660000	2.7932240000	-0.0363880000
H	1.2784960000	2.9313400000	0.4405300000

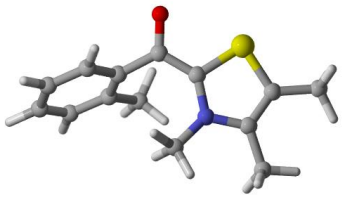
thermodynamic data

Zero-point correction= 0.233380 (Hartree/Particle)
Thermal correction to Energy= 0.249961
Thermal correction to Enthalpy= 0.250905
Thermal correction to Gibbs Free Energy= 0.187948
Sum of electronic and zero-point Energies= -1130.947682
Sum of electronic and thermal Energies= -1130.931101
Sum of electronic and thermal Enthalpies= -1130.930157
Sum of electronic and thermal Free Energies= -1130.993114

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.853	61.654	132.504

B3LYP/6-31G*	**Breslowintermediat radde *o*-Me**





xyz-matrix

33
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.5341800000	0.9163570000	0.9206230000
C	-4.4008750000	0.7037100000	-0.1513660000

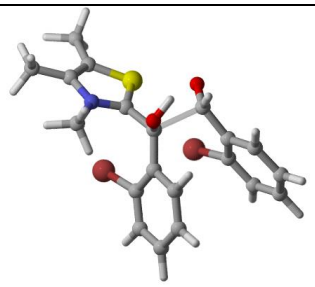
C	-4.0182670000	-0.1411170000	-1.1941550000
C	-2.7657060000	-0.7503560000	-1.1576100000
C	-1.8734510000	-0.5070210000	-0.1042800000
C	-2.2670930000	0.3188160000	0.9708580000
C	-0.5613230000	-1.2489050000	-0.1100320000
O	-0.5670300000	-2.5039230000	-0.0734910000
C	0.6997800000	-0.5809060000	-0.1388010000
S	2.1319830000	-1.5544130000	0.1440990000
C	3.1543590000	-0.1173200000	0.0367410000
C	2.4236570000	0.9940490000	-0.2397550000
N	1.0472270000	0.7433690000	-0.3636610000
C	4.6312130000	-0.2588840000	0.2432210000
C	2.9445520000	2.3912900000	-0.4103010000
C	0.1116820000	1.7098910000	-0.9387040000
C	-1.3830900000	0.5275650000	2.1822890000
H	-3.8506650000	1.5477420000	1.7482460000
H	-5.3766010000	1.1825550000	-0.1622040000
H	-4.6928790000	-0.3308310000	-2.0248280000
H	-2.4616550000	-1.4293870000	-1.9494040000
H	5.1476170000	0.6986060000	0.1343080000
H	4.8611490000	-0.6507440000	1.2421490000
H	5.0670040000	-0.9544190000	-0.4853410000
H	2.4056880000	3.1038590000	0.2254390000
H	3.9997540000	2.4370440000	-0.1356660000
H	2.8633040000	2.7432480000	-1.4468600000
H	0.6705970000	2.5238900000	-1.3990030000
H	-0.4939060000	1.2208450000	-1.7047970000
H	-0.5620830000	2.1235710000	-0.1830340000
H	-1.0167750000	-0.4278500000	2.5737680000
H	-0.4972880000	1.1366180000	1.9615130000
H	-1.9369010000	1.0306480000	2.9813180000

thermodynamic data

Zero-point correction= 0.269338 (Hartree/Particle)
Thermal correction to Energy= 0.286839
Thermal correction to Enthalpy= 0.287783
Thermal correction to Gibbs Free Energy= 0.222993
Sum of electronic and zero-point Energies= -1070.988491
Sum of electronic and thermal Energies= -1070.970991
Sum of electronic and thermal Enthalpies= -1070.970046
Sum of electronic and thermal Free Energies= -1071.034837

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.994	64.739	136.362

B3LYP/6-31G*	**TST3 *o*-Br**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	2.7339110000	-0.5959320000	-1.0622790000
C	3.8983350000	0.0625680000	-0.6635700000
C	2.7403960000	-1.9873100000	-1.5336770000
C	3.6206170000	1.2817510000	-0.1211260000
S	1.9131010000	1.6419390000	-0.1875240000
C	1.5830000000	0.0894880000	-0.8757150000
C	5.2427560000	-0.5756030000	-0.8497780000
C	4.5746430000	2.3054770000	0.4216420000
C	0.2663870000	-0.3897660000	-1.3506490000
C	-0.5086330000	-1.3846710000	-0.5488010000
O	0.4451830000	-0.9031470000	-2.6766930000
C	-0.3587760000	-1.7403430000	0.8075860000
C	-1.2034330000	-2.6538670000	1.4424240000
C	-2.2215310000	-3.2823190000	0.7347170000
C	-2.3761330000	-2.9914300000	-0.6217860000
C	-1.5409270000	-2.0698930000	-1.2360770000
C	-0.8197220000	1.3404470000	-1.6598170000
O	-0.2027800000	2.3493680000	-1.2174140000
C	-2.2245880000	1.0555410000	-1.1629420000
C	-3.2059210000	0.7380490000	-2.1122040000
C	-4.5410390000	0.5426260000	-1.7629160000
C	-4.9244880000	0.6609200000	-0.4277970000
C	-3.9704400000	0.9755170000	0.5404420000
C	-2.6422330000	1.1756140000	0.1690150000
H	3.6313220000	-2.4847640000	-1.1536620000
H	1.8551590000	-2.4925540000	-1.1509630000
H	2.7166640000	-2.0199690000	-2.6241020000
H	5.3717320000	-1.4664150000	-0.2224020000
H	6.0297790000	0.1310090000	-0.5798720000
H	5.4113510000	-0.8740620000	-1.8911140000
H	5.5349170000	1.8541670000	0.6865300000
H	4.7670440000	3.1051050000	-0.3043220000
H	4.1700490000	2.7753100000	1.3246250000
H	0.3317040000	-0.1463620000	-3.2784010000
Br	1.0619720000	-1.0778120000	1.9275780000
H	-1.0392160000	-2.8768850000	2.4908620000
H	-2.8713900000	-3.9946140000	1.2347560000
H	-3.1535870000	-3.4784690000	-1.2040330000
H	-1.6654870000	-1.8535700000	-2.2891350000
H	-0.7857500000	1.1451880000	-2.7665900000

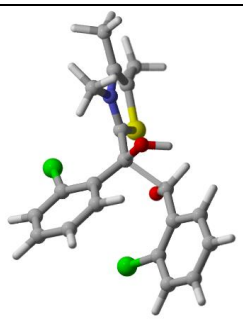
H	-2.9041130000	0.6581580000	-3.1549170000
H	-5.2753630000	0.3048190000	-2.5278730000
H	-5.9601120000	0.5138030000	-0.1333340000
H	-4.2509940000	1.0682730000	1.5843070000
Br	-1.4028160000	1.5791210000	1.5699930000

thermodynamic data

Zero-point correction= 0.343677 (Hartree/Particle)
Thermal correction to Energy= 0.369339
Thermal correction to Enthalpy= 0.370283
Thermal correction to Gibbs Free Energy= 0.285979
Sum of electronic and zero-point Energies= -6519.928936
Sum of electronic and thermal Energies= -6519.903274
Sum of electronic and thermal Enthalpies= -6519.902330
Sum of electronic and thermal Free Energies= -6519.986634

