Supporting Information

Detailed Transition State Geometries from ^{13}C Isotope Effects. The Experimental Transition State and Mechanism of Epoxidation of Alkenes with Oxaziridines

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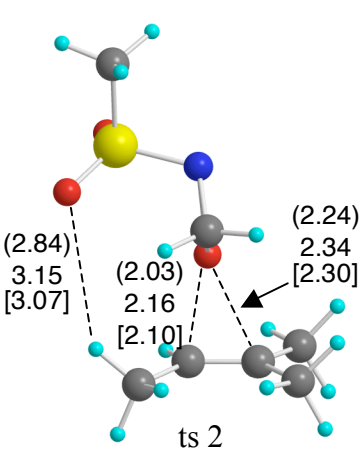
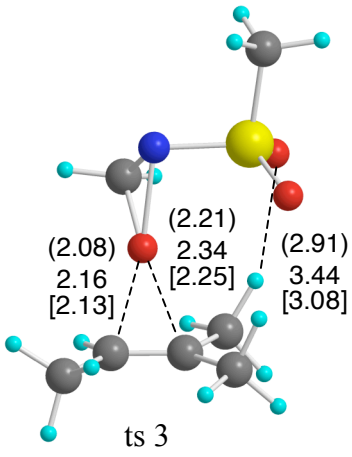
Figure of all B3LYP/6-31+G** Calculated Structures

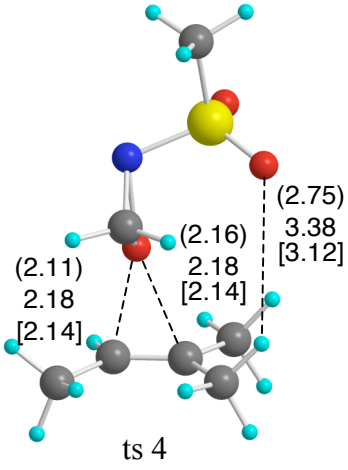
Transition structures for the epoxidation of 2-methyl-2-butene with 2-(methylsulfonyl)oxaziridine using B3LYP/6-31+G**. Bond distances in angstroms from gas-phase calculations are shown in parentheses, from calculations using a PCM solvent model are shown without parentheses, and from calculations using an Onsager solvent model are shown in brackets.



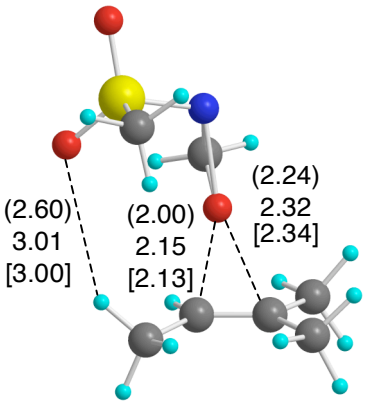
ts 2



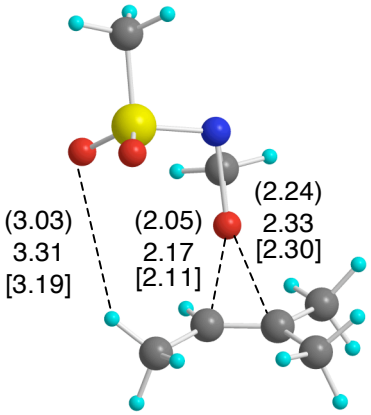
ts 3



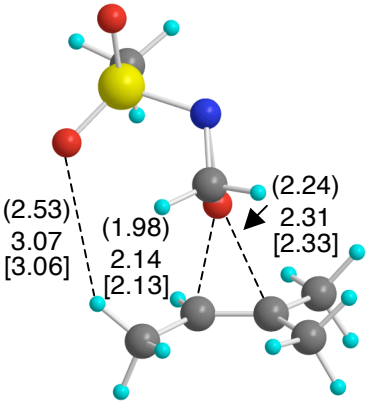
ts 4



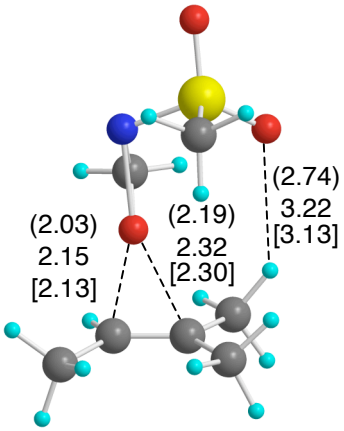
ts 5



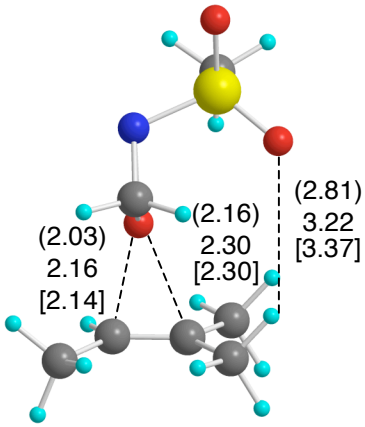
ts 6



ts 7

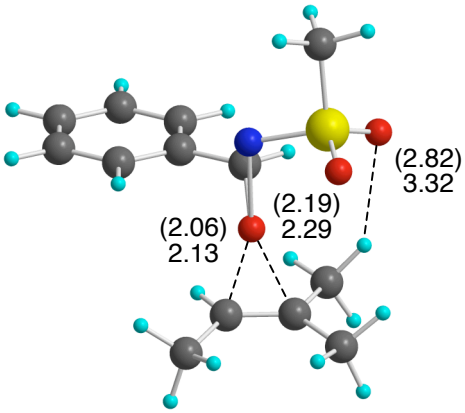


ts 8

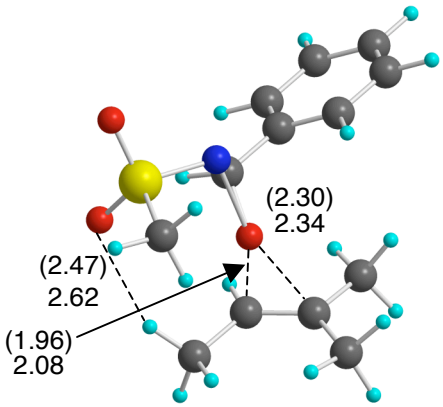


ts 9

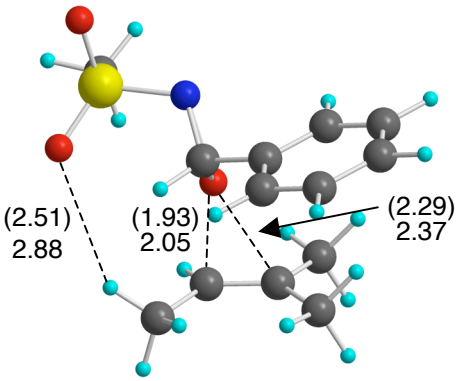
Transition structures for the epoxidation of 2-methyl-2-butene with *trans*- and *cis*-3-phenyl-2-methanesulfonyloxaziridine using B3LYP/6-31+G**. Bond distances in angstroms from gas-phase calculations are shown in parentheses, and distances from calculations using a PCM solvent model are shown without parentheses.



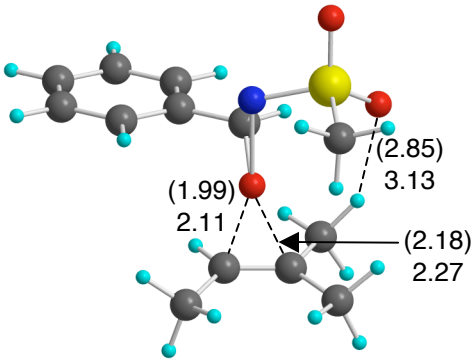
trans ts 3



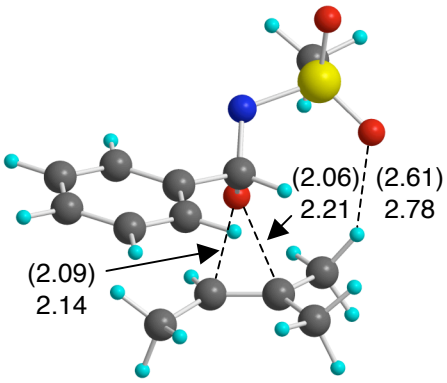
trans ts 5



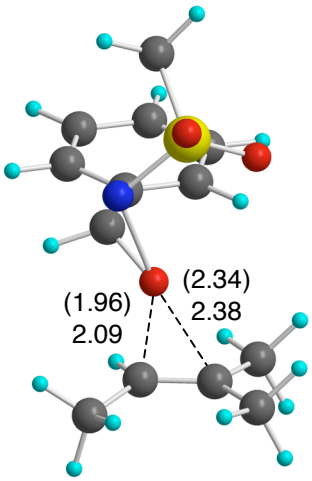
trans ts 7



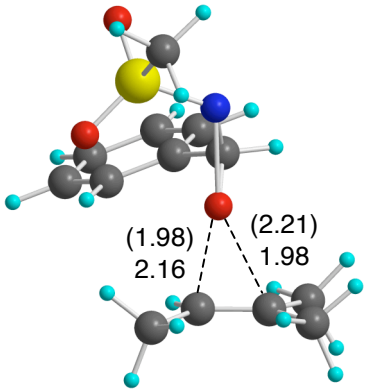
trans ts 8



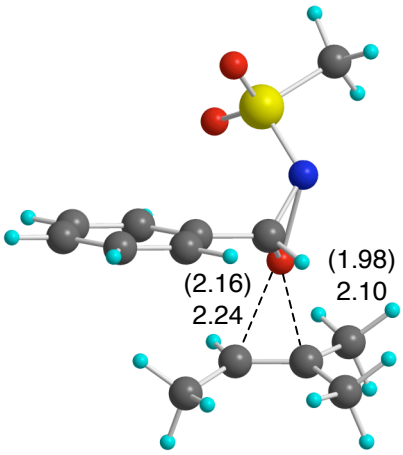
trans ts 9



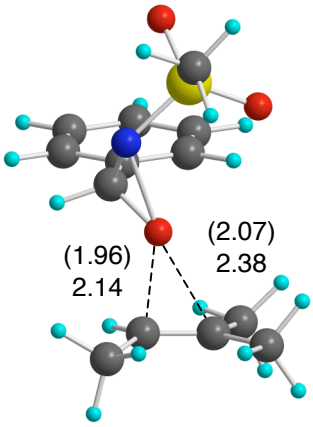
cis ts 3



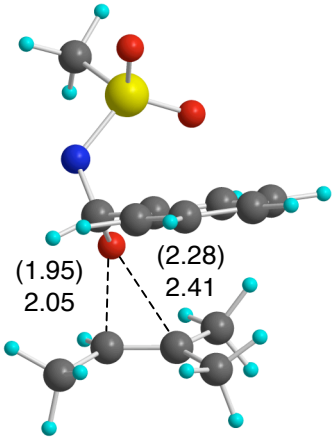
cis ts 5



cis ts 7



cis ts 8



cis ts 9

Technical Note on Frequency Calculations and KIE Predictions

As described in the main text, the program QUIVER (reference 27) was employed here to calculate the isotope effects. QUIVER works by calculating the vibrational frequencies for isotopologues then using these frequencies in the Bigeleisen equation (reference 26). QUIVER calculates frequencies by diagonalizing the full mass-weighted Cartesian Hessian, and this process is subject to error because it does not first project out the rotational and translation degrees of freedom. The program ISOEFF98 used in the Schramm process (reference 11a) employs the same process. In contrast, programs such as Gaussian03 (reference 24a) employ a more accurate process of projecting out the rotational and translational modes. The difference between the processes usually makes no significant difference in the calculated high-energy modes, but the lowest-energy vibrational modes can be contaminated by rotational and translational modes if they are not first projected out.

At stationary points, the difference between frequencies calculated with versus without projecting out the rotational and translational modes is small. For a set of 29 of the transition structures here, the average absolute error in the lowest-two real frequencies was 0.24 cm^{-1}. At non-stationary points, the error is greater. For the 38 non-stationary points associated with the grid discussed in the main text, the average absolute error was 3.4 cm^{-1}. It should be noted that the frequency predictions at non-stationary points do not project out the gradients at these points.

We next examine how this issue and related problems with low-energy modes impact kinetic isotope effect predictions. This was done by comparing kinetic isotope effects predicted in three ways: Method A – based on QUIVER, using the frequencies obtained without projecting out the rotational and translation modes in the Bigeleisen equation; Method B – using frequencies obtained with projecting out the rotational and translational modes in the Biegeleisen equation; and Method C – based on free-energies of activation, using the harmonic free energy estimates from Gaussian03. (It

should be noted that Method C is subject to a significant round-off error when using the default digits from Gaussian03.)

In a comparison of the three methods for 14 stationary point transition structures (gas phase structures ts 2 through ts 9 and PCM structures ts 4 through ts 9 from the previous section), the predicted KIEs from the three methods are identical within the round-off error of Method C. The average absolute difference between predictions of carbon KIEs by Method A versus Method B at these stationary points was only 0.000018, essentially negligible. The agreement of Method A and Method B at stationary points is unsurprising, as it has long been known that the incorporation of the Redlich-Teller product rule into the Bigeleisen equation minimizes the importance of the low frequencies (and errors therein, see reference 31). The agreement of Methods A and B with Method C is unsurprising as this is essentially based on the Redlich-Teller product rule.

The situation is more complicated at non-stationary points. Out of 76 KIEs based on the 38 non-stationary points associated with the grid discussed in the main text, a difference of > 0.001 between Method A and Method B is seen in 12 cases. The source of the discrepancy when it arises is a difference in the imaginary frequencies factored into the KIE prediction. In each of the 76 cases, there is a negligible difference between the reduced isotopic partition functions (as derived from the real frequencies and the Bigeleisen equation). However, the difference in the portion of the KIEs derived from the imaginary frequencies ranges up to 0.017 in the 12 bad cases. These bad cases have a common feature – the imaginary frequencies are all small, between -20 and -50 cm^{-1}, and there is significant rotational contamination of these modes. For the 64 KIEs derived from structures with imaginary frequencies ranging from -50 to -475 cm^{-1}, little rotational contamination of the imaginary frequency was apparent and Method A and Method B agreed within 0.0002 in all cases.

For the KIEs calculated at non-stationary points, Method C agreed (within round-off error) with Methods A and B in only 32 cases. The comparison failed uniformly when the structures exhibited two imaginary frequencies, and likewise failed when the lowest real frequency was below 25^{-1}. The predictions of KIEs based on free energies are subject to particularly large errors – in one case a carbon KIE of 7% was predicted.

The problems with KIE predictions at non-stationary points are not surprising and the general lesson is that care should be taken in applying the Schramm process, particularly when the constrained structures involve very small frequencies. Nonetheless, as described in main text, the inaccuracies in the derived geometries in our test cases appear to be small.