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	231.764	95.548	177.433

B3LYP/6-31G*	**TST3 *o*-Cl**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	2.7090130000	-0.0435620000	1.0663890000
C	3.9667600000	-0.4365170000	0.5835550000
C	2.5582950000	0.6627200000	2.3457410000
C	3.8782310000	-0.9627450000	-0.6657280000
S	2.2154110000	-1.0183650000	-1.2305260000
C	1.6583360000	-0.2927950000	0.2548960000
C	5.1930540000	-0.2389390000	1.4238240000
C	4.9727440000	-1.4781880000	-1.5519850000
C	0.2568800000	-0.1735650000	0.7088500000
C	-0.4935700000	1.1043660000	0.6107140000
O	0.1791330000	-0.6974670000	2.0355990000
C	-0.2281100000	2.2090680000	-0.2287810000
C	-1.0451320000	3.3399160000	-0.2576150000

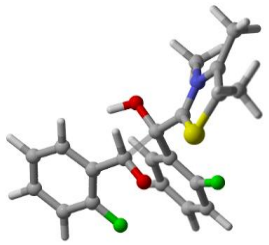
C	-2.1569060000	3.4292710000	0.5734950000
C	-2.4349020000	2.3727670000	1.4412770000
C	-1.6236440000	1.2463170000	1.4535150000
C	-0.6299060000	-1.5917330000	-0.5078060000
O	-0.2660210000	-1.3648860000	-1.6868300000
C	-2.0850400000	-1.5788230000	-0.0942270000
C	-2.4594690000	-2.3954860000	0.9858370000
C	-3.7722950000	-2.4854470000	1.4400470000
C	-4.7672720000	-1.7514460000	0.7947810000
C	-4.4349040000	-0.9450000000	-0.2918750000
C	-3.1117970000	-0.8592790000	-0.7320850000
H	3.4376670000	1.2861060000	2.5079280000
H	1.6720350000	1.2918560000	2.3010300000
H	2.4386770000	-0.0490570000	3.1652530000
H	5.4273690000	0.8223040000	1.5752210000
H	6.0563570000	-0.6975730000	0.9382440000
H	5.0868880000	-0.6995620000	2.4130700000
H	5.9597570000	-1.2894000000	-1.1213820000
H	4.8797020000	-2.5581640000	-1.7174860000
H	4.9404100000	-0.9939980000	-2.5348690000
H	0.0177510000	-1.6521520000	1.9377480000
Cl	1.1934690000	2.2892480000	-1.2827540000
H	-0.7898830000	4.1509310000	-0.9313870000
H	-2.7861140000	4.3141760000	0.5462100000
H	-3.2902510000	2.4203320000	2.1098810000
H	-1.8451620000	0.4332810000	2.1324090000
H	-0.0979870000	-2.3924610000	0.0810830000
H	-1.6914240000	-3.0045410000	1.4598770000
H	-4.0176200000	-3.1327570000	2.2774410000
H	-5.8009880000	-1.8110220000	1.1242790000
H	-5.1981000000	-0.3741770000	-0.8104990000
Cl	-2.8147490000	0.1805580000	-2.1136630000

thermodynamic data

Zero-point correction= 0.344571 (Hartree/Particle)
Thermal correction to Energy= 0.369711
Thermal correction to Enthalpy= 0.370655
Thermal correction to Gibbs Free Energy= 0.288573
Sum of electronic and zero-point Energies= -2296.903501
Sum of electronic and thermal Energies= -2296.878361
Sum of electronic and thermal Enthalpies= -2296.877417
Sum of electronic and thermal Free Energies= -2296.959499

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	231.997	94.972	172.757

B3LYP/6-31G*	**TST3 *o*-F**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	2.5696810000	-0.1235280000	1.1022920000
C	3.8511130000	-0.3972340000	0.5932830000
C	2.3661830000	0.2410870000	2.5121540000
C	3.8292320000	-0.5535340000	-0.7554900000
S	2.1995730000	-0.4166380000	-1.3998830000
C	1.5672620000	-0.1360100000	0.1980680000
C	5.0291170000	-0.4691750000	1.5186190000
C	4.9685130000	-0.8275600000	-1.6915280000
C	0.1393640000	-0.1034430000	0.5591550000
C	-0.6061560000	1.1898710000	0.4835370000
O	-0.0322610000	-0.7572880000	1.8122050000
C	-0.3703060000	2.2026130000	-0.4593410000
C	-1.1401710000	3.3532850000	-0.5489310000
C	-2.2031930000	3.5411160000	0.3336430000
C	-2.4601390000	2.5715790000	1.3026830000
C	-1.6762070000	1.4212360000	1.3706430000
C	-0.5728930000	-1.2748460000	-0.8558210000
O	-0.3000420000	-0.7387900000	-1.9695110000
C	-2.0052440000	-1.4943950000	-0.4161510000
C	-2.3190730000	-2.5953690000	0.3980120000
C	-3.6232730000	-2.8560670000	0.8266710000
C	-4.6577250000	-2.0121800000	0.4244850000
C	-4.3821720000	-0.9186650000	-0.3989740000
C	-3.0748370000	-0.6742810000	-0.8045240000
H	3.2410250000	0.7922030000	2.8584570000
H	1.4834560000	0.8705290000	2.5932410000
H	2.2133940000	-0.6508350000	3.1230740000
H	5.2781840000	0.5059410000	1.9563390000
H	5.9095260000	-0.8167400000	0.9750290000
H	4.8540530000	-1.1680940000	2.3448790000
H	4.9967070000	-0.0881030000	-2.5003770000
H	5.9310690000	-0.7904770000	-1.1743440000
H	4.8757240000	-1.8159570000	-2.1572250000
H	-0.7477740000	-1.4059530000	1.6818330000
F	0.6901640000	2.1110780000	-1.2992050000
H	-0.8869740000	4.0853330000	-1.3091840000
H	-2.8133450000	4.4372950000	0.2664360000
H	-3.2745910000	2.7052740000	2.0095410000
H	-1.8751990000	0.6791080000	2.1346210000
H	0.0361020000	-2.1522460000	-0.5116480000

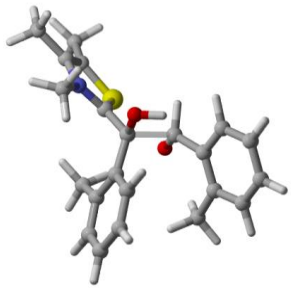
H	-1.5192180000	-3.2871870000	0.6600620000
H	-3.8294030000	-3.7206180000	1.4514230000
H	-5.6793990000	-2.2031800000	0.7410270000
H	-5.1643350000	-0.2443370000	-0.7331200000
F	-2.8577060000	0.3910770000	-1.5908740000

thermodynamic data

Zero-point correction= 0.347863 (Hartree/Particle)
Thermal correction to Energy= 0.372169
Thermal correction to Enthalpy= 0.373113
Thermal correction to Gibbs Free Energy= 0.293962
Sum of electronic and zero-point Energies= -1576.189024
Sum of electronic and thermal Energies= -1576.164718
Sum of electronic and thermal Enthalpies= -1576.163774
Sum of electronic and thermal Free Energies= -1576.242925