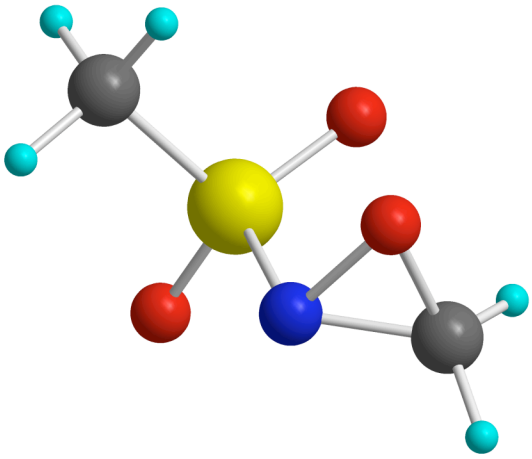
Calculational Results

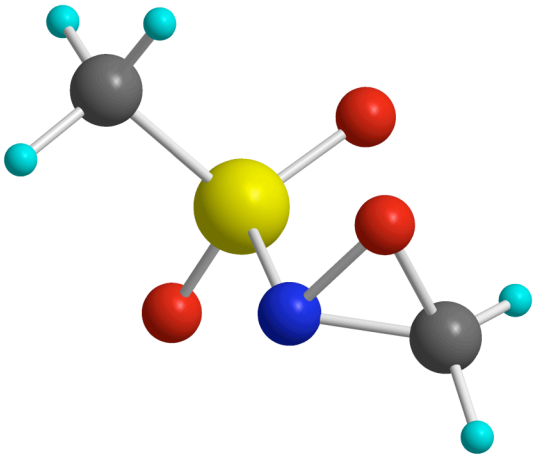
Unless otherwise stated, structures were fully optimized in B3LYP calculations with a 6-31+G** basis set. All structures and energies were obtained using standard procedures in Gaussian03[1]. Vibrational frequency analyses were carried out on all stationary points.

1. (this is the complete reference for 24a in the paper) Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

Sulfonyloxaziridine 1 (isomer-1)

B3LYP/6-31+G**





```
filename: oxazsm
E(RB+HF-LYP) = -757.691699168

 Zero-point correction=                           0.082933 (Hartree/Particle)
 Thermal correction to Energy=                    0.090437
 Thermal correction to Enthalpy=                  0.091381
 Thermal correction to Gibbs Free Energy=         0.050972
 Sum of electronic and zero-point Energies=           -757.608766
 Sum of electronic and thermal Energies=              -757.601262
 Sum of electronic and thermal Enthalpies=            -757.600318
 Sum of electronic and thermal Free Energies=         -757.640727

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  56.750             26.234             85.048

 O,0,0.0510295943,-0.0631016628,0.551056526
 C,0,1.0659746458,0.1652402616,1.5026383323
 N,0,0.2048728469,1.2742926093,1.16762624
 S,0,-1.094790091,1.5032099844,2.386676419
 C,0,-2.4621150901,1.8385486661,1.2697825365
 O,0,-0.6967249473,2.7272990609,3.0853317425
 O,0,-1.3603136555,0.2614766713,3.1230503371
 H,0,2.0803873729,0.2445758007,1.1165486816
 H,0,0.9267347058,-0.3390582996,2.4580279768
 H,0,-3.327278103,2.0532692747,1.8998436992
 H,0,-2.6336452451,0.9493418598,0.6624631688
 H,0,-2.1988400338,2.7023867735,0.6591793405
```

B3LYP/6-31G*

```
E(RB+HF-LYP) =  -757.667456767
E (Cosmo, CHCl3) E(RB+HF-LYP) =  -757.667550533

Zero-point correction=                           0.083602 (Hartree/Particle)
 Thermal correction to Energy=                    0.091041
 Thermal correction to Enthalpy=                  0.091985
 Thermal correction to Gibbs Free Energy=         0.051732
 Sum of electronic and zero-point Energies=           -757.583855
 Sum of electronic and thermal Energies=              -757.576416
 Sum of electronic and thermal Enthalpies=            -757.575471
```

```
 Sum of electronic and thermal Free Energies=         -757.615724

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  57.129             26.017             84.719

                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0    C    2.013609   -0.501011   -0.069320
    2          8             0    O    1.781746    0.873103    0.116506
    3          7             0    N    0.906620    0.085603   -0.785959
    4         16             0    S   -0.649755   -0.206362    0.053851
    5          8             0    O   -0.441562   -0.476347    1.479520
    6          8             0    O   -1.335497   -1.167760   -0.809231
    7          6             0    C   -1.368658    1.430368   -0.138918
    8          1             0    H    1.808859   -1.130883    0.795470
    9          1             0    H    2.865690   -0.770158   -0.691766
   10          1             0    H   -1.419763    1.662899   -1.203434
   11          1             0    H   -0.743418    2.145934    0.397069
   12          1             0    H   -2.368824    1.386665    0.297819
 ---------------------------------------------------------------------
```

MPW1K/6-31+G*

```
E(RmPW+HF-PW91) =  -757.552901408

 Zero-point correction=                           0.087141 (Hartree/Particle)
 Thermal correction to Energy=                    0.094225
 Thermal correction to Enthalpy=                  0.095169
 Thermal correction to Gibbs Free Energy=         0.055665
 Sum of electronic and zero-point Energies=           -757.465760
 Sum of electronic and thermal Energies=              -757.458677
 Sum of electronic and thermal Enthalpies=            -757.457732
 Sum of electronic and thermal Free Energies=         -757.497236

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  59.127             24.772             83.143

 C,0,1.9781565355,-0.5068712977,-0.0718440475
 O,0,1.7384140003,0.8452185559,0.1232013037
 N,0,0.8802993346,0.08854669,-0.7522985666
 S,0,-0.6322404206,-0.193776241,0.0480146317
 O,0,-0.4277587449,-0.4614706488,1.4524787186
 O,0,-1.3015900402,-1.1496393682,-0.7974375596
 C,0,-1.3498695248,1.4046535387,-0.1432322189
 H,0,1.7822753933,-1.1364725363,0.78638809
 H,0,2.8187365646,-0.7580354094,-0.7032966835
 H,0,-1.4071929101,1.6345653233,-1.201667302
 H,0,-0.7382242896,2.1257018989,0.3889840204
 H,0,-2.3440871571,1.3552719919,0.2919656313
```

B3LYP/6-31+G** (PCM)

```
Filename: oxazsmaPCM
E(RB+HF-LYP) = -757.701663066
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```
 Zero-point correction=                           0.082586 (Hartree/Particle)
 Thermal correction to Energy=                    0.090106
 Thermal correction to Enthalpy=                  0.091050
 Thermal correction to Gibbs Free Energy=         0.050608
 Sum of electronic and zero-point Energies=           -757.619077
 Sum of electronic and thermal Energies=              -757.611557
 Sum of electronic and thermal Enthalpies=            -757.610613
 Sum of electronic and thermal Free Energies=         -757.651055

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  56.542             26.319             85.117

 O,0,-1.8062755333,0.8616262667,0.1496599331
 C,0,-2.0277700743,-0.5158308305,-0.0784592386
 N,0,-0.9164856919,0.1090517677,-0.7592679321
 S,0,0.6460137463,-0.1837411535,0.0634270608
 C,0,1.3966937924,1.4302350065,-0.1509899463
 O,0,1.3013100682,-1.1755925821,-0.8002232666
 O,0,0.4608128646,-0.4599871182,1.4959230036
 H,0,-2.8694393858,-0.7689022736,-0.7212637174
 H,0,-1.829310362,-1.1652776526,0.7738164406
 H,0,2.4030395811,1.3590608539,0.2684784827
 H,0,0.7982729484,2.1614623144,0.3948618055
 H,0,1.4311740463,1.6498754014,-1.2189996253
```

MPW1K/6-31+G** (PCM)

```
Filename: mpBBoxazsmPCM
E(RmPW-PW91) = -757.683169025

 Zero-point correction=                           0.082004 (Hartree/Particle)
 Thermal correction to Energy=                    0.088474
 Thermal correction to Enthalpy=                  0.089419
 Thermal correction to Gibbs Free Energy=         0.051117
 Sum of electronic and zero-point Energies=           -757.601165
 Sum of electronic and thermal Energies=              -757.594695
 Sum of electronic and thermal Enthalpies=            -757.593750
 Sum of electronic and thermal Free Energies=         -757.632052

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  55.519             22.767             80.612

 O,0,-1.7468448939,0.8483593551,0.1461559456
 C,0,-1.990533982,-0.5037152042,-0.0727040867
 N,0,-0.8876059875,0.1070309983,-0.7365710847
 S,0,0.6252094929,-0.1743329415,0.0507666544
 C,0,1.3642142541,1.4074775652,-0.1507659542
 O,0,1.2751075884,-1.1531246958,-0.792183783
 O,0,0.434901224,-0.4493337624,1.4589692947
 H,0,-2.8281254773,-0.7425693622,-0.7140490802
 H,0,-1.8001404177,-1.1490810646,0.7759787475
 H,0,2.3608701579,1.3418313936,0.2770497884
 H,0,0.7669073004,2.1379243509,0.3853174892
 H,0,1.4140777405,1.6315123677,-1.211001931
```

B3PW91/6-31G* (gas phase)

```
E(RB+HF-PW91) = -757.487217816
```

```
Zero-point correction=                           0.084121 (Hartree/Particle)
 Thermal correction to Energy=                    0.091491
 Thermal correction to Enthalpy=                  0.092435
 Thermal correction to Gibbs Free Energy=         0.052324
 Sum of electronic and zero-point Energies=           -757.403097
 Sum of electronic and thermal Energies=              -757.395727
 Sum of electronic and thermal Enthalpies=            -757.394783
 Sum of electronic and thermal Free Energies=         -757.434894

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   57.411             25.761             84.421

 O,0,-1.7716766501,0.8685495412,0.131962634
 C,0,-2.0033817581,-0.4975856174,-0.0699806019
 N,0,-0.9053390121,0.1061225667,-0.7745130141
 S,0,0.6394633125,-0.2021219516,0.0524744096
 C,0,1.3740569123,1.4137569593,-0.1461881716
 O,0,1.3069743792,-1.1716178602,-0.8084795337
 O,0,0.432829649,-0.4637422942,1.4753043663
 H,0,-2.8553136676,-0.7590294783,-0.695948213
 H,0,-1.7937854336,-1.138197997,0.786401006
 H,0,2.3768284482,1.3586744175,0.2836920125
 H,0,0.7645194609,2.1406519986,0.3932525711
 H,0,1.4228603591,1.6465197153,-1.2110144653
```

BB1K/6-31G* (gas phase)

```
E(RB+HF-B95) = -757.546275417

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   92.200             23.293             78.787
 Zero-point correction=                           0.087091 (Hartree/Particle)
 Thermal correction to Energy=                    0.094120
 Thermal correction to Enthalpy=                  0.095064
 Thermal correction to Gibbs Free Energy=         0.055757
 Sum of electronic and zero-point Energies=           -757.459184
 Sum of electronic and thermal Energies=              -757.452155
 Sum of electronic and thermal Enthalpies=            -757.451211
 Sum of electronic and thermal Free Energies=         -757.490518

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   59.061             24.725             82.729

 O,0,-1.7077348974,0.8645345123,0.1223202686
 C,0,-1.9730151384,-0.4826593944,-0.0606116642
 N,0,-0.879126293,0.0874384197,-0.7704347672
 S,0,0.6295243764,-0.2030131957,0.0348399862
 C,0,1.3434861421,1.3979576586,-0.1445077505
 O,0,1.3061549667,-1.1561829224,-0.805785909
 O,0,0.4044831673,-0.4691010856,1.4353732632
 H,0,-2.8306962696,-0.725327718,-0.6724906517
 H,0,-1.7677511797,-1.11211701,0.7955496977
 H,0,2.3318429666,1.3549731,0.303029357
 H,0,0.7190818235,2.112931832,0.3806465684
 H,0,1.4117863355,1.6325458036,-1.2009653984
```

BPW91/6-31G* (gas phase)

E(RB-PW91) = -757.653205225

Zero-point correction= 0.080914 (Hartree/Particle)
Thermal correction to Energy= 0.088658
Thermal correction to Enthalpy= 0.089602
Thermal correction to Gibbs Free Energy= 0.048671
Sum of electronic and zero-point Energies= -757.572291
Sum of electronic and thermal Energies= -757.564547
Sum of electronic and thermal Enthalpies= -757.563603
Sum of electronic and thermal Free Energies= -757.604534

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	55.634	26.942	86.147

O,0,-1.8231618254,0.8774926257,0.1356261667
C,0,-2.0298525203,-0.5067676112,-0.0756053747
N,0,-0.9377367654,0.1247396839,-0.7980203366
S,0,0.6524123874,-0.2087963145,0.0627548157
C,0,1.4005087371,1.4269789542,-0.1454196826
O,0,1.3232165381,-1.190579981,-0.8159007817
O,0,0.4486488122,-0.4639328552,1.5079528165
H,0,-2.8892132353,-0.7859725734,-0.6974860014
H,0,-1.7984572011,-1.1543954986,0.7798813359
H,0,2.4113453531,1.3683820016,0.2808799636
H,0,0.789633967,2.1577577643,0.3999431148
H,0,1.4406917525,1.6570738043,-1.2176430362

MPWLYP1M/6-31G* (gas phase)

E(RmPW+HF-LYP) = -757.671368410

Zero-point correction= 0.083646 (Hartree/Particle)
Thermal correction to Energy= 0.091073
Thermal correction to Enthalpy= 0.092018
Thermal correction to Gibbs Free Energy= 0.051797
Sum of electronic and zero-point Energies= -757.587722
Sum of electronic and thermal Energies= -757.580295
Sum of electronic and thermal Enthalpies= -757.579351
Sum of electronic and thermal Free Energies= -757.619572

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	57.149	25.993	84.652

O,0,-1.7650904369,0.8824946068,0.1120572889
C,0,-2.0113600005,-0.4901580821,-0.0643672856
N,0,-0.9033615119,0.0820583443,-0.7900799249
S,0,0.6518159719,-0.2162197067,0.0457471276
C,0,1.3723197375,1.4188514756,-0.1426671308
O,0,1.3348535262,-1.1767371537,-0.8193957477
O,0,0.4428045719,-0.4890782133,1.4702535634
H,0,-2.8697048213,-0.7539742791,-0.6800158093
H,0,-1.8067138549,-1.116162437,0.8030889296
H,0,2.371745116,1.3743986435,0.295349014
H,0,0.7460161754,2.1331962751,0.3935871358
H,0,1.4247115265,1.6533105264,-1.2065941609

MPWB1K/6-31G* (gas phase)

```
E(RmPW+HF-B95) = -757.545147172

Zero-point correction=                           0.087374 (Hartree/Particle)
 Thermal correction to Energy=                    0.094381
 Thermal correction to Enthalpy=                  0.095325
 Thermal correction to Gibbs Free Energy=         0.056059
 Sum of electronic and zero-point Energies=           -757.457773
 Sum of electronic and thermal Energies=              -757.450766
 Sum of electronic and thermal Enthalpies=            -757.449822
 Sum of electronic and thermal Free Energies=         -757.489088

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  59.225             24.633             82.643


 O,0,-1.7005167334,0.8648264001,0.1202813309
 C,0,-1.9698253106,-0.4804419831,-0.0594376691
 N,0,-0.8760974873,0.0849418008,-0.7702414467
 S,0,0.629074011,-0.2036450041,0.032870295
 C,0,1.339794981,1.3960885069,-0.144185724
 O,0,1.3068568854,-1.1546823004,-0.8060809426
 O,0,0.4027439357,-0.4705972908,1.4312428768
 H,0,-2.8281032035,-0.721306316,-0.6697767775
 H,0,-1.7653449455,-1.1082770795,0.7972151416
 H,0,2.3265042112,1.3550848635,0.3055204988
 H,0,0.7128932885,2.1091281951,0.3793497045
 H,0,1.4100563676,1.6308602073,-1.1997942876
```