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.540	93.062	166.588

B3LYP/6-31G*	**TST3 *o*-Me**

xyz-matrix

51
XYZ file generated by gabedit : coordinates in Angstrom

N	2.5730320000	0.0438390000	1.0592040000
C	3.8517660000	-0.3385240000	0.6203830000
C	2.3579700000	0.6140230000	2.3969670000
C	3.8430440000	-0.7118930000	-0.6850080000
S	2.2248670000	-0.6381170000	-1.3669490000
C	1.5741080000	-0.0804030000	0.1571470000
C	5.0178220000	-0.2836670000	1.5618430000
C	4.9865790000	-1.1526970000	-1.5492980000
C	0.1487100000	0.0030850000	0.5215290000
C	-0.6224020000	1.2911560000	0.4069220000
O	0.0238390000	-0.5859770000	1.8162910000
C	-0.4186890000	2.3233420000	-0.5523070000
C	-1.2714430000	3.4357230000	-0.5333710000
C	-2.3115900000	3.5765550000	0.3833370000

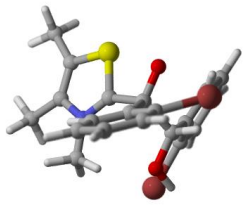
C	-2.5074630000	2.5730270000	1.3274130000
C	-1.6756080000	1.4572030000	1.3315310000
C	-0.5912180000	-1.2774890000	-0.8420810000
O	-0.3185410000	-0.7714310000	-1.9752480000
C	-2.0021450000	-1.5335370000	-0.3589860000
C	-2.1507110000	-2.5284850000	0.6255940000
C	-3.3921030000	-2.8543950000	1.1726290000
C	-4.5261010000	-2.1937490000	0.7069760000
C	-4.3983230000	-1.2346270000	-0.2988030000
C	-3.1590840000	-0.8785550000	-0.8482740000
H	3.2314530000	1.2077420000	2.6688870000
H	1.4763550000	1.2505000000	2.3719380000
H	2.1919470000	-0.1785310000	3.1291410000
H	5.2765860000	0.7438900000	1.8470650000
H	5.8989350000	-0.7237610000	1.0913170000
H	4.8204890000	-0.8434610000	2.4834380000
H	4.8652410000	-2.1928710000	-1.8743490000
H	5.0562230000	-0.5353190000	-2.4526550000
H	5.9406640000	-1.0767940000	-1.0208790000
H	-0.6755900000	-1.2605090000	1.7376220000
H	-1.1049970000	4.2190570000	-1.2696920000
H	-2.9487480000	4.4567310000	0.3598110000
H	-3.3048350000	2.6494940000	2.0624500000
H	-1.8325160000	0.6912090000	2.0796340000
H	0.0616680000	-2.1061420000	-0.4715800000
H	-1.2723180000	-3.0995780000	0.9273370000
H	-3.4712520000	-3.6290240000	1.9310220000
H	-5.5082680000	-2.4354470000	1.1053370000
H	-5.2910440000	-0.7419630000	-0.6786560000
C	0.6690800000	2.3147620000	-1.6031810000
H	0.6120660000	3.2258980000	-2.2076110000
H	0.5701880000	1.4535950000	-2.2677100000
H	1.6725570000	2.2854730000	-1.1599070000
C	-3.1202670000	0.1617030000	-1.9436270000
H	-4.0994290000	0.2341400000	-2.4305710000
H	-2.3517910000	-0.0774490000	-2.6792590000
H	-2.8766680000	1.1500520000	-1.5377300000

thermodynamic data

Zero-point correction= 0.420648 (Hartree/Particle)
Thermal correction to Energy= 0.446243
Thermal correction to Enthalpy= 0.447188
Thermal correction to Gibbs Free Energy= 0.365935
Sum of electronic and zero-point Energies= -1456.277986
Sum of electronic and thermal Energies= -1456.252391
Sum of electronic and thermal Enthalpies= -1456.251446
Sum of electronic and thermal Free Energies= -1456.332699

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	280.022	98.680	171.010

B3LYP/6-31G*	**Zwitterion2 *o*-Br**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

C	3.2238940000	-2.4534170000	0.4859570000
C	3.0032400000	-2.8939190000	1.7866130000
C	1.7291740000	-2.7701110000	2.3416930000
C	0.6975830000	-2.2071150000	1.5992520000
C	0.8885700000	-1.7230910000	0.2847720000
C	2.1782360000	-1.8783560000	-0.2421680000
C	-0.3568590000	-1.1210940000	-0.3575170000
C	-0.8614570000	0.2046220000	0.4000410000
C	-2.1315860000	0.7608300000	-0.3173460000
C	0.3104220000	1.2589080000	0.4145770000
O	-1.0958060000	-0.0051830000	1.6943790000
S	0.6486670000	1.5994030000	2.0551540000
C	1.9421310000	2.6952840000	1.5745650000
C	2.0706820000	2.7430320000	0.2187210000
N	1.1249680000	1.9157910000	-0.4221220000
C	-3.3658680000	0.0892110000	-0.2449510000
C	-4.5259850000	0.6045370000	-0.8217810000
C	-4.5031730000	1.8387090000	-1.4689350000
C	-3.3090030000	2.5496610000	-1.5245890000
C	-2.1549320000	2.0087780000	-0.9571000000
C	2.7503810000	3.4150280000	2.6130630000
C	3.0550420000	3.5183580000	-0.6056550000
H	3.8176530000	-3.3426710000	2.3487850000
H	-5.4134000000	2.2370640000	-1.9083320000
H	4.1981580000	-2.5585820000	0.0214080000
H	1.5334470000	-3.1194730000	3.3516300000
H	-0.2902660000	-2.0852070000	2.0263360000
Br	2.6775610000	-1.3951470000	-2.0590710000
H	-1.1695690000	-1.8292450000	-0.1727080000
Br	-3.6026640000	-1.5830700000	0.6753000000
H	-5.4476990000	0.0376800000	-0.7465410000
H	-3.2678150000	3.5243530000	-2.0036750000
H	-1.2474330000	2.5998170000	-0.9976640000
H	3.4950610000	4.0760980000	2.1616390000
H	2.1088410000	4.0272720000	3.2576330000
H	3.2814790000	2.7074250000	3.2608030000
H	2.5614350000	4.2280750000	-1.2806060000
H	3.7182050000	4.0905050000	0.0456170000

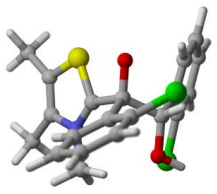
H	3.6811040000	2.8592740000	-1.2189630000
C	1.0792050000	1.8230410000	-1.8898700000
H	0.8959530000	2.8157680000	-2.3090420000
H	0.2983080000	1.1227270000	-2.1723920000
H	2.0334370000	1.4328880000	-2.2473130000
O	-0.2924350000	-0.8420160000	-1.7494350000
H	0.1260230000	-1.5869130000	-2.2078310000

thermodynamic data

Zero-point correction= 0.346430 (Hartree/Particle)
Thermal correction to Energy= 0.372050
Thermal correction to Enthalpy= 0.372994
Thermal correction to Gibbs Free Energy= 0.287891
Sum of electronic and zero-point Energies= -6519.941962
Sum of electronic and thermal Energies= -6519.916342
Sum of electronic and thermal Enthalpies= -6519.915398
Sum of electronic and thermal Free Energies= -6520.000502

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.465	96.360	179.116

B3LYP/6-31G*	**Zwitterion2 *o*-Cl**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.4500830000	-2.2775810000	0.4113340000
C	-3.5480830000	-2.8314670000	-0.8603930000
C	-2.4061470000	-2.9162930000	-1.6576990000
C	-1.1864440000	-2.4542930000	-1.1766860000
C	-1.0500830000	-1.8675210000	0.1014790000
C	-2.2190470000	-1.8026900000	0.8751040000
C	0.3652720000	-1.4138570000	0.4499940000
C	0.8697060000	-0.2013450000	-0.4737770000
C	2.2998390000	0.2590170000	-0.0430660000
C	-0.1730820000	0.9734520000	-0.3372030000
O	0.8313160000	-0.5061660000	-1.7682040000
S	-0.8340530000	1.2491030000	-1.8877400000
C	-1.8862030000	2.5009490000	-1.2307420000
C	-1.6992630000	2.6487610000	0.1112620000

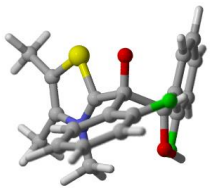
N	-0.7128790000	1.7657820000	0.5977990000
C	3.4308160000	-0.5713920000	-0.1724390000
C	4.7187870000	-0.1244230000	0.1245390000
C	4.9353050000	1.1899410000	0.5320240000
C	3.8484900000	2.0522250000	0.6280860000
C	2.5666690000	1.5821670000	0.3430670000
C	-2.8460170000	3.2293200000	-2.1238180000
C	-2.3972430000	3.5748130000	1.0621020000
H	-4.5061970000	-3.2013420000	-1.2152310000
H	5.9426570000	1.5303030000	0.7545310000
H	-4.3180720000	-2.2126190000	1.0588600000
H	-2.4606720000	-3.3508580000	-2.6519480000
H	-0.2985060000	-2.4911180000	-1.7963680000
Cl	-2.2661330000	-1.1503330000	2.5363650000
H	1.0243700000	-2.2341670000	0.1577720000
Cl	3.3445280000	-2.2393540000	-0.7530700000
H	5.5499380000	-0.8136490000	0.0182320000
H	3.9892870000	3.0899220000	0.9188760000
H	1.7473730000	2.2894680000	0.4015210000
H	-3.3674920000	4.0298030000	-1.5919570000
H	-2.3262960000	3.6800230000	-2.9771820000
H	-3.6048130000	2.5481660000	-2.5274850000
H	-1.6943330000	4.2278900000	1.5928040000
H	-3.0946510000	4.2141570000	0.5176900000
H	-2.9729490000	3.0249780000	1.8166850000
C	-0.3058770000	1.7894580000	2.0122740000
H	0.1553230000	2.7546680000	2.2399110000
H	0.3859690000	0.9714660000	2.1928580000
H	-1.1886310000	1.6449630000	2.6369800000
O	0.6117350000	-1.0768450000	1.8092060000
H	0.2917050000	-1.7948540000	2.3760170000

thermodynamic data

Zero-point correction= 0.347137 (Hartree/Particle)
Thermal correction to Energy= 0.372325
Thermal correction to Enthalpy= 0.373269
Thermal correction to Gibbs Free Energy= 0.291555
Sum of electronic and zero-point Energies= -2296.916615
Sum of electronic and thermal Energies= -2296.891427
Sum of electronic and thermal Enthalpies= -2296.890483
Sum of electronic and thermal Free Energies= -2296.972197

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.637	95.861	171.981

B3LYP/6-31G*	**Zwitterion2 *o*-F**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

C	-3.4629610000	-2.0113780000	0.8751630000
C	-3.8774520000	-2.4366270000	-0.3853100000
C	-2.9317730000	-2.6029630000	-1.3998390000
C	-1.5827070000	-2.3578760000	-1.1517290000
C	-1.1298260000	-1.9221790000	0.1087150000
C	-2.1128960000	-1.7594860000	1.0870260000
C	0.3554170000	-1.6659440000	0.2865270000
C	0.8507900000	-0.4035010000	-0.5626890000
C	2.3213490000	-0.0454230000	-0.2002310000
C	-0.0936280000	0.8045170000	-0.2570310000
O	0.6976460000	-0.6130310000	-1.8714920000
S	-0.8367350000	1.2823480000	-1.7168100000
C	-1.7359830000	2.5348950000	-0.8586180000
C	-1.4398860000	2.5317310000	0.4720590000
N	-0.4955900000	1.5335880000	0.7895940000
C	3.3372520000	-1.0025310000	-0.3256950000
C	4.6828940000	-0.7163390000	-0.1420530000
C	5.0721360000	0.5892350000	0.1590500000
C	4.0998430000	1.5797780000	0.2696340000
C	2.7521800000	1.2565820000	0.0886200000
C	-2.6922750000	3.4223890000	-1.5982820000
C	-1.9800240000	3.4103060000	1.5607290000
H	-4.9287350000	-2.6412130000	-0.5677380000
H	6.1235840000	0.8233990000	0.2998880000
H	-4.1582090000	-1.8750820000	1.6974090000
H	-3.2435810000	-2.9328110000	-2.3867720000
H	-0.8428280000	-2.4553200000	-1.9376180000
F	-1.7620230000	-1.3451590000	2.3507420000
H	0.8881860000	-2.4926630000	-0.1878140000
F	3.0273720000	-2.2855120000	-0.6282590000
H	5.4034060000	-1.5215090000	-0.2456190000
H	4.3826450000	2.6056660000	0.4899940000
H	2.0195920000	2.0552180000	0.1607790000
H	-3.1580590000	4.1576520000	-0.9364720000
H	-2.1838830000	3.9710390000	-2.3998560000
H	-3.4943680000	2.8365710000	-2.0628370000
H	-2.5064910000	2.8317910000	2.3295650000
H	-1.1871320000	3.9792020000	2.0612970000
H	-2.6886890000	4.1292470000	1.1456280000
C	-0.0015080000	1.3443680000	2.1621170000
H	0.4792420000	2.2641560000	2.5050270000
H	0.6982260000	0.5113760000	2.1670220000

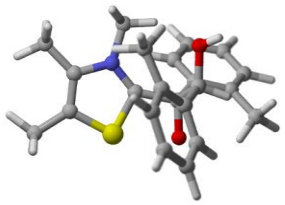
H	-0.8426820000	1.0987790000	2.8138820000
O	0.7971040000	-1.5410930000	1.6394760000
H	0.1648640000	-1.9864730000	2.2208410000

thermodynamic data

Zero-point correction= 0.349708 (Hartree/Particle)
Thermal correction to Energy= 0.374438
Thermal correction to Enthalpy= 0.375383
Thermal correction to Gibbs Free Energy= 0.294620
Sum of electronic and zero-point Energies= -1576.202220
Sum of electronic and thermal Energies= -1576.177489
Sum of electronic and thermal Enthalpies= -1576.176545
Sum of electronic and thermal Free Energies= -1576.257308

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.964	94.215	169.979

B3LYP/6-31G*	**Zwitterion2 *o*-Me**

xyz-matrix

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XYZ file generated by gabedit : coordinates in Angstrom