MPW1B95/6-31G* (gas phase)

```
E(RmPW+HF-B95) = -757.574510652

Thermal correction to Energy=                    0.092738
 Thermal correction to Enthalpy=                  0.093682
 Thermal correction to Gibbs Free Energy=         0.054104
 Sum of electronic and zero-point Energies=           -757.488935
 Sum of electronic and thermal Energies=              -757.481773
 Sum of electronic and thermal Enthalpies=            -757.480829
 Sum of electronic and thermal Free Energies=         -757.520407

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  58.194             25.208             83.298

 O,0,-1.715932445,0.8727951558,0.1188413942
 C,0,-1.9798979123,-0.4818313279,-0.0599676523
 N,0,-0.8858165293,0.0876713929,-0.783696495
 S,0,0.6361051069,-0.2097734375,0.0355492682
 C,0,1.3481377829,1.401725092,-0.1434977591
 O,0,1.3177652235,-1.1648486229,-0.8121261961
 O,0,0.4086162089,-0.4766179827,1.4437043859
 H,0,-2.8439326629,-0.7293944351,-0.6673864804
 H,0,-1.7679697327,-1.1109843003,0.7994718201
 H,0,2.3385266988,1.36209545,0.3068876998
 H,0,0.7164293588,2.1144853015,0.38221486
 H,0,1.4160049024,1.6366577142,-1.2030318453
```

MPWLYP1M/6-31G* (gas phase)

```
E(RmPW+HF-LYP) = -757.566197933

Zero-point correction=                           0.080988 (Hartree/Particle)
 Thermal correction to Energy=                    0.088725
 Thermal correction to Enthalpy=                  0.089669
 Thermal correction to Gibbs Free Energy=         0.048792
 Sum of electronic and zero-point Energies=           -757.485210
 Sum of electronic and thermal Energies=              -757.477473
 Sum of electronic and thermal Enthalpies=            -757.476529
 Sum of electronic and thermal Free Energies=         -757.517406

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  55.676             26.989             86.033

 O,0,-1.7977697477,0.8971127316,0.1033322238
 C,0,-2.0344114234,-0.491882615,-0.0645594832
 N,0,-0.9270121285,0.0835686117,-0.8180631274
 S,0,0.6683617819,-0.2294508003,0.049515987
 C,0,1.389758918,1.4309526071,-0.140116968
 O,0,1.3619618626,-1.1940076229,-0.8310272652
 O,0,0.4592456088,-0.5031836484,1.4913992994
 H,0,-2.9026917386,-0.770037857,-0.6713531972
 H,0,-1.8139217298,-1.1167761218,0.8077132033
 H,0,2.3929258731,1.3904562579,0.3023567005
 H,0,0.7513845441,2.1413927903,0.3975645886
 H,0,1.4402041795,1.6638356667,-1.2097989615
```

PBE1KCIS/6-31G* (gas phase)

```
E(RPBE+HF-KCIS) = -757.175662918

Zero-point correction=                           0.084163 (Hartree/Particle)
 Thermal correction to Energy=                    0.091481
 Thermal correction to Enthalpy=                  0.092425
 Thermal correction to Gibbs Free Energy=         0.052446
 Sum of electronic and zero-point Energies=           -757.091500
 Sum of electronic and thermal Energies=              -757.084182
 Sum of electronic and thermal Enthalpies=            -757.083237
 Sum of electronic and thermal Free Energies=         -757.123217

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  57.405             25.669             84.143

 O,0,-1.7685861902,0.8688769686,0.129418888
 C,0,-2.0008113927,-0.4959303702,-0.0701646302
 N,0,-0.904586183,0.1079834768,-0.7714645986
 S,0,0.6391819194,-0.2013685146,0.0518319492
 C,0,1.3709638584,1.4103627871,-0.1459382956
 O,0,1.3053800406,-1.1702009513,-0.8108704672
 O,0,0.4359037637,-0.4635153494,1.4751813793
 H,0,-2.853052158,-0.759481265,-0.6967260836
 H,0,-1.7935029103,-1.1360833691,0.7883904484
 H,0,2.3735452133,1.3577575691,0.28584652
 H,0,0.7609608969,2.1387249698,0.3921261228
 H,0,1.4226391418,1.6448540482,-1.2106682327
```

PBE1W/6-31G* (gas phase)

```
E(RPBE+HF-PBE) = -809.235346079
```

```
Zero-point correction=                           0.128924 (Hartree/Particle)
 Thermal correction to Energy=                    0.134531
 Thermal correction to Enthalpy=                  0.135475
 Thermal correction to Gibbs Free Energy=         0.099134
 Sum of electronic and zero-point Energies=           -809.106422
 Sum of electronic and thermal Energies=              -809.100815
 Sum of electronic and thermal Enthalpies=            -809.099871
 Sum of electronic and thermal Free Energies=         -809.136212

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  84.419             18.684             76.486

 O,0,-1.5164177096,0.7457977907,0.1221151658
 C,0,-1.7306664358,-0.4023858917,-0.072235177
 N,0,-0.7628712184,0.1309850992,-0.5729385686
 S,0,0.5205705122,-0.0971244143,0.0291554529
 C,0,1.1656335455,1.251995731,-0.1441350945
 O,0,1.0741428171,-0.9477688989,-0.6959641324
 O,0,0.3699012038,-0.3289848412,1.2483567763
 H,0,-2.4245586412,-0.6055429865,-0.6397036693
 H,0,-1.6034366854,-0.9584336087,0.6501329827
 H,0,2.0096753389,1.1847160334,0.2151714833
 H,0,0.6743881629,1.8774026233,0.3165811408
 H,0,1.21167511,1.4513233638,-1.03957336
```

PBELYP1W/6-31G* (gas phase)

```
E(RPBE+HF-V5LYP) = -795.032006542

Zero-point correction=                           0.118909 (Hartree/Particle)
 Thermal correction to Energy=                    0.124733
 Thermal correction to Enthalpy=                  0.125677
 Thermal correction to Gibbs Free Energy=         0.088848
 Sum of electronic and zero-point Energies=           -794.913098
 Sum of electronic and thermal Energies=              -794.907273
 Sum of electronic and thermal Enthalpies=            -794.906329
 Sum of electronic and thermal Free Energies=         -794.943158

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  78.271             19.604             77.513

 O,0,-1.545532779,0.7747362958,0.1094123433
 C,0,-1.788135855,-0.4176867757,-0.0652395644
 N,0,-0.7810523459,0.1014375613,-0.6164939928
 S,0,0.5494081326,-0.1262949495,0.0234260139
 C,0,1.2008739434,1.2858882221,-0.1424958558
 O,0,1.1404369936,-0.99141025,-0.7252402687
 O,0,0.3815824134,-0.3751829616,1.2788522392
 H,0,-2.5193689026,-0.6253722058,-0.6390426728
 H,0,-1.6547031863,-0.978557372,0.6943928293
 H,0,2.074097572,1.231187386,0.2414005129
 H,0,0.6733020035,1.9265592715,0.3292815806
 H,0,1.2571280103,1.4966757779,-1.0712901645
```

RHF/6-31G* (gas phase)

```
E(RHF) = -755.005421421
```

```
Zero-point correction=                           0.091519 (Hartree/Particle)
 Thermal correction to Energy=                    0.098258
 Thermal correction to Enthalpy=                  0.099202
 Thermal correction to Gibbs Free Energy=         0.060398
 Sum of electronic and zero-point Energies=           -754.913902
 Sum of electronic and thermal Energies=              -754.907163
 Sum of electronic and thermal Enthalpies=            -754.906219
 Sum of electronic and thermal Free Energies=         -754.945023

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  61.658             23.489             81.670

 O,0,-1.7297821441,0.8383020502,0.1386037649
 C,0,-1.991491587,-0.4968554966,-0.0678168216
 N,0,-0.8722882947,0.0740846645,-0.7175584012
 S,0,0.628323131,-0.1877777585,0.0453365441
 C,0,1.3570161984,1.4071894454,-0.1514082297
 O,0,1.2890325263,-1.139379122,-0.7870735742
 O,0,0.4418434641,-0.4565120805,1.4360452404
 H,0,-2.819854389,-0.7241883715,-0.7123178186
 H,0,-1.8360899523,-1.1343602207,0.7820299886
 H,0,2.3510575995,1.3488311666,0.2712230816
 H,0,0.7630213303,2.1325469368,0.3844212319
 H,0,1.4072481175,1.6400987864,-1.204522006
```

TPSS1KCIS/6-31G* (gas phase)

```
E(RTPSS+HF-KCIS) = -757.709022254

Zero-point correction=                           0.083893 (Hartree/Particle)
 Thermal correction to Energy=                    0.091347
 Thermal correction to Enthalpy=                  0.092291
 Thermal correction to Gibbs Free Energy=         0.052021
 Sum of electronic and zero-point Energies=           -757.625129
 Sum of electronic and thermal Energies=              -757.617675
 Sum of electronic and thermal Enthalpies=            -757.616731
 Sum of electronic and thermal Free Energies=         -757.657001

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  57.321             26.004             84.755

 O,0,-1.7696099804,0.879214646,0.1211147622
 C,0,-2.0064460411,-0.4936699933,-0.0672360128
 N,0,-0.9070661397,0.0948494535,-0.7904785495
 S,0,0.6467844849,-0.2119806429,0.0487384637
 C,0,1.3730556959,1.4168442451,-0.1435653925
 O,0,1.3258308865,-1.1773758859,-0.8182801829
 O,0,0.4342607246,-0.4776080997,1.4765340071
 H,0,-2.8636347252,-0.7559206708,-0.6814324106
 H,0,-1.7931399659,-1.1229110607,0.79376008
 H,0,2.371686967,1.3681897416,0.2917447833
 H,0,0.752237197,2.1336221998,0.3925148734
 H,0,1.4240768963,1.6487260675,-1.2064514216
```

TPSSLYP1W/6-31G* (gas phase)

```
E(RTPSS+HF-V5LYP) = -809.827205703
```

```
 Zero-point correction=                           0.129909 (Hartree/Particle)
 Thermal correction to Energy=                    0.135525
 Thermal correction to Enthalpy=                  0.136469
 Thermal correction to Gibbs Free Energy=         0.100106
 Sum of electronic and zero-point Energies=           -809.697297
 Sum of electronic and thermal Energies=              -809.691681
 Sum of electronic and thermal Enthalpies=            -809.690737
 Sum of electronic and thermal Free Energies=         -809.727099

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  85.043             18.689             76.531


 O,0,-1.5052568812,0.7535611574,0.110767914
 C,0,-1.7363302011,-0.3979372138,-0.0680671803
 N,0,-0.7558600801,0.1090880849,-0.5811664324
 S,0,0.5288057752,-0.108183776,0.0238589932
 C,0,1.1629664167,1.2557620296,-0.1420049006
 O,0,1.0962477119,-0.9500440701,-0.7009267141
 O,0,0.3737107744,-0.346698698,1.241528813
 H,0,-2.4332330769,-0.5960069264,-0.6279728047
 H,0,-1.6169894095,-0.9427164365,0.6595571321
 H,0,2.0035000105,1.1975836225,0.2213238889
 H,0,0.6601666118,1.8713897732,0.3149366476
 H,0,1.2103083483,1.4561824531,-1.0348723568
```

BP86/6-31G* (gas phase)

```
E(RB-P86) = -757.720514557

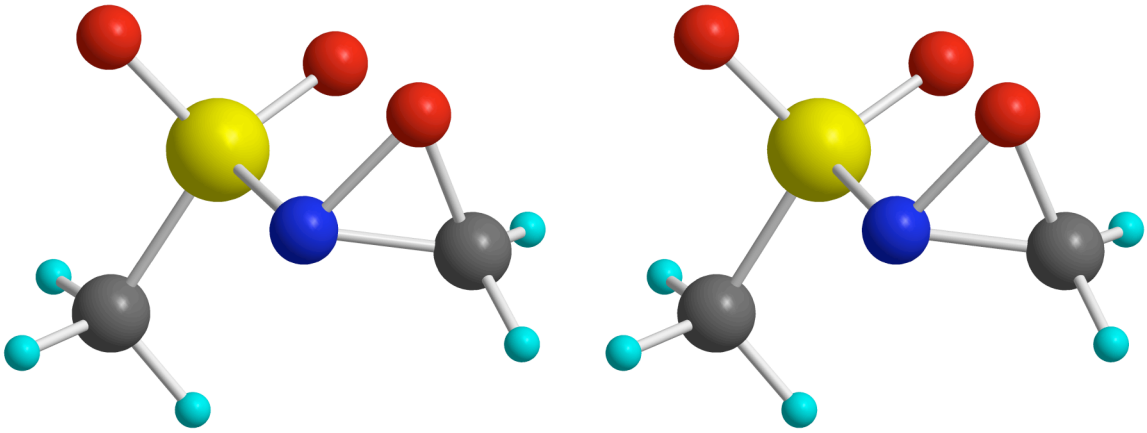
Zero-point correction=                           0.132948 (Hartree/Particle)
 Thermal correction to Energy=                    0.139904
 Thermal correction to Enthalpy=                  0.140849
 Thermal correction to Gibbs Free Energy=         0.103135
 Sum of electronic and zero-point Energies=           -196.395054
 Sum of electronic and thermal Energies=              -196.388098
 Sum of electronic and thermal Enthalpies=            -196.387154
 Sum of electronic and thermal Free Energies=         -196.424867

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  87.791             24.265             79.374

 C,0,1.2819616616,0.050005017,-0.9182584002
 C,0,0.0901423395,0.1712741934,-0.0063676226
 C,0,0.0369062392,0.0164948498,1.336449644
 C,0,-1.2714235648,0.1811302623,2.0804998677
 C,0,1.2213190565,-0.3233431679,2.2132858135
 H,0,1.0425366657,-1.2659505147,2.7678180305
 H,0,2.1620238797,-0.4384001989,1.6514790044
 H,0,1.3806017477,0.4604625925,2.9802689071
 H,0,-1.2026857771,0.9835444548,2.842241796
 H,0,-2.1046260643,0.428148383,1.4001688538
 H,0,-1.5409682961,-0.7434118325,2.6295074057
 H,0,1.1171701932,-0.7330053928,-1.6845073234
 H,0,1.4554347584,0.9937344136,-1.4720462193
 H,0,2.2140980887,-0.1982975725,-0.3843047544
 H,0,-0.8536929278,0.4188355128,-0.5163890027
```

Sulfonyloxaziridine 2 (isomer-2)

B3LYP/6-31+G**



Filename: oxazsmb
E(RB+HF-LYP) = -757.686780445

Zero-point correction=	0.082777 (Hartree/Particle)
Thermal correction to Energy=	0.090345
Thermal correction to Enthalpy=	0.091289
Thermal correction to Gibbs Free Energy=	0.050542
Sum of electronic and zero-point Energies=	-757.604003
Sum of electronic and thermal Energies=	-757.596436
Sum of electronic and thermal Enthalpies=	-757.595491
Sum of electronic and thermal Free Energies=	-757.636238