C	-3.5797780000	-2.0582540000	0.8065110000
C	-3.7634320000	-2.8674680000	-0.3085910000
C	-2.6583960000	-3.2038550000	-1.0898950000
C	-1.3992810000	-2.7378690000	-0.7289490000
C	-1.1956970000	-1.9112830000	0.3942370000
C	-2.3192980000	-1.5553520000	1.1767630000
C	0.2646740000	-1.5180400000	0.6283840000
C	0.8208320000	-0.4272410000	-0.4038010000
C	2.3327590000	-0.1351040000	-0.1361470000
C	-0.0586620000	0.8606990000	-0.2815330000
O	0.6024110000	-0.8243270000	-1.6671960000
S	-0.8402610000	1.0843100000	-1.7822820000
C	-1.6579770000	2.5164650000	-1.1523090000
C	-1.3113710000	2.7546800000	0.1439220000
N	-0.3950620000	1.7932060000	0.6208950000
C	3.3081760000	-1.1386400000	-0.3741890000
C	4.6588020000	-0.8294490000	-0.1680510000

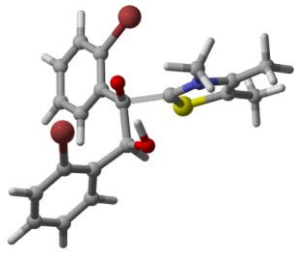
C	5.0873280000	0.4364430000	0.2281930000
C	4.1399640000	1.4383190000	0.4012430000
C	2.7883320000	1.1429440000	0.2148570000
C	-2.6092300000	3.2878420000	-2.0180460000
C	-1.7747800000	3.8523270000	1.0553200000
H	-4.7550520000	-3.2366310000	-0.5584690000
H	6.1459080000	0.6381160000	0.3706850000
H	-4.4381720000	-1.7974500000	1.4229840000
H	-2.7714620000	-3.8344380000	-1.9678960000
H	-0.5392230000	-2.9864530000	-1.3386760000
H	0.8584800000	-2.3993810000	0.3772520000
H	5.3970840000	-1.6083110000	-0.3490570000
H	4.4408530000	2.4480450000	0.6702690000
H	2.0812340000	1.9576290000	0.3188940000
H	-2.9824280000	4.1840320000	-1.5146990000
H	-2.1256710000	3.6060520000	-2.9489690000
H	-3.4758530000	2.6754660000	-2.2949190000
H	-0.9412680000	4.4620950000	1.4244100000
H	-2.4569430000	4.5163980000	0.5214750000
H	-2.3114400000	3.4631770000	1.9294640000
C	0.1453630000	1.8699760000	1.9870200000
H	0.7376030000	2.7826620000	2.0952810000
H	0.7561800000	0.9918490000	2.1766520000
H	-0.6822920000	1.8881940000	2.6987400000
O	0.5954490000	-1.1287630000	1.9679820000
H	0.5203350000	-1.9150250000	2.5307540000
C	2.9832080000	-2.5246970000	-0.8941980000
H	3.8431260000	-2.9308510000	-1.4381480000
H	2.1237620000	-2.4778450000	-1.5657410000
H	2.7622620000	-3.2325010000	-0.0830810000
C	-2.3028070000	-0.6373770000	2.3862910000
H	-1.3499640000	-0.6416410000	2.9107660000
H	-3.0958720000	-0.9206030000	3.0873240000
H	-2.5068140000	0.4003370000	2.0864640000

thermodynamic data

Zero-point correction= 0.422808 (Hartree/Particle)
Thermal correction to Energy= 0.448552
Thermal correction to Enthalpy= 0.449496
Thermal correction to Gibbs Free Energy= 0.367851
Sum of electronic and zero-point Energies= -1456.282498
Sum of electronic and thermal Energies= -1456.256754
Sum of electronic and thermal Enthalpies= -1456.255810
Sum of electronic and thermal Free Energies= -1456.337455

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	281.470	99.640	171.836

B3LYP/6-31G*	**TST5 *o*-Br**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	-2.3629530000	-1.5001830000	-0.4644430000
C	-3.5661710000	-1.9377070000	0.1314590000
C	-2.0109980000	-1.8637990000	-1.8502540000
C	-3.7105010000	-1.4607890000	1.3966860000
S	-2.3230720000	-0.4642740000	1.8005900000
C	-1.5749050000	-0.7208900000	0.2718990000
C	-4.4992670000	-2.8229660000	-0.6365720000
C	-4.8276470000	-1.6650940000	2.3747430000
C	0.1053270000	-0.0289170000	-0.2184290000
C	-0.0198160000	1.3752400000	0.3983300000
O	0.2543440000	-0.0596090000	-1.4840390000
C	0.7524530000	1.8008800000	1.4883980000
C	0.6792790000	3.1013460000	1.9916800000
C	-0.1857720000	4.0241530000	1.4126520000
C	-0.9840590000	3.6304660000	0.3385520000
C	-0.8959070000	2.3301020000	-0.1505670000
C	0.9764090000	-1.1657510000	0.5145000000
O	0.9072710000	-2.2653780000	-0.3702530000
C	2.4304090000	-0.8730690000	0.9078230000
C	2.7395130000	-0.9418440000	2.2794690000
C	4.0239910000	-0.7433740000	2.7780700000
C	5.0673490000	-0.4786100000	1.8923650000
C	4.8062890000	-0.4313240000	0.5255220000
C	3.5102460000	-0.6319830000	0.0423230000
H	-2.8790340000	-1.6952050000	-2.4907930000
H	-1.1825470000	-1.2216020000	-2.1526820000
H	-1.7144950000	-2.9150860000	-1.8856330000
H	-3.9904700000	-3.7222660000	-1.0017640000
H	-4.9261450000	-2.3080290000	-1.5056300000
H	-5.3279590000	-3.1434060000	-0.0023150000
H	-5.5811420000	-2.3494000000	1.9755290000
H	-4.4601980000	-2.0872530000	3.3171560000
H	-5.3287250000	-0.7187040000	2.6100770000
H	1.4449210000	1.1096290000	1.9477840000
H	1.3063600000	3.3858220000	2.8321750000
H	-0.2506110000	5.0413650000	1.7889460000
H	-1.6789180000	4.3252000000	-0.1206660000
Br	-2.1038380000	1.8976690000	-1.5796160000

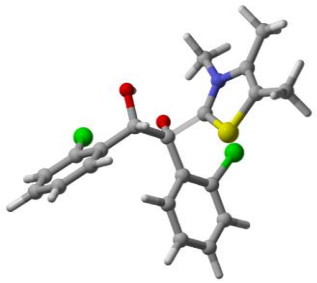
H	0.4777410000	-1.4591560000	1.4435860000
H	0.8853830000	-1.8107930000	-1.2469400000
H	1.9319250000	-1.1630760000	2.9745710000
H	4.2076410000	-0.8061880000	3.8471050000
H	6.0798930000	-0.3230010000	2.2542050000
H	5.6066330000	-0.2446260000	-0.1822040000
Br	3.3295320000	-0.5931290000	-1.8620530000

thermodynamic data

Zero-point correction= 0.345639 (Hartree/Particle)
Thermal correction to Energy= 0.370927
Thermal correction to Enthalpy= 0.371871
Thermal correction to Gibbs Free Energy= 0.287442
Sum of electronic and zero-point Energies= -6519.942615
Sum of electronic and thermal Energies= -6519.917327
Sum of electronic and thermal Enthalpies= -6519.916383
Sum of electronic and thermal Free Energies= -6520.000812