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	56.692	26.285	85.758

O,0,1.4507635538,1.4353719409,-0.0641396064
S,0,0.8005504522,0.132505253,0.0520511878
O,0,0.5942575935,-0.4997975131,1.3637783803
N,0,-0.7545752759,0.2481830137,-0.8572205316
C,0,-1.9025180001,-0.1665859158,-0.0841509807
O,0,-1.6138236211,1.2121650468,-0.1488842427
C,0,1.6016878532,-1.0415871254,-1.0529816988
H,0,-2.7501087019,-0.5089747687,-0.6762284744
H,0,-1.7380158935,-0.6343874342,0.8852971064
H,0,2.6040106776,-1.1975978871,-0.6492090614
H,0,1.0385565232,-1.9758821856,-1.0486896639
H,0,1.6471558391,-0.6020514246,-2.0492984146

B3LYP/6-31G*

E(RB+HF-LYP) = -757.662692619
E (Cosmo, $CHCl_3$) E(RB+HF-LYP) = -757.664493634

Zero-point correction=	0.083417 (Hartree/Particle)
Thermal correction to Energy=	0.090939
Thermal correction to Enthalpy=	0.091883
Thermal correction to Gibbs Free Energy=	0.051215
Sum of electronic and zero-point Energies=	-757.579275
Sum of electronic and thermal Energies=	-757.571754
Sum of electronic and thermal Enthalpies=	-757.570810
Sum of electronic and thermal Free Energies=	-757.611477

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	57.065	26.082	85.592

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.957079	-0.674503	0.172367
2	8	0	1.936076	0.653067	-0.292488
3	7	0	0.892307	-0.296792	-0.726659
4	16	0	-0.625158	0.158330	0.129087
5	8	0	-0.986264	1.493087	-0.336650
6	8	0	-0.531566	-0.149567	1.561801
7	6	0	-1.682236	-1.063187	-0.667813
8	1	0	1.727036	-0.810141	1.228137
9	1	0	2.710963	-1.329100	-0.264464
10	1	0	-1.338434	-2.064426	-0.401249
11	1	0	-1.647517	-0.905142	-1.746297
12	1	0	-2.690691	-0.893479	-0.283547

B3LYP/6-31+G** (PCM)

Filename: oxazsmbPCM
E(RB+HF-LYP) = -757.698209050

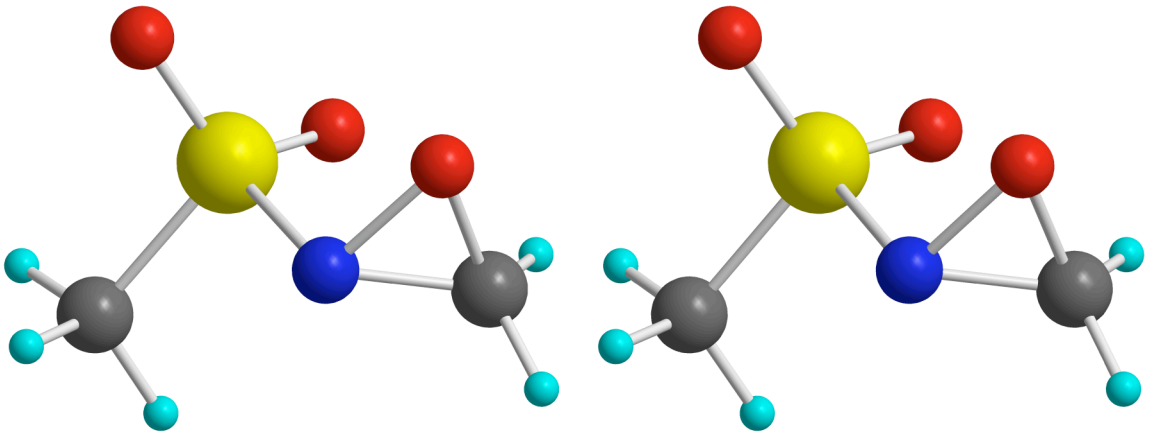
Zero-point correction= 0.082484 (Hartree/Particle)
Thermal correction to Energy= 0.090043
Thermal correction to Enthalpy= 0.090987
Thermal correction to Gibbs Free Energy= 0.050352
Sum of electronic and zero-point Energies= -757.615725
Sum of electronic and thermal Energies= -757.608166
Sum of electronic and thermal Enthalpies= -757.607222
Sum of electronic and thermal Free Energies= -757.647857

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	56.503	26.347	85.524

O,0,1.4851011133,1.4605253236,-0.1096171595
S,0,0.8131381304,0.1658134024,0.0417011232
O,0,0.6155657564,-0.4036719927,1.3851514864
N,0,-0.7452420981,0.3266250787,-0.8377946414
C,0,-1.8834393462,-0.1982106648,-0.1171365405
O,0,-1.6215834859,1.1887436685,-0.0256246375
C,0,1.5726893268,-1.0527048496,-1.0356434245
H,0,-2.7240661776,-0.487497385,-0.7465880439
H,0,-1.7128549899,-0.7647348198,0.7974486682
H,0,2.5813462468,-1.2125774941,-0.6464652161
H,0,0.9919524081,-1.9758858028,-0.9881268746
H,0,1.6053341158,-0.6450634645,-2.0469807396

Sulfonyloxaziridine 3 (isomer-3)

B3LYP/6-31+G**



oxazsmc
E(RB+HF-LYP) = -757.683377244

Zero-point correction=	0.082630 (Hartree/Particle)
Thermal correction to Energy=	0.090274
Thermal correction to Enthalpy=	0.091218
Thermal correction to Gibbs Free Energy=	0.049883
Sum of electronic and zero-point Energies=	-757.600747
Sum of electronic and thermal Energies=	-757.593104
Sum of electronic and thermal Enthalpies=	-757.592159
Sum of electronic and thermal Free Energies=	-757.633494

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	56.648	26.428	86.995

O,0,-2.5832063288,1.957104767,1.3412005613
S,0,-1.4020732098,1.5524258672,2.0960669195
C,0,-1.7990596278,0.0306505267,2.9899133627
N,0,-0.183692772,1.117405536,0.847638495
C,0,0.9329875196,0.3528767541,1.3237395162
O,0,-0.1032714287,-0.3489527733,0.6637565156
O,0,-0.7034959743,2.4810544309,2.9913740753
H,0,1.8569971101,0.486889989,0.7639717441
H,0,1.0431232222,0.1587195439,2.3905923012
H,0,-0.9147180502,-0.3561448557,3.495577236
H,0,-2.5467327141,0.3389318078,3.7237549063
H,0,-2.2139577461,-0.6933875936,2.2905703668

B3LYP/6-31G*

E(RB+HF-LYP) = -757.659048503
E (Cosmo, $CHCl_3$) E(RB+HF-LYP) = -757.660376666

Zero-point correction=	0.083379 (Hartree/Particle)
Thermal correction to Energy=	0.090919
Thermal correction to Enthalpy=	0.091863
Thermal correction to Gibbs Free Energy=	0.050980
Sum of electronic and zero-point Energies=	-757.575669
Sum of electronic and thermal Energies=	-757.568130
Sum of electronic and thermal Enthalpies=	-757.567185
Sum of electronic and thermal Free Energies=	-757.608069

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	57.053	26.182	86.046

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.951858	-0.436367	-0.401462
2	8	0	-1.825178	0.649534	0.490187
3	7	0	-0.941534	-0.535172	0.612801
4	16	0	0.720429	-0.147605	0.043107
5	8	0	1.024322	-1.153328	-0.977660
6	8	0	1.513366	-0.022206	1.259145
7	6	0	0.615124	1.483595	-0.733327
8	1	0	-1.662913	-0.253044	-1.437058
9	1	0	-2.816881	-1.082532	-0.257912
10	1	0	0.301274	2.215321	0.009889
11	1	0	-0.069257	1.463915	-1.582052
12	1	0	1.631964	1.688850	-1.076817

B3LYP/6-31+G** (PCM)

Filename: oxazsmcPCM
E(RB+HF-LYP) = -757.698208830

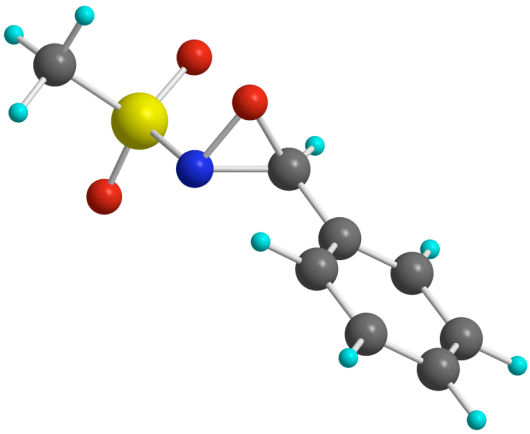
Zero-point correction=	0.082483 (Hartree/Particle)
Thermal correction to Energy=	0.090042
Thermal correction to Enthalpy=	0.090986
Thermal correction to Gibbs Free Energy=	0.050351
Sum of electronic and zero-point Energies=	-757.615726
Sum of electronic and thermal Energies=	-757.608167
Sum of electronic and thermal Enthalpies=	-757.607223
Sum of electronic and thermal Free Energies=	-757.647857

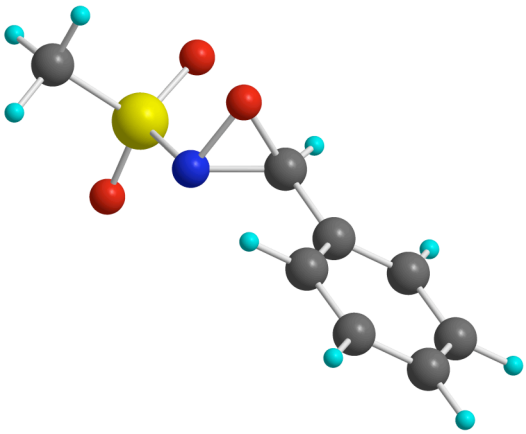
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	56.502	26.348	85.523

O,0,1.4863353053,1.4599522414,-0.1098993244
S,0,0.8137012285,0.1655049747,0.0413325305
O,0,0.6168002592,-0.4046837293,1.3845840422
N,0,-0.7453627592,0.3280018666,-0.8367712897
C,0,-1.8829311997,-0.1975567106,-0.115622594
O,0,-1.6206161455,1.1892257479,-0.0225120311
C,0,1.5715658281,-1.0530197992,-1.0371938512
H,0,-2.7242519706,-0.4857966286,-0.7446175388
H,0,-1.7115384111,-0.7654030642,0.7979843848
H,0,2.579640157,-1.2155394692,-0.6476494822
H,0,0.9890181196,-1.9751572322,-0.991313353
H,0,1.6055805883,-0.6441671974,-2.0479974931

trans-3-phenyl-2-methanesulfonyloxaziridine (isomer-1)

B3LYP/6-31+G**





```
Filename: b3BBoxsmtransa
E(RB+HF-LYP) = -988.767780998

 Zero-point correction=                           0.163589 (Hartree/Particle)
 Thermal correction to Energy=                    0.175721
 Thermal correction to Enthalpy=                  0.176665
 Thermal correction to Gibbs Free Energy=         0.123718
 Sum of electronic and zero-point Energies=           -988.604192
 Sum of electronic and thermal Energies=              -988.592060
 Sum of electronic and thermal Enthalpies=            -988.591116
 Sum of electronic and thermal Free Energies=         -988.644063

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 110.267             45.299           111.436

 C,0,-2.3477575362,-0.4687138084,-1.1536662221
 C,0,-1.7342456481,-0.3428417621,0.0914442543
 C,0,-2.4369012551,-0.6893010526,1.2541886049
 C,0,-3.7522937098,-1.1590076734,1.1599360206
 C,0,-4.3640220545,-1.2871579776,-0.0895075172
 C,0,-3.6620357182,-0.9420584215,-1.2464000816
 C,0,-1.8126824954,-0.5637137713,2.5964958148
 O,0,-0.8904217932,0.4888125217,2.8341241585
 N,0,-0.405277992,-0.9032659844,2.7493224904
 S,0,-0.0149325456,-1.4880020791,4.4019258807
 O,0,0.2288591478,-2.920576211,4.2170077926
 O,0,-0.9920059228,-1.007640864,5.3874656482
 C,0,1.5400300712,-0.6172912177,4.6421174421
 H,0,-2.4575060566,-0.7737179579,3.4500989589
 H,0,1.9143497446,-0.9236637253,5.6207123277
 H,0,1.3379418464,0.4540573852,4.6209656719
 H,0,2.225360578,-0.9170545464,3.8491861994
 H,0,-4.2974939017,-1.4246909329,2.0620310602
 H,0,-5.3840539434,-1.6529546423,-0.1572853518
 H,0,-4.1363100166,-1.0396216378,-2.2185760707
 H,0,-1.8027037571,-0.1993638762,-2.0534252958
 H,0,-0.7161920419,0.0235232348,0.1725282141
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B3LYP/6-31G*

```
E(RB+HF-LYP) = -988.729652244
E (Cosmo, CHCl3) E(RB+HF-LYP) =  -988.727489141

Zero-point correction=                           0.164511 (Hartree/Particle)
 Thermal correction to Energy=                    0.176548
 Thermal correction to Enthalpy=                  0.177492
 Thermal correction to Gibbs Free Energy=         0.124909
```

```
 Sum of electronic and zero-point Energies=           -988.565141
 Sum of electronic and thermal Energies=              -988.553104
 Sum of electronic and thermal Enthalpies=            -988.552160
 Sum of electronic and thermal Free Energies=         -988.604744

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 110.786             45.018            110.672


                  Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0    C   -0.123327   -0.216316   -0.597181
    2          8             0    O    0.529902    0.880662   -1.208324
    3          7             0    N    0.842728    0.533238    0.195214
    4         16             0    S    2.445917   -0.263936    0.240188
    5          8             0    O    2.635223   -1.156506   -0.908059
    6          8             0    O    2.554457   -0.760945    1.612027
    7          6             0    C    3.476027    1.195125    0.021125
    8          6             0    C   -1.563743   -0.098107   -0.255765
    9          6             0    C   -2.362681   -1.245854   -0.265839
   10          6             0    C   -3.716774   -1.160078    0.060165
   11          6             0    C   -4.274778    0.074836    0.392060
   12          6             0    C   -3.478481    1.224530    0.397578
   13          6             0    C   -2.126636    1.141165    0.075469
   14          1             0    H    0.206901   -1.184510   -0.974082
   15          1             0    H    3.265346    1.893286    0.832252
   16          1             0    H    3.248100    1.632160   -0.952247
   17          1             0    H    4.513317    0.855203    0.059128
   18          1             0    H   -1.924898   -2.206251   -0.527828
   19          1             0    H   -4.332735   -2.054788    0.052207
   20          1             0    H   -5.329420    0.143900    0.644431
   21          1             0    H   -3.914221    2.186342    0.653297
   22          1             0    H   -1.500445    2.027487    0.072509
 ---------------------------------------------------------------------
```

MPW1K/6-31+G*

```
E(RmPW+HF-PW91) =  -988.556345263

 Zero-point correction=                           0.170493 (Hartree/Particle)
 Thermal correction to Energy=                    0.182066
 Thermal correction to Enthalpy=                  0.183010
 Thermal correction to Gibbs Free Energy=         0.131347
 Sum of electronic and zero-point Energies=           -988.385852
 Sum of electronic and thermal Energies=              -988.374280
 Sum of electronic and thermal Enthalpies=            -988.373336
 Sum of electronic and thermal Free Energies=         -988.424999

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 114.248             43.161            108.734

 C,0,-0.1064574627,-0.2528239486,-0.5836175316
 O,0,0.5406681916,0.8122389902,-1.2093131184
 N,0,0.8466302826,0.5125890068,0.1638534865
 S,0,2.4091093967,-0.2326726364,0.2452583347
 O,0,2.6039239917,-1.1451176858,-0.8580529629
 O,0,2.5136054491,-0.689831911,1.6079923704
 C,0,3.4120669521,1.196354921,-0.002851901
 C,0,-1.5374168597,-0.1202267009,-0.2463718356
```

C,0,-2.3485027481,-1.2452747285,-0.2903108258
C,0,-3.6957022969,-1.1433663644,0.02284592
C,0,-4.2301404429,0.0849830039,0.3764482845
C,0,-3.4186688911,1.212174738,0.4180075131
C,0,-2.0744202338,1.1119322974,0.1089836222
H,0,0.222102224,-1.2230959735,-0.9373788433
H,0,3.1976546507,1.9121898911,0.7832547804
H,0,3.1967935449,1.6047190589,-0.9848078151
H,0,4.4454926273,0.865595354,0.0518796576
H,0,-1.9285906461,-2.2022199327,-0.5690560538
H,0,-4.3243803545,-2.0209529368,-0.0111763485
H,0,-5.2796911153,0.1669879492,0.6193827813
H,0,-3.837012358,2.1692266609,0.6934938495
H,0,-1.4346600593,1.981354609,0.1394904428

B3LYP/6-31+G** (PCM)

E(RB+HF-LYP) = -988.780890618

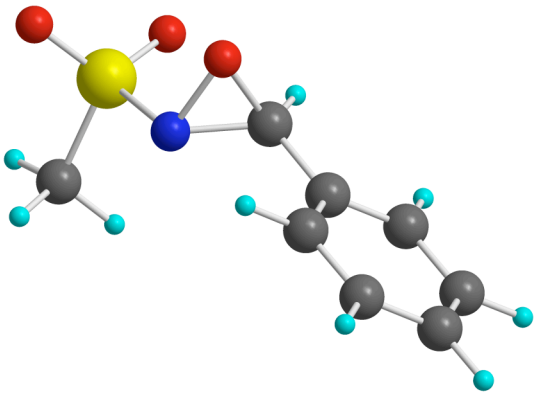
Zero-point correction=	0.162652 (Hartree/Particle)
Thermal correction to Energy=	0.174800
Thermal correction to Enthalpy=	0.175745
Thermal correction to Gibbs Free Energy=	0.122835
Sum of electronic and zero-point Energies=	-988.618239
Sum of electronic and thermal Energies=	-988.606090
Sum of electronic and thermal Enthalpies=	-988.605146
Sum of electronic and thermal Free Energies=	-988.658055

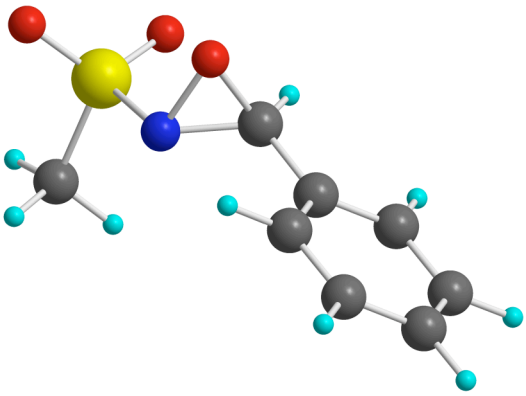
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	109.689	45.429	111.357

C,0,3.4670188439,1.2483947734,0.3791480003
C,0,2.1142370119,1.1384631451,0.0582689849
C,0,1.5700623429,-0.1179938551,-0.247904479
C,0,2.3856731759,-1.2569323574,-0.2320900102
C,0,3.7403444383,-1.1435834599,0.0930996492
C,0,4.281069363,0.1083869341,0.3985544054
C,0,0.1357885721,-0.2750083483,-0.5989507226
O,0,-0.5203491891,0.7674692294,-1.3122771385
N,0,-0.8500243951,0.5373659061,0.1051001475
S,0,-2.4579709854,-0.2390521761,0.2171808886
O,0,-2.5248033594,-0.6950758624,1.6132471827
O,0,-2.6844986583,-1.1931345686,-0.879939053
C,0,-3.4963611036,1.2042677704,-0.02126893
H,0,-0.1775642751,-1.2760393174,-0.9029938353
H,0,-4.5285874993,0.8585898181,0.0724694046
H,0,-3.3081496987,1.5991781111,-1.0210114643
H,0,-3.2531013235,1.931258865,0.7547438045
H,0,1.9620499981,-2.2306817113,-0.4739774075
H,0,4.3701440015,-2.0304656552,0.1050218128
H,0,5.3359390895,0.1984825064,0.6501111027
H,0,3.8887309683,2.2230662629,0.6153132533
H,0,1.4804206525,2.0216520751,0.04134625

trans-3-phenyl-2-methanesulfonyloxaziridine (Isomer 2)

B3LYP/6-31+G**





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Filename: b3BBoxazsmtransisb
E(RB+HF-LYP) = -988.725677463

 Zero-point correction=                           0.164417 (Hartree/Particle)
 Thermal correction to Energy=                    0.176491
 Thermal correction to Enthalpy=                  0.177435
 Thermal correction to Gibbs Free Energy=         0.124741
 Sum of electronic and zero-point Energies=           -988.561261
 Sum of electronic and thermal Energies=              -988.549187
 Sum of electronic and thermal Enthalpies=            -988.548243
 Sum of electronic and thermal Free Energies=         -988.600936

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 110.749             45.054           110.902
 C,0,4.2824310038,0.0769839778,0.4037466668
 C,0,3.4673666895,1.2122730183,0.455817421
 C,0,2.1208309598,1.1242668432,0.1125256091
 C,0,1.5819896994,-0.1061068276,-0.2861296345
 C,0,2.4002464896,-1.2390673137,-0.3436468401
 C,0,3.7488557105,-1.1485486611,0.003332086
 C,0,0.1469978706,-0.2284650867,-0.6487030793
 N,0,-0.8377217916,0.4513508517,0.1849538239
 S,0,-2.4673162581,-0.3068755553,0.1412076364
 O,0,-3.4135818895,0.74791343,-0.2112308411
 O,0,-0.5227632194,0.8984138553,-1.1825166986
 C,0,-2.5795583271,-0.6511550561,1.9065106879
 O,0,-2.442098745,-1.5782321446,-0.5944302178
 H,0,-0.1674193345,-1.1770359971,-1.0838463728
 H,0,1.9821751254,-2.1911173652,-0.6627784605
 H,0,4.3802220777,-2.0313127242,-0.0436699792
 H,0,5.3330802389,0.1504421073,0.6711485668
 H,0,3.8848453651,2.1673701152,0.7622422651
 H,0,1.4806483233,2.0001875501,0.1416924315
 H,0,-3.5641458237,-1.0947854038,2.0712375709
 H,0,-1.7936736575,-1.3558965446,2.1848731321
 H,0,-2.481509507,0.2877709311,2.4524862265
```

B3LYP/6-31+G** (PCM)

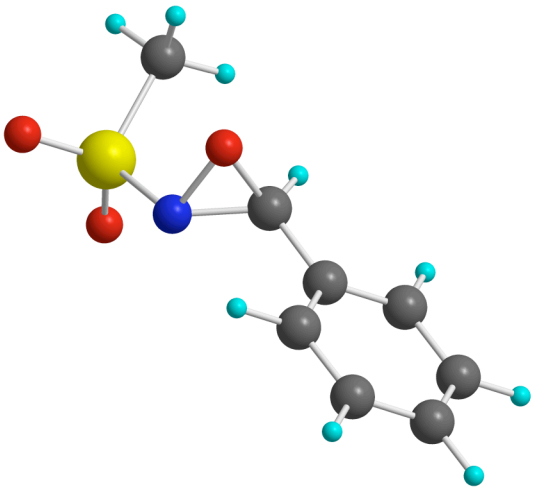
```
E(RB+HF-LYP) = -988.777909821
Zero-point correction=                           0.162577 (Hartree/Particle)
 Thermal correction to Energy=                    0.174753
 Thermal correction to Enthalpy=                  0.175697
 Thermal correction to Gibbs Free Energy=         0.122733
 Sum of electronic and zero-point Energies=           -988.615333
 Sum of electronic and thermal Energies=              -988.603157
 Sum of electronic and thermal Enthalpies=            -988.602213
 Sum of electronic and thermal Free Energies=         -988.655177
```

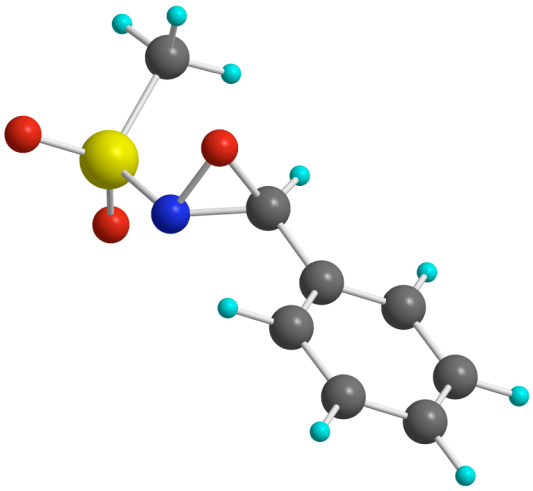
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	109.659	45.452	111.473

```
C,0,4.2810651976,0.0915018153,0.4082195934
C,0,3.4589537863,1.2252555046,0.4466254829
C,0,2.109201164,1.1248801619,0.1097158081
C,0,1.5763396347,-0.1166931104,-0.2701231234
C,0,2.4004701495,-1.2490008971,-0.3132872011
C,0,3.7519778161,-1.1450154439,0.0277093777
C,0,0.1448567714,-0.263967095,-0.635745559
N,0,-0.8492274417,0.4793936853,0.1334616873
S,0,-2.4873075688,-0.2536269433,0.1492331187
O,0,-3.4185825472,0.8457484872,-0.1309731432
O,0,-0.5259277764,0.8273307921,-1.2568665306
C,0,-2.5436259737,-0.679656867,1.8925297925
O,0,-2.5441061237,-1.4782626647,-0.6681299245
H,0,-0.1623760145,-1.2395802207,-1.0174233221
H,0,1.9868462213,-2.2096120127,-0.6176262518
H,0,4.388855636,-2.0262167864,-0.0083184904
H,0,5.3337622473,0.1749239226,0.67104798
H,0,3.8724557276,2.1883423103,0.7385052066
H,0,1.4691908254,2.0036424828,0.1344714854
H,0,-3.5334830234,-1.1087699487,2.0666522732
H,0,-1.7640037203,-1.4149129848,2.1008499799
H,0,-2.4054339875,0.2326698127,2.4742937606
```

trans-3-phenyl-2-methanesulfonyloxaziridine (Isomer 3)

B3LYP/6-31+G**





```
b3BBoxazsmtransisc
E(RB+HF-LYP) = -988.760076529

Zero-point correction=                           0.163415 (Hartree/Particle)
 Thermal correction to Energy=                    0.175632
 Thermal correction to Enthalpy=                  0.176576
 Thermal correction to Gibbs Free Energy=         0.123060
 Sum of electronic and zero-point Energies=           -988.596661
 Sum of electronic and thermal Energies=              -988.584445
 Sum of electronic and thermal Enthalpies=            -988.583501
 Sum of electronic and thermal Free Energies=         -988.637017
```

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	110.211	45.425	112.635

C,0,4.3111090541,0.1933617643,0.4000429459
C,0,3.4615220277,1.2990403625,0.2748096521
C,0,2.1132922435,1.1171382753,-0.027629583
C,0,1.6091625568,-0.1785385888,-0.2092782031
C,0,2.4598631297,-1.2832199608,-0.0853455708
C,0,3.8102465955,-1.0978538304,0.2206432271
C,0,0.1765782729,-0.3995680751,-0.5350428586
N,0,-0.8140757588,0.4796912174,0.0421564322
S,0,-2.4398807421,-0.2184429687,0.3248256987
O,0,-3.3336980723,0.932896568,0.4136300574
O,0,-0.4862716774,0.5260696535,-1.3953083489
O,0,-2.2593747105,-1.1411518789,1.4503467273
C,0,-2.885799699,-1.1504519737,-1.1617325618
H,0,-0.1035124751,-1.4410665581,-0.6975903882
H,0,2.0679419062,-2.2877555526,-0.2248631445
H,0,4.4661672204,-1.9575978451,0.3175488981
H,0,5.3607500938,0.3399873564,0.6372386171
H,0,3.8515748828,2.3025276316,0.4157907283
H,0,1.4466720105,1.9677896594,-0.123295055
H,0,-3.9045948979,-1.4921177196,-0.9678361073
H,0,-2.8570075188,-0.4826103147,-2.0213771496
H,0,-2.2216144419,-2.0050512219,-1.2884810134

B3LYP/6-31+G** (PCM)

E(RB+HF-LYP) = -988.774902412

Zero-point correction= 0.162505 (Hartree/Particle)
Thermal correction to Energy= 0.174746
Thermal correction to Enthalpy= 0.175690
Thermal correction to Gibbs Free Energy= 0.122271
Sum of electronic and zero-point Energies= -988.612398
Sum of electronic and thermal Energies= -988.600157
Sum of electronic and thermal Enthalpies= -988.599213
Sum of electronic and thermal Free Energies= -988.652631

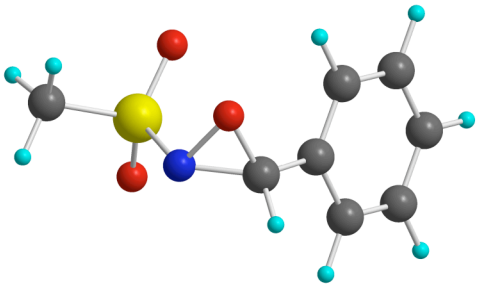
	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	109.655	45.554	112.428

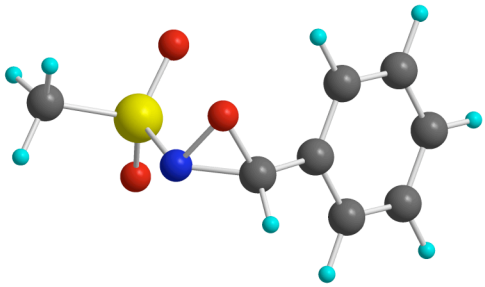
C,0,4.3081073035,0.1722423074,0.4046050381
C,0,3.463057866,1.2876917165,0.3384896821
C,0,2.1134988206,1.1278889763,0.0254981185
C,0,1.6049209512,-0.1553555737,-0.2262107656
C,0,2.45099257,-1.2702034523,-0.1631738811
C,0,3.8022136123,-1.1062401756,0.1541564087
C,0,0.1744289989,-0.3621367669,-0.5662608537
N,0,-0.8204343669,0.4858281774,0.0623582759
S,0,-2.4574510347,-0.1748056949,0.2944475009
O,0,-3.3374743026,0.9968143734,0.2341272691
O,0,-0.494993748,0.6168190136,-1.3661578482
O,0,-2.3577511932,-0.9671149443,1.5283126387
C,0,-2.8515094427,-1.2443965985,-1.1036526391
H,0,-0.1015147697,-1.3922515263,-0.7970005156
H,0,2.054616995,-2.2652546615,-0.3613395156
H,0,4.456067095,-1.9742281583,0.2035529401
H,0,5.3602334419,0.3020158516,0.6504013623
H,0,3.8577585341,2.282661336,0.5330653734
H,0,1.4554536307,1.9918786266,-0.0257336804
H,0,-3.9003362903,-1.5136439115,-0.9551733976

```
 H,0,-2.7253232805,-0.6782449089,-2.0268760847
 H,0,-2.2255113905,-2.1368880063,-1.0781824261
```

cis-3-phenyl-2-methanesulfonyloxaziridine (Isomer 1)