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	232.760	94.277	177.696

B3LYP/6-31G*	**TST5 *o*-Cl**



xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	-2.4724870000	-1.1924440000	-0.5240370000
C	-3.6921920000	-1.3937770000	0.1600550000
C	-2.2262710000	-1.7898460000	-1.8519540000
C	-3.7110320000	-0.7615600000	1.3639680000
S	-2.1873440000	0.0775890000	1.6007900000
C	-1.5521270000	-0.4534130000	0.0910750000
C	-4.7706670000	-2.2249010000	-0.4651460000
C	-4.7974350000	-0.6989170000	2.3946560000
C	0.1620720000	-0.0316340000	-0.5533720000
C	0.2481970000	1.4288240000	-0.0784560000
O	0.2210860000	-0.2173710000	-1.8129560000
C	1.0660520000	1.8258250000	0.9894360000

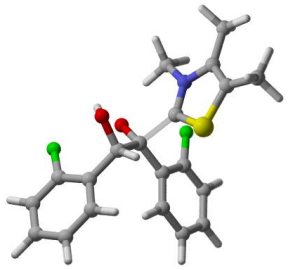
C	1.1883890000	3.1593240000	1.3832050000
C	0.4784780000	4.1487010000	0.7104220000
C	-0.3633970000	3.7895200000	-0.3413130000
C	-0.4760530000	2.4532540000	-0.7214990000
C	0.9462260000	-1.1856410000	0.2551620000
O	0.7243210000	-2.3434240000	-0.5223390000
C	2.4393640000	-1.0231270000	0.5717350000
C	2.8068900000	-1.0785760000	1.9291750000
C	4.1279770000	-1.0013060000	2.3614900000
C	5.1486170000	-0.8782960000	1.4201720000
C	4.8278590000	-0.8456820000	0.0658420000
C	3.4956670000	-0.9227360000	-0.3510760000
H	-3.1081950000	-1.6396500000	-2.4770910000
H	-1.3602320000	-1.2811900000	-2.2781210000
H	-2.0228380000	-2.8573490000	-1.7359020000
H	-4.4006170000	-3.2165500000	-0.7487500000
H	-5.1773070000	-1.7523800000	-1.3674990000
H	-5.5962120000	-2.3650960000	0.2352600000
H	-5.6523050000	-1.3154680000	2.1041770000
H	-4.4438960000	-1.0565390000	3.3685290000
H	-5.1582400000	0.3274070000	2.5308580000
H	1.6410530000	1.0784740000	1.5181170000
H	1.8447720000	3.4160930000	2.2100620000
H	0.5671050000	5.1925610000	0.9985340000
H	-0.9413470000	4.5398510000	-0.8706020000
Cl	-1.6350070000	2.1198940000	-2.0102220000
H	0.4607100000	-1.3381170000	1.2245630000
H	0.6744800000	-1.9547880000	-1.4317590000
H	2.0155460000	-1.1911080000	2.6676460000
H	4.3562250000	-1.0481170000	3.4227120000
H	6.1881270000	-0.8191530000	1.7304970000
H	5.6069490000	-0.7646740000	-0.6848180000
Cl	3.2331380000	-0.9115630000	-2.0885960000

thermodynamic data

Zero-point correction= 0.346571 (Hartree/Particle)
Thermal correction to Energy= 0.371311
Thermal correction to Enthalpy= 0.372255
Thermal correction to Gibbs Free Energy= 0.290164
Sum of electronic and zero-point Energies= -2296.918547
Sum of electronic and thermal Energies= -2296.893806
Sum of electronic and thermal Enthalpies= -2296.892862
Sum of electronic and thermal Free Energies= -2296.974954

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.001	93.505	172.777

B3LYP/6-31G*	**TST5 *o*-F**

xyz-matrix

45
XYZ file generated by gabedit : coordinates in Angstrom

N	-2.5273780000	-0.6934900000	-0.7275370000
C	-3.7439710000	-0.9549310000	-0.0557760000
C	-2.4485000000	-0.7440420000	-2.2019480000
C	-3.6201870000	-0.8326280000	1.2922460000
S	-1.9661070000	-0.3899580000	1.6786210000
C	-1.4745900000	-0.3858230000	0.0286620000
C	-4.9655870000	-1.3188490000	-0.8429170000
C	-4.6436250000	-1.0242460000	2.3701890000
C	0.2749920000	-0.0149510000	-0.5846500000
C	0.3687280000	1.4583820000	-0.1675770000
O	0.3593540000	-0.2616690000	-1.8329900000
C	1.2272240000	1.9517360000	0.8230380000
C	1.3131010000	3.3163670000	1.1139220000
C	0.5310630000	4.2318750000	0.4137520000
C	-0.3454330000	3.7739230000	-0.5714100000
C	-0.4078020000	2.4140490000	-0.8385640000
C	1.0151800000	-1.1217930000	0.2849940000
O	0.6245450000	-2.3432590000	-0.3139000000
C	2.5362020000	-1.0219660000	0.3683450000
C	3.1605110000	-0.8478940000	1.6126760000
C	4.5477120000	-0.7997270000	1.7533520000
C	5.3589310000	-0.9479020000	0.6282610000
C	4.7734100000	-1.1544200000	-0.6200680000
C	3.3872540000	-1.1981000000	-0.7296500000
H	-3.1174310000	0.0122350000	-2.6193500000
H	-1.4146030000	-0.5336290000	-2.4817440000
H	-2.7529360000	-1.7372660000	-2.5413400000
H	-4.8216320000	-2.2482720000	-1.4066240000
H	-5.2323350000	-0.5356670000	-1.5619270000
H	-5.8180080000	-1.4635640000	-0.1765560000
H	-5.6231130000	-1.2615170000	1.9462400000
H	-4.3645120000	-1.8434480000	3.0431920000
H	-4.7546620000	-0.1197450000	2.9793660000
H	1.8597000000	1.2637870000	1.3680890000
H	1.9997310000	3.6579360000	1.8834440000
H	0.5939870000	5.2947460000	0.6299250000
H	-0.9830690000	4.4488310000	-1.1336170000
F	-1.3089050000	2.0111450000	-1.7674110000
H	0.6443250000	-1.1200640000	1.3163370000
H	0.5685740000	-2.0792490000	-1.2637770000

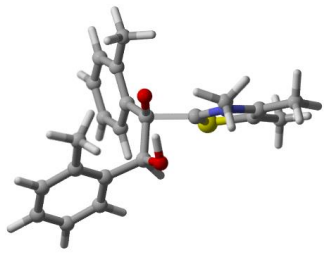
H	2.5325470000	-0.7547130000	2.4969380000
H	4.9893670000	-0.6604830000	2.7360470000
H	6.4411070000	-0.9142610000	0.7185410000
H	5.3692570000	-1.2915890000	-1.5168220000
F	2.8749250000	-1.4395080000	-1.9512180000

thermodynamic data

Zero-point correction= 0.349433 (Hartree/Particle)
Thermal correction to Energy= 0.373463
Thermal correction to Enthalpy= 0.374407
Thermal correction to Gibbs Free Energy= 0.294126
Sum of electronic and zero-point Energies= -1576.201502
Sum of electronic and thermal Energies= -1576.177473
Sum of electronic and thermal Enthalpies= -1576.176529
Sum of electronic and thermal Free Energies= -1576.256809