B3LYP/6-31+G**





```
b3BBoxazsmcisisb
E(RB+HF-LYP) = -988.757855848

Zero-point correction=                           0.163511 (Hartree/Particle)
 Thermal correction to Energy=                    0.175586
 Thermal correction to Enthalpy=                  0.176530
 Thermal correction to Gibbs Free Energy=         0.123944
 Sum of electronic and zero-point Energies=           -988.594345
 Sum of electronic and thermal Energies=              -988.582270
 Sum of electronic and thermal Enthalpies=            -988.581325
 Sum of electronic and thermal Free Energies=         -988.633912

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 110.182             45.355           110.678
 Zero-point correction=                           0.162637 (Hartree/Particle)

 C,0,3.1126753765,-3.9781463527,-1.5889125085
 C,0,3.296047926,-3.4912121895,-0.288851802
 C,0,4.4640627652,-3.8114650362,0.4178474206
 C,0,5.42865286,-4.6379198254,-0.1581285574
 C,0,5.2408892734,-5.1292974344,-1.4533703404
 C,0,4.0865436285,-4.7942978783,-2.1663037468
 C,0,2.3218903725,-2.5617165352,0.3574077992
 O,0,1.1556094052,-2.1662331844,-0.3341088143
 N,0,1.0271749581,-2.8999911529,0.939475798
 S,0,0.4011779689,-4.5622371023,0.7161573176
 O,0,1.0985673997,-5.3506776962,1.7374389906
 O,0,0.3595007136,-4.9811251027,-0.6868752879
 C,0,-1.2808985569,-4.2337313755,1.2657306326
 H,0,2.7908728118,-1.7619248317,0.9348202234
 H,0,4.6143967868,-3.4210735301,1.4213093761
 H,0,6.3250859709,-4.8924645145,0.3991447582
 H,0,5.9936910982,-5.7679726008,-1.9062102424
 H,0,3.940219982,-5.1717042017,-3.1738461473
 H,0,2.2091148753,-3.7283845301,-2.1318450801
 H,0,-1.802899678,-5.1918856953,1.2290761348
 H,0,-1.2443553177,-3.8439416788,2.2825795883
 H,0,-1.7355026202,-3.5198845511,0.5776574877
```

B3LYP/6-31G*

```
E(RB+HF-LYP) =  -988.720366144
E (Cosmo, CHCl3) E(RB+HF-LYP) =  -988.664369180
```

```
Zero-point correction=                           0.164421 (Hartree/Particle)
Thermal correction to Energy=                    0.176420
Thermal correction to Enthalpy=                  0.177364
Thermal correction to Gibbs Free Energy=         0.125017
Sum of electronic and zero-point Energies=           -988.555945
Sum of electronic and thermal Energies=              -988.543947
Sum of electronic and thermal Enthalpies=            -988.543002
Sum of electronic and thermal Free Energies=         -988.595349

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                  110.705             45.075            110.174

                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0       -0.005453    1.598521    0.074951
   2          8             0        0.854266    1.709867   -1.036889
   3          7             0        1.385703    1.195069    0.241559
   4         16             0        1.760858   -0.549835    0.163692
   5          8             0        1.294768   -1.185163   -1.068917
   6          8             0        1.398083   -1.059694    1.487628
   7          6             0        3.549660   -0.370880    0.063874
   8          6             0       -1.200535    0.705665    0.012377
   9          6             0       -2.037659    0.643227    1.133826
  10          6             0       -3.190123   -0.139158    1.104907
  11          6             0       -3.521899   -0.846660   -0.052626
  12          6             0       -2.697431   -0.771596   -1.176834
  13          6             0       -1.537144    0.000924   -1.148694
  14          1             0       -0.183936    2.541763    0.597074
  15          1             0        3.898621    0.181613    0.936694
  16          1             0        3.796110    0.153448   -0.861063
  17          1             0        3.961988   -1.382466    0.052094
  18          1             0       -1.783081    1.203005    2.030877
  19          1             0       -3.829951   -0.192100    1.981187
  20          1             0       -4.423725   -1.452336   -0.078989
  21          1             0       -2.956363   -1.317352   -2.079713
  22          1             0       -0.886752    0.055966   -2.013405
---------------------------------------------------------------------
```

B3LYP/6-31+G** (PCM)

```
E(RB+HF-LYP) = -988.770552935
Zero-point correction=                           0.162637 (Hartree/Particle)
 Thermal correction to Energy=                    0.174717
 Thermal correction to Enthalpy=                  0.175661
 Thermal correction to Gibbs Free Energy=         0.123112
 Sum of electronic and zero-point Energies=           -988.607916
 Sum of electronic and thermal Energies=              -988.595836
 Sum of electronic and thermal Enthalpies=            -988.594892
 Sum of electronic and thermal Free Energies=         -988.647441

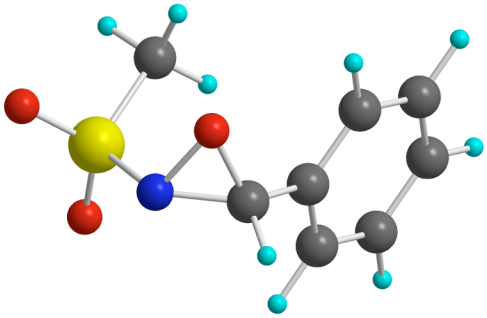
                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  109.636             45.442            110.599

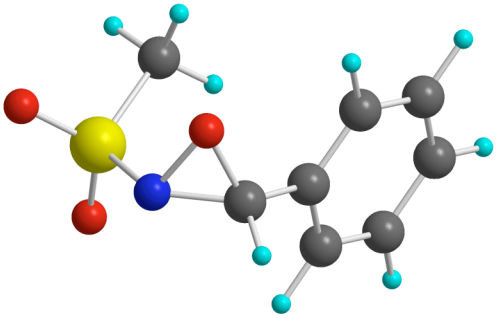
 C,0,3.133906729,-3.9432699102,-1.6244419285
 C,0,3.2887122086,-3.493334842,-0.3070744507
 C,0,4.4337391732,-3.8455956244,0.4229763175
 C,0,5.4019901151,-4.6722614956,-0.1491962995
 C,0,5.2430096264,-5.1281606139,-1.4623803777
```

```
C,0,4.1132119377,-4.7571107767,-2.1984877476
C,0,2.3151790485,-2.5580141944,0.3309252195
O,0,1.1285778335,-2.1985278845,-0.3534221651
N,0,1.0306569946,-2.8991402718,0.9401673099
S,0,0.4088798847,-4.5626819013,0.770899514
O,0,1.1033554001,-5.3111872481,1.8297030056
O,0,0.4046046848,-5.0508821142,-0.6130296871
C,0,-1.2819609444,-4.2327280111,1.278126963
H,0,2.7789341147,-1.7344215976,0.8822967122
H,0,4.564781253,-3.4770764314,1.439570642
H,0,6.2820044494,-4.9525707681,0.4256509324
H,0,6.0011829519,-5.7657677164,-1.9126541102
H,0,3.9910602131,-5.1035060712,-3.222574495
H,0,2.2519069198,-3.6612959138,-2.1910281354
H,0,-1.7974319717,-5.1959309414,1.2611961365
H,0,-1.2659196787,-3.8111122913,2.2835200857
H,0,-1.7278629435,-3.5427103808,0.5594495586
```

cis-3-phenyl-2-methanesulfonyloxaziridine (Isomer 2)

B3LYP/6-31+G**





```
b3BBoxazsmcisisc
E(RB+HF-LYP) = -988.751621168

Zero-point correction=                           0.163578 (Hartree/Particle)
 Thermal correction to Energy=                    0.175633
 Thermal correction to Enthalpy=                  0.176577
 Thermal correction to Gibbs Free Energy=         0.124400
 Sum of electronic and zero-point Energies=           -988.588043
 Sum of electronic and thermal Energies=              -988.575988
 Sum of electronic and thermal Enthalpies=            -988.575044
 Sum of electronic and thermal Free Energies=         -988.627221

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 110.211             45.351            109.816

 C,0,3.553787426,-3.667132354,-1.6399833367
 C,0,3.4962012157,-3.0963821004,-0.3619372037
 C,0,4.131543115,-3.7291058514,0.7153349166
 C,0,4.7984252581,-4.9395200665,0.515867979
 C,0,4.8491963646,-5.5131156361,-0.7585149224
 C,0,4.2292269282,-4.8741660309,-1.8361128825
 C,0,2.8513973008,-1.7587958553,-0.1745064827
 O,0,1.7328395056,-1.4129405474,-0.9779647733
 N,0,1.6010149548,-1.4752431255,0.4929296447
 S,0,0.5051317245,-2.7585916851,1.0686429003
 C,0,0.4195997534,-4.1035945776,-0.1370166964
 O,0,-0.8035494231,-2.1103677463,1.0810448495
 O,0,1.1410756429,-3.2255864439,2.3047709561
 H,0,3.5548552824,-0.9350329857,-0.0283840473
 H,0,4.0829405747,-3.2907701398,1.7074407883
```

```
 H,0,5.2756652966,-5.4345028916,1.3561180717
 H,0,5.3714960379,-6.4529429755,-0.9108488299
 H,0,4.2707943853,-5.3135696399,-2.8283025922
 H,0,3.0680846873,-3.1690048188,-2.4736884998
 H,0,-0.4417877757,-4.693540784,0.1837757317
 H,0,0.2432410413,-3.6758340637,-1.1237529746
 H,0,1.3355297037,-4.6889766805,-0.1041185963
```

B3LYP/6-31+G** (PCM)

```
E(RB+HF-LYP) = -988.766629937
Zero-point correction=                           0.162703 (Hartree/Particle)
 Thermal correction to Energy=                    0.174731
 Thermal correction to Enthalpy=                  0.175676
 Thermal correction to Gibbs Free Energy=         0.123527
 Sum of electronic and zero-point Energies=           -988.603927
 Sum of electronic and thermal Energies=              -988.591899
 Sum of electronic and thermal Enthalpies=            -988.590954
 Sum of electronic and thermal Free Energies=         -988.643103

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 109.646             45.414           109.756

 C,0,3.5070346922,-3.6692398876,-1.6220677144
 C,0,3.5047533836,-3.0917208697,-0.3455254746
 C,0,4.1843454733,-3.7165412525,0.7102130077
 C,0,4.8355655234,-4.9330084637,0.4933717652
 C,0,4.8291803231,-5.5164187457,-0.7786978385
 C,0,4.1695409193,-4.8813247969,-1.8357102605
 C,0,2.8751819874,-1.7539934278,-0.1280478857
 O,0,1.7705317107,-1.3683411087,-0.9383072378
 N,0,1.6068092915,-1.4815372019,0.5227010133
 S,0,0.4667325117,-2.746203701,1.0164193806
 C,0,0.4577710986,-4.1379820587,-0.1310256867
 O,0,-0.836273199,-2.0813284345,0.9064306452
 O,0,0.9747484272,-3.1664753904,2.3296709559
 H,0,3.5798941264,-0.9392332684,0.0686523565
 H,0,4.1942556159,-3.261309104,1.6990714926
 H,0,5.3491689863,-5.4233920992,1.3175267728
 H,0,5.3412125177,-6.4618296609,-0.9458273086
 H,0,4.1695753003,-5.3279771987,-2.8277546029
 H,0,2.9927171365,-3.1736480811,-2.4427985986
 H,0,-0.4202314542,-4.7199679208,0.1619847062
 H,0,0.3413805064,-3.7531370497,-1.1445956956
 H,0,1.3728141217,-4.7141072781,-0.0148897922
```

2-methyl-2-butene

B3LYP/6-31+G**

```
b3BBgassm1
E(RB+HF-LYP) = -196.564442449

 Zero-point correction=                           0.135787 (Hartree/Particle)
 Thermal correction to Energy=                    0.142700
 Thermal correction to Enthalpy=                  0.143644
 Thermal correction to Gibbs Free Energy=         0.105915
 Sum of electronic and zero-point Energies=           -196.428655
 Sum of electronic and thermal Energies=              -196.421743
 Sum of electronic and thermal Enthalpies=            -196.420798
```

```
 Sum of electronic and thermal Free Energies=         -196.458528

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.545             23.867             79.408

 C,0,1.281173637,0.0498317609,-0.9134809796
 C,0,0.0906984563,0.1704043374,-0.0019835532
 C,0,0.0373073543,0.016731378,1.3325516874
 C,0,-1.2670696654,0.1805374912,2.0785472407
 C,0,1.2183796602,-0.3226361701,2.210294032
 H,0,1.0358362145,-1.2569079589,2.7581246555
 H,0,2.151257366,-0.437980225,1.655190508
 H,0,1.3723723812,0.4571417807,2.9681831662
 H,0,-1.193454096,0.9772319833,2.8313496747
 H,0,-2.0940151587,0.4251311512,1.4053925413
 H,0,-1.5295315415,-0.7379256536,2.6210750781
 H,0,1.1147216205,-0.7271747466,-1.6711257403
 H,0,1.4495372609,0.9870102794,-1.4602202041
 H,0,2.2055576881,-0.1956460031,-0.3852302755
 H,0,-0.8439721773,0.4154725952,-0.5088228313
```

mPW1K/6-31+G**

```
mpBBgassm1
E(RmPW+HF-PW91) = -196.512416150

 Zero-point correction=                           0.139640 (Hartree/Particle)
 Thermal correction to Energy=                    0.146473
 Thermal correction to Enthalpy=                  0.147417
 Thermal correction to Gibbs Free Energy=         0.109820
 Sum of electronic and zero-point Energies=           -196.372776
 Sum of electronic and thermal Energies=              -196.365943
 Sum of electronic and thermal Enthalpies=            -196.364999
 Sum of electronic and thermal Free Energies=         -196.402596

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  91.913             23.387             79.130

 C,0,1.2739378348,0.0489152973,-0.8960023934
 C,0,0.0908762048,0.1697380582,0.0047481617
 C,0,0.0394597382,0.0168869741,1.3286479859
 C,0,-1.2529961737,0.1787839109,2.0700670237
 C,0,1.2108743156,-0.3194941659,2.1980443902
 H,0,1.0277837237,-1.2481200646,2.7408164902
 H,0,2.1379847299,-0.4334222071,1.6459707701
 H,0,1.3618914083,0.4563863177,2.9501588974
 H,0,-1.1772430272,0.9703081182,2.8175569491
 H,0,-2.0753429386,0.4220623436,1.401743689
 H,0,-1.5112390567,-0.7351056735,2.6077486675
 H,0,1.1090490277,-0.7241045001,-1.6474595484
 H,0,1.4427464399,0.9802791316,-1.4377613475
 H,0,2.1902881135,-0.1955563226,-0.3671167478
 H,0,-0.8392723403,0.4136637821,-0.4973169877
```