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.351	91.771	168.965

B3LYP/6-31G*	**TST5 *o*-Me**

xyz-matrix

51
XYZ file generated by gabedit : coordinates in Angstrom

N	-2.5731400000	-1.0992010000	-0.4301220000
C	-3.8397110000	-0.9607390000	0.1822610000
C	-2.3306190000	-2.1201100000	-1.4695160000
C	-3.8450440000	0.0276380000	1.1160590000
S	-2.2534190000	0.7616700000	1.1952950000
C	-1.6011750000	-0.2890650000	-0.0044790000
C	-4.9743220000	-1.8513830000	-0.2246180000
C	-4.9664870000	0.5179800000	1.9816710000
C	0.1941890000	-0.2110980000	-0.6743670000
C	0.4678390000	1.2817850000	-0.4769290000
O	0.1913470000	-0.6707890000	-1.8711560000
C	0.8149330000	1.7608150000	0.7958630000
C	1.0637450000	3.1106140000	1.0396110000
C	0.9645810000	4.0201490000	-0.0089850000
C	0.6081420000	3.5615500000	-1.2757750000

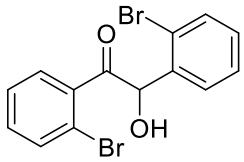
C	0.3491050000	2.2089350000	-1.5432500000
C	0.8646550000	-1.2458930000	0.3561710000
O	0.5612600000	-2.5228670000	-0.1777490000
C	2.3647250000	-1.0818160000	0.6319500000
C	2.7334730000	-0.7795850000	1.9512520000
C	4.0622810000	-0.6275520000	2.3429930000
C	5.0684850000	-0.7933930000	1.3956660000
C	4.7222080000	-1.1263510000	0.0868670000
C	3.3906790000	-1.2875700000	-0.3218900000
H	-3.2110150000	-2.1916300000	-2.1095100000
H	-1.4625360000	-1.7948000000	-2.0430340000
H	-2.1264310000	-3.0830600000	-0.9957170000
H	-4.7032780000	-2.9103820000	-0.1476870000
H	-5.2924710000	-1.6643410000	-1.2575490000
H	-5.8381300000	-1.6818360000	0.4211210000
H	-4.6997530000	0.4695040000	3.0436350000
H	-5.2194040000	1.5600020000	1.7528600000
H	-5.8691480000	-0.0819910000	1.8378160000
H	0.9082070000	1.0642850000	1.6197200000
H	1.3401940000	3.4397700000	2.0377980000
H	1.1598850000	5.0771730000	0.1531510000
H	0.5219170000	4.2742130000	-2.0931520000
H	0.3613710000	-1.1708780000	1.3260680000
H	0.4849600000	-2.3122750000	-1.1403530000
H	1.9507720000	-0.6713620000	2.7004370000
H	4.3035120000	-0.3904710000	3.3760610000
H	6.1140070000	-0.6789370000	1.6706530000
H	5.5093560000	-1.2764870000	-0.6490310000
C	-0.0557490000	1.8402420000	-2.9547280000
H	-0.1607690000	2.7485900000	-3.5591650000
H	-1.0030930000	1.2942010000	-2.9794520000
H	0.6771990000	1.1822180000	-3.4268350000
C	3.1295770000	-1.7218670000	-1.7466130000
H	4.0500450000	-1.6673680000	-2.3371280000
H	2.3599080000	-1.1161400000	-2.2292820000
H	2.7774600000	-2.7607820000	-1.7693440000

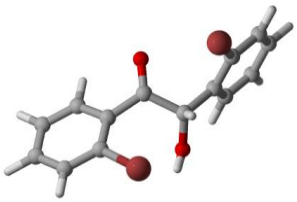
thermodynamic data

Zero-point correction= 0.422581 (Hartree/Particle)
Thermal correction to Energy= 0.447771
Thermal correction to Enthalpy= 0.448715
Thermal correction to Gibbs Free Energy= 0.366821
Sum of electronic and zero-point Energies= -1456.295265
Sum of electronic and thermal Energies= -1456.270076
Sum of electronic and thermal Enthalpies= -1456.269131
Sum of electronic and thermal Free Energies= -1456.351025

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	280.980	97.169	172.360

B3LYP/6-31G*	***o*-Br-Benzoin**





xyz-matrix

28
XYZ file generated by gabedit : coordinates in Angstrom

C	4.1722440000	0.2341000000	-0.0744760000
C	4.6314670000	1.3545370000	-0.7648200000
C	3.7193280000	2.2160010000	-1.3750420000
C	2.3572030000	1.9523280000	-1.2853540000
C	1.8582820000	0.8469720000	-0.5723780000
C	2.8022060000	-0.0043550000	0.0189710000
C	0.3486430000	0.7084690000	-0.5884960000
C	-0.4017650000	0.2282410000	0.6845440000
O	-0.2583680000	1.0492120000	-1.5844990000
C	-1.8529180000	0.6666740000	0.6579920000
O	0.2350900000	0.7444880000	1.8453470000
C	-2.8285760000	-0.0180410000	-0.0741800000
C	-4.1586830000	0.3960440000	-0.0968720000
C	-4.5356970000	1.5254010000	0.6284550000
C	-3.5830520000	2.2239390000	1.3705510000
C	-2.2574300000	1.7944440000	1.3824660000
Br	2.3006930000	-1.6151350000	0.9544450000
Br	-2.3685650000	-1.5903180000	-1.0712180000
H	4.8692500000	-0.4569880000	0.3863410000
H	5.6993390000	1.5431620000	-0.8278740000
H	4.0676530000	3.0864290000	-1.9229860000
H	1.6350400000	2.5996760000	-1.7716610000
H	-0.3686910000	-0.8681200000	0.6676360000
H	0.8733900000	0.0794030000	2.1497230000
H	-4.8860540000	-0.1640210000	-0.6741600000
H	-5.5722420000	1.8506230000	0.6136680000
H	-3.8708280000	3.1014960000	1.9426000000
H	-1.5126270000	2.3210530000	1.9688170000

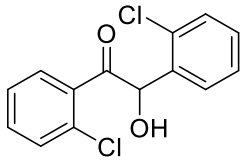
thermodynamic data

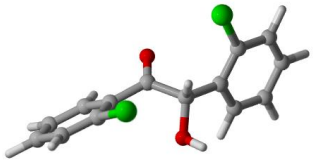
Zero-point correction= 0.203994 (Hartree/Particle)
Thermal correction to Energy= 0.220146
Thermal correction to Enthalpy= 0.221091
Thermal correction to Gibbs Free Energy= 0.157244
Sum of electronic and zero-point Energies= -5833.147829
Sum of electronic and thermal Energies= -5833.131677
Sum of electronic and thermal Enthalpies= -5833.130733