B3LYP/6-31G*

```
E(RB+HF-LYP) =  -196.543583745

 Zero-point correction=                           0.134493 (Hartree/Particle)
 Thermal correction to Energy=                    0.142040
 Thermal correction to Enthalpy=                  0.142984
```

```
 Thermal correction to Gibbs Free Energy=         0.103815
 Sum of electronic and zero-point Energies=           -196.409091
 Sum of electronic and thermal Energies=              -196.401544
 Sum of electronic and thermal Enthalpies=            -196.400600
 Sum of electronic and thermal Free Energies=         -196.439769

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  89.131             25.076             82.438

                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number              X           Y           Z
 ---------------------------------------------------------------------
    1          6      C     0.734302   -0.671522   -0.000002
    2          6      C    -0.449608   -0.040352   -0.000003
    3          6      C    -0.629993    1.458176    0.000000
    4          6      C     2.115263   -0.077846    0.000000
    5          1      H     0.714160   -1.762813    0.000002
    6          6      C    -1.741324   -0.824199    0.000000
    7          1      H    -1.205424    1.779740   -0.879540
    8          1      H    -1.205280    1.779752    0.879630
    9          1      H     0.313768    2.008357   -0.000083
   10          1      H    -1.563937   -1.904444    0.000030
   11          1      H    -2.353788   -0.580559   -0.879961
   12          1      H    -2.353810   -0.580515    0.879935
   13          1      H     2.683510   -0.410228    0.879861
   14          1      H     2.115417    1.015466   -0.000043
   15          1      H     2.683543   -0.410297   -0.879813
 ---------------------------------------------------------------------
```

MPW1K/6-31+G*

```
E(RmPW+HF-PW91) =  -196.495886934

 Zero-point correction=                           0.140385 (Hartree/Particle)
 Thermal correction to Energy=                    0.147199
 Thermal correction to Enthalpy=                  0.148143
 Thermal correction to Gibbs Free Energy=         0.110576
 Sum of electronic and zero-point Energies=           -196.355502
 Sum of electronic and thermal Energies=              -196.348688
 Sum of electronic and thermal Enthalpies=            -196.347744
 Sum of electronic and thermal Free Energies=         -196.385311

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  92.369             23.258             79.065

 C,0,-0.1975509345,-0.063112104,0.9684390342
 C,0,-0.2583931984,0.088259349,-0.3551860693
 C,0,0.990100254,-0.3859539872,1.8121255407
 C,0,0.9052063516,-0.0422347963,-1.2882819494
 C,0,-1.5559123039,0.4147690668,-1.030693869
 H,0,-1.1234812885,0.0612645302,1.5206744534
 H,0,1.1616519299,0.3966579254,2.5533070775
 H,0,1.9051781321,-0.5016277588,1.2376939211
 H,0,0.828919794,-1.3116853774,2.3675034211
 H,0,0.7158031292,-0.8220784746,-2.0287783277
 H,0,1.8372447184,-0.2812906448,-0.7851295655
 H,0,1.0544164026,0.885280612,-1.8449035842
 H,0,-1.4846927402,1.3552018262,-1.581441681
 H,0,-2.3736690512,0.502006813,-0.3180603027
 H,0,-1.8220720391,-0.3540946208,-1.7592815352
```

MP2/6-31G*

EUMP2= -0.19579496015743D+03

Zero-point correction= 0.139534 (Hartree/Particle)
Thermal correction to Energy= 0.146471
Thermal correction to Enthalpy= 0.147415
Thermal correction to Gibbs Free Energy= 0.109447
Sum of electronic and zero-point Energies= -195.655426
Sum of electronic and thermal Energies= -195.648489
Sum of electronic and thermal Enthalpies= -195.647545
Sum of electronic and thermal Free Energies= -195.685514

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	91.912	23.473	79.911

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.735969	-0.675499	0.000000
2	6	0	0.000000	0.451358	0.000000
3	6	0	-1.503765	0.504132	0.000000
4	6	0	0.257823	-2.097251	0.000000
5	1	0	1.820710	-0.559766	0.000000
6	6	0	0.667195	1.801440	0.000000
7	1	0	-1.865236	1.049177	0.879975
8	1	0	-1.865236	1.049177	-0.879975
9	1	0	-1.969367	-0.482220	0.000000
10	1	0	1.756846	1.711502	0.000000
11	1	0	0.371085	2.384230	0.880498
12	1	0	0.371085	2.384230	-0.880498
13	1	0	0.633501	-2.631229	-0.880021
14	1	0	-0.830215	-2.178949	0.000000
15	1	0	0.633501	-2.631229	0.880021

HF/6-31G*

E(RHF) = -195.145768089

Zero-point correction= 0.145805 (Hartree/Particle)
Thermal correction to Energy= 0.152444
Thermal correction to Enthalpy= 0.153388
Thermal correction to Gibbs Free Energy= 0.116105
Sum of electronic and zero-point Energies= -194.999963
Sum of electronic and thermal Energies= -194.993324
Sum of electronic and thermal Enthalpies= -194.992380
Sum of electronic and thermal Free Energies= -195.029663

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	95.660	22.361	78.469

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.731264	-0.661217	0.000000

2	6	0	0.000000	0.443471	0.000000
3	6	0	-1.508819	0.493200	0.000000
4	6	0	0.277045	-2.095671	0.000000
5	1	0	1.804077	-0.542333	0.000000
6	6	0	0.655555	1.804655	0.000000
7	1	0	-1.868830	1.032923	0.872944
8	1	0	-1.868830	1.032923	-0.872944
9	1	0	-1.971745	-0.483407	0.000000
10	1	0	1.736766	1.732621	0.000000
11	1	0	0.355358	2.379606	0.873344
12	1	0	0.355358	2.379606	-0.873344
13	1	0	0.663267	-2.616267	-0.873015
14	1	0	-0.798959	-2.206026	0.000000
15	1	0	0.663267	-2.616267	0.873015

BP86/6-31G*

E(RB-P86) = -196.527990360

Zero-point correction= 0.132898 (Hartree/Particle)
Thermal correction to Energy= 0.139864
Thermal correction to Enthalpy= 0.140808
Thermal correction to Gibbs Free Energy= 0.103077
Sum of electronic and zero-point Energies= -196.395093
Sum of electronic and thermal Energies= -196.388127
Sum of electronic and thermal Enthalpies= -196.387183
Sum of electronic and thermal Free Energies= -196.424913

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	87.766	24.292	79.411

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.738333	-0.677805	0.000000
2	6	0	0.000000	0.455544	0.000000
3	6	0	-1.511844	0.500590	0.000000
4	6	0	0.263242	-2.106635	0.000000
5	1	0	1.832943	-0.559002	0.000000
6	6	0	0.669639	1.813413	0.000000
7	1	0	-1.888381	1.049400	0.886033
8	1	0	-1.888381	1.049400	-0.886033
9	1	0	-1.979308	-0.497034	0.000000
10	1	0	1.770195	1.730648	0.000000
11	1	0	0.371532	2.408712	0.886308
12	1	0	0.371532	2.408712	-0.886308
13	1	0	0.644545	-2.651176	-0.886236
14	1	0	-0.835440	-2.199119	0.000000
15	1	0	0.644545	-2.651176	0.886236

B3LYP/6-311+G**

E(RB+HF-LYP) = -196.600890884

Zero-point correction= 0.135233 (Hartree/Particle)
Thermal correction to Energy= 0.142170
Thermal correction to Enthalpy= 0.143115

```
Thermal correction to Gibbs Free Energy=         0.105324
Sum of electronic and zero-point Energies=           -196.465658
Sum of electronic and thermal Energies=              -196.458720
Sum of electronic and thermal Enthalpies=            -196.457776
Sum of electronic and thermal Free Energies=         -196.495567

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                   89.213             23.924             79.538

                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0   C     0.737583   -0.667280    0.000000
   2          6             0   C     0.000000    0.450525    0.000000
   3          6             0   C    -1.507532    0.488390    0.000000
   4          6             0   C     0.272348   -2.095574    0.000000
   5          1             0   H     1.819896   -0.544698    0.000000
   6          6             0   C     0.656109    1.810013    0.000000
   7          1             0   H    -1.877811    1.030376    0.878305
   8          1             0   H    -1.877811    1.030376   -0.878305
   9          1             0   H    -1.965186   -0.500421    0.000000
  10          1             0   H     1.745402    1.735025    0.000000
  11          1             0   H     0.354133    2.392335    0.878856
  12          1             0   H     0.354133    2.392335   -0.878856
  13          1             0   H     0.654969   -2.628501   -0.878106
  14          1             0   H    -0.813739   -2.194774    0.000000
  15          1             0   H     0.654969   -2.628501    0.878106
---------------------------------------------------------------------
```

B3LYP/6-31+G** (PCM)

```
b3BBpcmsm1
E(RB+HF-LYP) = -196.565413359

 Zero-point correction=                           0.135524 (Hartree/Particle)
 Thermal correction to Energy=                    0.142437
 Thermal correction to Enthalpy=                  0.143381
 Thermal correction to Gibbs Free Energy=         0.105656
 Sum of electronic and zero-point Energies=           -196.429889
 Sum of electronic and thermal Energies=              -196.422976
 Sum of electronic and thermal Enthalpies=            -196.422032
 Sum of electronic and thermal Free Energies=         -196.459758

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.381             23.896             79.400

 C,0,1.281864642,0.0496491806,-0.9140792386
 C,0,0.0902577949,0.1707152675,-0.0031265418
 C,0,0.0372370738,0.0167487062,1.3323929634
 C,0,-1.2671473053,0.180419384,2.0793085333
 C,0,1.2182376559,-0.3225553854,2.2106855238
 H,0,1.0347765864,-1.2566080371,2.7588129871
 H,0,2.1517704635,-0.437719254,1.6563701709
 H,0,1.3709489953,0.4572369069,2.9690703298
 H,0,-1.1926650207,0.9765230788,2.8328287942
 H,0,-2.0946384272,0.425126832,1.4064358393
```

H,0,-1.5284993516,-0.7382672381,2.6222706618
H,0,1.115054752,-0.726888968,-1.672384843
H,0,1.4502957192,0.9866350563,-1.461406583
H,0,2.2063934161,-0.1962384694,-0.3858261108
H,0,-0.8450889944,0.4164439397,-0.5115064865

mPW1k/6-31+G** (PCM)

mpBBPCMsm
E(RmPW+HF-PW91) = -196.513563299

Zero-point correction=	0.139364 (Hartree/Particle)
Thermal correction to Energy=	0.146197
Thermal correction to Enthalpy=	0.147141
Thermal correction to Gibbs Free Energy=	0.109548
Sum of electronic and zero-point Energies=	-196.374199
Sum of electronic and thermal Energies=	-196.367366
Sum of electronic and thermal Enthalpies=	-196.366422
Sum of electronic and thermal Free Energies=	-196.404015

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.740	23.415	79.122

C,0,1.2745748936,0.0488636388,-0.8966117963
C,0,0.0903210638,0.1699483218,0.0036031332
C,0,0.0392781353,0.0169139186,1.3285684439
C,0,-1.2529955609,0.178710361,2.0707541493
C,0,1.2106137898,-0.3195119864,2.1986015729
H,0,1.0265986166,-1.2478354292,2.7418579321
H,0,2.1383255748,-0.4336096285,1.6472347625
H,0,1.3605917247,0.4563087085,2.951187837
H,0,-1.1761263156,0.9697474179,2.8188330384
H,0,-2.0758985933,0.4220851166,1.4026533373
H,0,-1.5100808845,-0.7352883123,2.6090691646
H,0,1.1097587899,-0.723675248,-1.648837097
H,0,1.4432940341,0.9799730343,-1.4391941418
H,0,2.191198512,-0.1956559704,-0.3678217955
H,0,-0.84065578,0.4142460573,-0.5000525407

B3LYP/6-31+G** (onsager)

b3BBonssm
E(RB+HF-LYP) = -196.564448855

Zero-point correction=	0.135775 (Hartree/Particle)
Thermal correction to Energy=	0.142688
Thermal correction to Enthalpy=	0.143632
Thermal correction to Gibbs Free Energy=	0.105902
Sum of electronic and zero-point Energies=	-196.428674
Sum of electronic and thermal Energies=	-196.421761
Sum of electronic and thermal Enthalpies=	-196.420817
Sum of electronic and thermal Free Energies=	-196.458547

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.538	23.871	79.410

C,0,1.281174,0.049832,-0.913481
C,0,0.090698,0.170404,-0.001984
C,0,0.037307,0.016731,1.332552
C,0,-1.26707,0.180537,2.078547

```
C,0,1.21838,-0.322636,2.210294
H,0,1.035836,-1.256908,2.758125
H,0,2.151257,-0.43798,1.655191
H,0,1.372372,0.457142,2.968183
H,0,-1.193454,0.977232,2.83135
H,0,-2.094015,0.425131,1.405393
H,0,-1.529532,-0.737926,2.621075
H,0,1.114722,-0.727175,-1.671126
H,0,1.449537,0.98701,-1.46022
H,0,2.205558,-0.195646,-0.38523
H,0,-0.843972,0.415473,-0.508823
```

mPW1k/6-31+G** (onsager)

```
mpBBonssm
E(RmPW+HF-PW91) = -196.512422621

 Zero-point correction=                           0.139628 (Hartree/Particle)
 Thermal correction to Energy=                    0.146462
 Thermal correction to Enthalpy=                  0.147406
 Thermal correction to Gibbs Free Energy=         0.109808
 Sum of electronic and zero-point Energies=           -196.372795
 Sum of electronic and thermal Energies=              -196.365961
 Sum of electronic and thermal Enthalpies=            -196.365017
 Sum of electronic and thermal Free Energies=         -196.402615

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  91.906             23.391             79.132

 C,0,1.273938,0.048915,-0.896002
 C,0,0.090876,0.169738,0.004748
 C,0,0.03946,0.016887,1.328648
 C,0,-1.252996,0.178784,2.070067
 C,0,1.210874,-0.319494,2.198044
 H,0,1.027784,-1.24812,2.740816
 H,0,2.137985,-0.433422,1.645971
 H,0,1.361891,0.456386,2.950159
 H,0,-1.177243,0.970308,2.817557
 H,0,-2.075343,0.422062,1.401744
 H,0,-1.511239,-0.735106,2.607749
 H,0,1.109049,-0.724105,-1.64746
 H,0,1.442746,0.980279,-1.437761
 H,0,2.190288,-0.195556,-0.367117
 H,0,-0.839272,0.413664,-0.497317
```

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

```
E(RB+HF-LYP) = -196.601942835

 Zero-point correction=                           0.134986 (Hartree/Particle)
 Thermal correction to Energy=                    0.141932
 Thermal correction to Enthalpy=                  0.142876
 Thermal correction to Gibbs Free Energy=         0.105043
 Sum of electronic and zero-point Energies=           -196.466957
 Sum of electronic and thermal Energies=              -196.460011
 Sum of electronic and thermal Enthalpies=            -196.459067
 Sum of electronic and thermal Free Energies=         -196.496900

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.064             23.942             79.626
```

```
 C,0,1.2803710245,0.0492798883,-0.9089243198
 C,0,0.0900458354,0.1704180326,0.0003264173
 C,0,0.0377003568,0.0169581716,1.3307180847
 C,0,-1.2647711101,0.1802491098,2.0768923456
 C,0,1.2174265384,-0.3219358739,2.2071777465
 H,0,1.0335452273,-1.2543357832,2.7542440738
 H,0,2.1489447446,-0.4366721806,1.6534850005
 H,0,1.3690948364,0.4567153288,2.9642520319
 H,0,-1.1895227829,0.9749439934,2.8290671489
 H,0,-2.0899007956,0.4244829207,1.4044194046
 H,0,-1.5247928275,-0.7372919801,2.6186183881
 H,0,1.113296835,-0.7257362089,-1.6661154493
 H,0,1.4480843964,0.9846479556,-1.4556118891
 H,0,2.2029901871,-0.196206838,-0.3815268617
 H,0,-0.8437144658,0.4157044638,-0.5071761221
```