Sum of electronic and thermal Free Energies= -5833.194579

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.144	60.336	134.376

B3LYP/6-31G*	***o*-Cl-Benzoin**





xyz-matrix

28
XYZ file generated by gabedit : coordinates in Angstrom

C	4.1482230000	-0.2480580000	0.3001460000
C	4.6923860000	0.9077890000	-0.2568730000
C	3.8657180000	1.8224160000	-0.9100500000
C	2.4999050000	1.5757110000	-0.9909700000
C	1.9162210000	0.4369150000	-0.4078780000
C	2.7740520000	-0.4755970000	0.2272170000
C	0.4212890000	0.3289730000	-0.5807520000
C	-0.4505830000	-0.1875430000	0.5867770000
O	-0.0931680000	0.7087280000	-1.6144960000
C	-1.8980730000	0.2552670000	0.4438250000
O	0.1516820000	0.2917370000	1.7833210000
C	-2.8379150000	-0.4583410000	-0.3100560000
C	-4.1615010000	-0.0345050000	-0.4236340000
C	-4.5671520000	1.1302990000	0.2257580000
C	-3.6503790000	1.8595970000	0.9836830000
C	-2.3322630000	1.4206050000	1.0875530000
Cl	2.1988150000	-2.0052460000	0.8909280000
Cl	-2.3780740000	-1.9445370000	-1.1430700000
H	4.7826750000	-0.9815230000	0.7859800000
H	5.7622890000	1.0825230000	-0.1867860000
H	4.2828480000	2.7192130000	-1.3583420000
H	1.8430530000	2.2666840000	-1.5089950000
H	-0.4044640000	-1.2832320000	0.5405710000
H	-0.1780970000	-0.2474740000	2.5184350000
H	-4.8603020000	-0.6159990000	-1.0154920000
H	-5.5980660000	1.4615380000	0.1379260000
H	-3.9599980000	2.7678680000	1.4928000000
H	-1.6102180000	1.9718110000	1.6812450000

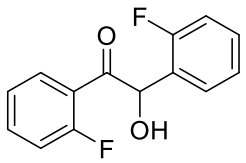
thermodynamic data

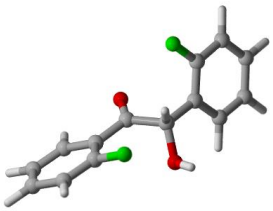
Zero-point correction= 0.204684 (Hartree/Particle)

Thermal correction to Energy= 0.220507
Thermal correction to Enthalpy= 0.221451
Thermal correction to Gibbs Free Energy= 0.159491
Sum of electronic and zero-point Energies= -1610.124311
Sum of electronic and thermal Energies= -1610.108488
Sum of electronic and thermal Enthalpies= -1610.107544
Sum of electronic and thermal Free Energies= -1610.169503

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.370	59.825	130.405

B3LYP/6-31G*	***o*-F-Benzoin**





xyz-matrix

28
XYZ file generated by gabedit : coordinates in Angstrom

C	3.9993420000	-0.8245070000	-0.3475050000
C	4.7401350000	0.2514250000	0.1381600000
C	4.0887550000	1.4042950000	0.5865580000
C	2.7007100000	1.4702800000	0.5492990000
C	1.9224810000	0.3956230000	0.0831100000
C	2.6128020000	-0.7373120000	-0.3648580000
C	0.4321020000	0.5817650000	0.0811800000
C	-0.4732320000	-0.6706700000	0.0145810000
O	-0.0449910000	1.6985090000	0.1568690000
C	-1.9415800000	-0.3237040000	0.1506860000
O	-0.0193140000	-1.5428020000	1.0459030000
C	-2.6328020000	0.2164990000	-0.9323410000
C	-3.9786370000	0.5482400000	-0.8804730000
C	-4.6707550000	0.3347450000	0.3134390000
C	-4.0097930000	-0.2036780000	1.4187380000
C	-2.6543630000	-0.5288180000	1.3342870000
F	1.9405810000	-1.7957580000	-0.8767060000
F	-1.9535180000	0.4116590000	-2.0896690000
H	4.4724020000	-1.7282920000	-0.7170190000
H	5.8244590000	0.1890620000	0.1600270000
H	4.6627920000	2.2462680000	0.9613970000
H	2.1729810000	2.3578830000	0.8823220000
H	-0.2994050000	-1.1153940000	-0.9739490000
H	-0.1509180000	-2.4541930000	0.7464970000
H	-4.4594660000	0.9646180000	-1.7595840000

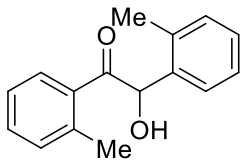
H	-5.7250490000	0.5895510000	0.3749400000
H	-4.5481180000	-0.3701990000	2.3473650000
H	-2.1298030000	-0.9531840000	2.1840410000

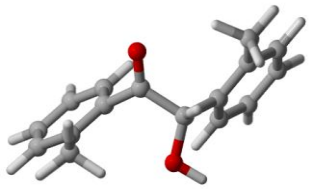
thermodynamic data

Zero-point correction= 0.207625 (Hartree/Particle)
Thermal correction to Energy= 0.222838
Thermal correction to Enthalpy= 0.223782
Thermal correction to Gibbs Free Energy= 0.163458
Sum of electronic and zero-point Energies= -889.405494
Sum of electronic and thermal Energies= -889.390281
Sum of electronic and thermal Enthalpies= -889.389337
Sum of electronic and thermal Free Energies= -889.449660

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.833	58.045	126.962

B3LYP/6-31G*	***o*-Me-Benzoin**





xyz-matrix

34
XYZ file generated by gabedit : coordinates in Angstrom

C	3.8998850000	0.4349050000	0.1800770000
C	3.7602560000	1.7237230000	-0.3376750000
C	2.5478170000	2.1188470000	-0.8991740000
C	1.4811280000	1.2197030000	-0.9351220000
C	1.6193780000	-0.0662650000	-0.4018270000
C	2.8425650000	-0.4807140000	0.1609600000
C	0.4540270000	-1.0185980000	-0.5170100000
C	-0.5464460000	-1.1292170000	0.6562760000
O	0.2560290000	-1.6593740000	-1.5326620000
C	-1.6976510000	-0.1489770000	0.4348950000
O	0.1561770000	-0.8789520000	1.8665640000
C	-2.8473890000	-0.5144330000	-0.3001480000
C	-3.8591200000	0.4402920000	-0.4590910000
C	-3.7517040000	1.7229510000	0.0802520000
C	-2.6118560000	2.0766760000	0.7992480000
C	-1.5914460000	1.1414310000	0.9712890000
C	3.0192980000	-1.8773890000	0.7105860000
C	-3.0146600000	-1.8924440000	-0.9016800000

H	4.8517620000	0.1274720000	0.6070870000
H	4.6001360000	2.4128540000	-0.3064930000
H	2.4300900000	3.1164000000	-1.3134340000
H	0.5357340000	1.5158600000	-1.3805570000
H	-0.9248660000	-2.1593650000	0.6323350000
H	-0.5037820000	-0.8010900000	2.5740630000
H	-4.7513050000	0.1674900000	-1.0179270000
H	-4.5562900000	2.4394470000	-0.0627490000
H	-2.5125280000	3.0725420000	1.2225270000
H	-0.6967180000	1.4050580000	1.5267540000
H	2.8235630000	-2.6354390000	-0.0577980000
H	4.0394790000	-2.0285340000	1.0764300000
H	2.3264050000	-2.0602340000	1.5392740000
H	-2.1809540000	-2.1487840000	-1.5620480000
H	-3.0583190000	-2.6682260000	-0.1246060000
H	-3.9445370000	-1.9517800000	-1.4752260000

thermodynamic data

Zero-point correction= 0.279722 (Hartree/Particle)
Thermal correction to Energy= 0.296463
Thermal correction to Enthalpy= 0.297408
Thermal correction to Gibbs Free Energy= 0.233934
Sum of electronic and zero-point Energies= -769.495450
Sum of electronic and thermal Energies= -769.478709
Sum of electronic and thermal Enthalpies= -769.477765
Sum of electronic and thermal Free Energies= -769.541238

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	186.034	63.946	133.590