B3PW91/6-31G* (gas phase)

```
E(RB+HF-PW91) = -196.470833317

Zero-point correction=                           0.137061 (Hartree/Particle)
 Thermal correction to Energy=                    0.143923
 Thermal correction to Enthalpy=                  0.144868
 Thermal correction to Gibbs Free Energy=         0.107285
 Sum of electronic and zero-point Energies=           -196.333772
 Sum of electronic and thermal Energies=              -196.326910
 Sum of electronic and thermal Enthalpies=            -196.325966
 Sum of electronic and thermal Free Energies=         -196.363548

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.313             23.682             79.098


 C,0,1.2769559226,0.049776088,-0.9078337885
 C,0,0.0921102799,0.169926714,0.0012253378
 C,0,0.0395426411,0.0163536661,1.3327951034
 C,0,-1.2616044151,0.1799907637,2.0739807798
 C,0,1.2160574818,-0.3216617777,2.2074074636
 H,0,1.0354054672,-1.2564942047,2.7561056454
 H,0,2.1502518172,-0.4365975409,1.6525867761
 H,0,1.3713264995,0.4574827964,2.9666491901
 H,0,-1.1913121314,0.9766610651,2.8281230632
 H,0,-2.0885614114,0.424865789,1.3997712649
 H,0,-1.5270981987,-0.7380293357,2.6172157657
 H,0,1.1103376898,-0.7272156996,-1.6665192308
 H,0,1.4460207076,0.9870553905,-1.4555621875
 H,0,2.2027602523,-0.196371947,-0.3807252325
 H,0,-0.8433946024,0.4154792327,-0.5053739506
```

BB1K/6-31G* (gas phase)

```
E(RB+HF-B95) = -196.417036669

Zero-point correction=                           0.140146 (Hartree/Particle)
 Thermal correction to Energy=                    0.146930
 Thermal correction to Enthalpy=                  0.147874
 Thermal correction to Gibbs Free Energy=         0.110440
 Sum of electronic and zero-point Energies=           -196.276891
 Sum of electronic and thermal Energies=              -196.270107
 Sum of electronic and thermal Enthalpies=            -196.269163
 Sum of electronic and thermal Free Energies=         -196.306597
```

```
                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  92.200             23.293            78.787

 C,0,1.2713390221,0.0492249314,-0.8939775406
 C,0,0.0913689914,0.1692543091,0.0078306844
 C,0,0.0412906085,0.0164364869,1.3291416033
 C,0,-1.2510987643,0.1787383301,2.0673329582
 C,0,1.2112137706,-0.3195721464,2.1977338338
 H,0,1.0294984114,-1.2483068426,2.7417498004
 H,0,2.1385865315,-0.4336717901,1.6450606706
 H,0,1.3637306135,0.4557625114,2.9508063052
 H,0,-1.1790730141,0.9707573314,2.8154426015
 H,0,-2.071361972,0.4218447258,1.3956446133
 H,0,-1.5128465073,-0.7342194066,2.6059806109
 H,0,1.1065165618,-0.7236173493,-1.6464261318
 H,0,1.4401532466,0.9806812632,-1.4366777746
 H,0,2.1887668893,-0.195311853,-0.3662205027
 H,0,-0.8392863891,0.4132204988,-0.4935757319
```

BPW91/6-31G* (gas phase)

```
E(RB-PW91) = -196.501309862

Zero-point correction=                           0.133575 (Hartree/Particle)
 Thermal correction to Energy=                    0.140534
 Thermal correction to Enthalpy=                  0.141478
 Thermal correction to Gibbs Free Energy=         0.103732
 Sum of electronic and zero-point Energies=           -196.367735
 Sum of electronic and thermal Energies=              -196.360776
 Sum of electronic and thermal Enthalpies=            -196.359831
 Sum of electronic and thermal Free Energies=         -196.397578

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  88.187             24.203            79.444

 C,0,1.2812528853,0.0502576621,-0.9188264109
 C,0,0.0921091315,0.1706806043,-0.004779528
 C,0,0.0382649845,0.0161072032,1.3371032636
 C,0,-1.2704938138,0.181071471,2.079403199
 C,0,1.2209369932,-0.3235464289,2.2151943027
 H,0,1.0416501213,-1.2641630494,2.7684136742
 H,0,2.1605263276,-0.4389090653,1.6562195293
 H,0,1.3792796843,0.4591214768,2.980256975
 H,0,-1.2026503753,0.9823810484,2.8390683588
 H,0,-2.1015954648,0.4274685185,1.3999541795
 H,0,-1.5402823342,-0.741563898,2.6268936496
 H,0,1.1140818128,-0.7307740025,-1.6834748922
 H,0,1.4516383901,0.9927472104,-1.4713899509
 H,0,2.2136950522,-0.1974263071,-0.3900679335
 H,0,-0.8496153946,0.4177685565,-0.5141224162
```

MPW3LYP/6-31G* (gas phase)

```
E(RmPW+HF-LYP) = -196.538789991

Zero-point correction=                           0.136962 (Hartree/Particle)
 Thermal correction to Energy=                    0.143791
 Thermal correction to Enthalpy=                  0.144736
```

```
 Thermal correction to Gibbs Free Energy=         0.107243
 Sum of electronic and zero-point Energies=           -196.401828
 Sum of electronic and thermal Energies=              -196.394999
 Sum of electronic and thermal Enthalpies=            -196.394054
 Sum of electronic and thermal Free Energies=         -196.431547

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.230             23.621             78.910


 C,0,1.2788994426,0.0498388004,-0.9113024445
 C,0,0.0910969893,0.1702192583,0.0005051554
 C,0,0.0387403197,0.016645675,1.3317690291
 C,0,-1.2647825263,0.1803779267,2.0758644653
 C,0,1.2179403818,-0.3222701114,2.2092279369
 H,0,1.0366118495,-1.2567388664,2.7583325028
 H,0,2.1519499679,-0.4373008901,1.6547637787
 H,0,1.3725434309,0.4567398913,2.9687488814
 H,0,-1.1938470767,0.9766930866,2.830313941
 H,0,-2.0917222832,0.4251672221,1.4019197419
 H,0,-1.5295083776,-0.7375907909,2.6195451066
 H,0,1.1122117054,-0.7270065644,-1.6700339495
 H,0,1.447797395,0.9870354767,-1.4591014032
 H,0,2.2041393882,-0.1962250452,-0.3837150496
 H,0,-0.8432726064,0.4156359313,-0.5069916923
```

mpwb1k/6-31G* (gas phase)

```
E(RmPW+HF-B95) = -196.413423684

 Zero-point correction=                           0.140507 (Hartree/Particle)
 Thermal correction to Energy=                    0.147276
 Thermal correction to Enthalpy=                  0.148220
 Thermal correction to Gibbs Free Energy=         0.110819
 Sum of electronic and zero-point Energies=           -196.272917
 Sum of electronic and thermal Energies=              -196.266148
 Sum of electronic and thermal Enthalpies=            -196.265204
 Sum of electronic and thermal Free Energies=         -196.302604

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  92.417             23.238             78.717

 C,0,1.2706690057,0.0491087276,-0.8919318431
 C,0,0.0910239324,0.1692657722,0.0083000157
 C,0,0.0412478441,0.016537987,1.3283912772
 C,0,-1.2495885307,0.1785304042,2.0666116881
 C,0,1.2103071619,-0.319182397,2.1959790997
 H,0,1.0283599581,-1.2472325242,2.7395879878
 H,0,2.1370214797,-0.4331995411,1.6435299707
 H,0,1.3623976248,0.4557315353,2.948488522
 H,0,-1.1769074533,0.9699062118,2.8142528771
 H,0,-2.0695506553,0.4214719768,1.3956628364
 H,0,-1.5104523714,-0.7339746646,2.6049472958
 H,0,1.1065081815,-0.7233663534,-1.6437468837
 H,0,1.4399269774,0.9798424346,-1.4341321041
 H,0,2.1868677675,-0.1952834473,-0.3633738069
 H,0,-0.8390329222,0.4130648781,-0.4927209326
```

MPWB195/6-31G* (gas phase)

```
E(RmPW+HF-B95) = -196.411756375
```

```
Zero-point correction=                           0.138408 (Hartree/Particle)
 Thermal correction to Energy=                    0.145232
 Thermal correction to Enthalpy=                  0.146176
 Thermal correction to Gibbs Free Energy=         0.108684
 Sum of electronic and zero-point Energies=           -196.273348
 Sum of electronic and thermal Energies=              -196.266524
 Sum of electronic and thermal Enthalpies=            -196.265580
 Sum of electronic and thermal Free Energies=         -196.303073

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   91.134             23.533             78.909

 C,0,1.2729447262,0.0493627109,-0.8978140249
 C,0,0.090982323,0.1696621569,0.0051453441
 C,0,0.040494904,0.0164246744,1.3305948031
 C,0,-1.2543479729,0.1791099099,2.0695277072
 C,0,1.2129122193,-0.3201673815,2.2000155329
 H,0,1.0316999989,-1.2514626163,2.7462410812
 H,0,2.1427756172,-0.4344265646,1.6453585753
 H,0,1.3666436462,0.4566959728,2.9559008434
 H,0,-1.1829712604,0.9730702448,2.820346119
 H,0,-2.0767497405,0.422949489,1.395699589
 H,0,-1.517588879,-0.7360238044,2.6102918841
 H,0,1.1085933595,-0.7254336576,-1.652983668
 H,0,1.4430752886,0.9830254346,-1.4427301495
 H,0,2.1928758055,-0.1959056052,-0.368226949
 H,0,-0.8425420357,0.4143400361,-0.4975206879
```

MPWLYP1M/6-31G* (gas phase)

```
E(RmPW+HF-LYP) = -196.402310024

 Zero-point correction=                           0.134116 (Hartree/Particle)
 Thermal correction to Energy=                    0.141022
 Thermal correction to Enthalpy=                  0.141966
 Thermal correction to Gibbs Free Energy=         0.104340
 Sum of electronic and zero-point Energies=           -196.268194
 Sum of electronic and thermal Energies=              -196.261288
 Sum of electronic and thermal Enthalpies=            -196.260344
 Sum of electronic and thermal Free Energies=         -196.297970

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   88.492             24.026             79.190


 C,0,1.2834393229,0.0501753475,-0.921089999
 C,0,0.0904286932,0.1709850765,-0.0049354639
 C,0,0.0370831564,0.0165612198,1.33462026
 C,0,-1.2733789116,0.181393051,2.0812644389
 C,0,1.2225241479,-0.3239760092,2.2156095283
 H,0,1.0419603701,-1.2631315279,2.7685852444
 H,0,2.1610003497,-0.4395180667,1.6577291714
 H,0,1.379452402,0.4581466756,2.9798474487
 H,0,-1.2037118803,0.9815227522,2.8402947482
 H,0,-2.104334457,0.4273682832,1.4036885866
 H,0,-1.5408944434,-0.7405325103,2.6286856917
 H,0,1.116422002,-0.7301041694,-1.6846910453
 H,0,1.4535182058,0.9917541094,-1.4727443092
 H,0,2.2139043513,-0.1971518122,-0.3915990795
 H,0,-0.8486153088,0.4177285804,-0.5154192211
```

PBE1KCIS/6-31G* (gas phase)

```
E(RPBE+HF-KCIS) = -196.265451800

Zero-point correction=                           0.137043 (Hartree/Particle)
 Thermal correction to Energy=                    0.143840
 Thermal correction to Enthalpy=                  0.144784
 Thermal correction to Gibbs Free Energy=         0.107416
 Sum of electronic and zero-point Energies=           -196.128409
 Sum of electronic and thermal Energies=              -196.121612
 Sum of electronic and thermal Enthalpies=            -196.120668
 Sum of electronic and thermal Free Energies=         -196.158036

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.261             23.663             78.647

C,0,1.2755619175,0.0498341809,-0.9061491009
 C,0,0.0928883683,0.1697788953,0.0012030319
 C,0,0.0394214747,0.01640248,1.3326347901
 C,0,-1.2592565922,0.1796881326,2.0727175429
 C,0,1.2140480116,-0.3210479004,2.2056730494
 H,0,1.0339774147,-1.2553807828,2.7556520178
 H,0,2.1494271025,-0.4364004442,1.6526321887
 H,0,1.3695712961,0.4571058495,2.9660518736
 H,0,-1.1896253086,0.9756144268,2.8278976433
 H,0,-2.0875190834,0.424646563,1.4000139071
 H,0,-1.5251434413,-0.7376736936,2.6171374264
 H,0,1.1105539749,-0.726618305,-1.6658418476
 H,0,1.4459855278,0.9862636391,-1.4550525619
 H,0,2.202299746,-0.1963674298,-0.3801954177
 H,0,-0.8433924085,0.4153753886,-0.5045285431
```

PBE1W/6-31G* (gas phase)

```
E(RPBE+HF-PBE) = -219.042651887

Zero-point correction=                           0.204598 (Hartree/Particle)
 Thermal correction to Energy=                    0.210222
 Thermal correction to Enthalpy=                  0.211166
 Thermal correction to Gibbs Free Energy=         0.176386
 Sum of electronic and zero-point Energies=           -218.838054
 Sum of electronic and thermal Energies=              -218.832430
 Sum of electronic and thermal Enthalpies=            -218.831486
 Sum of electronic and thermal Free Energies=         -218.866265

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 131.916             18.349             73.200

C,0,1.14782813,0.0416006425,-0.6359230473
 C,0,0.1224817908,0.1469632,0.1396677467
 C,0,0.0775216831,0.0148331207,1.2848739208
 C,0,-1.0387787587,0.1547122257,1.9247395193
 C,0,1.0924600034,-0.2758362243,2.0317736258
 H,0,0.9404224729,-1.0615199565,2.4875957593
 H,0,1.8724589001,-0.3704829598,1.5578890626
 H,0,1.2229949538,0.3802976378,2.6647317959
 H,0,-0.9724815435,0.8240748747,2.5539745497
 H,0,-1.7353096322,0.3603601238,1.3617213197
 H,0,-1.2549179592,-0.6182866874,2.3765526922
 H,0,1.0089440409,-0.6129847859,-1.2686467412
```

```
 H,0,1.2913690389,0.8291581221,-1.0911811743
 H,0,1.9179542558,-0.1651138669,-0.1816848366
 H,0,-0.6641493761,0.3534455336,-0.2862381927
```

PBELYP1W/6-31G* (gas phase)

```
E(RPBE+HF-V5LYP) = -212.754028832

Zero-point correction=                           0.188890 (Hartree/Particle)
 Thermal correction to Energy=                    0.194731
 Thermal correction to Enthalpy=                  0.195676
 Thermal correction to Gibbs Free Energy=         0.160349
 Sum of electronic and zero-point Energies=           -212.565138
 Sum of electronic and thermal Energies=              -212.559297
 Sum of electronic and thermal Enthalpies=            -212.558353
 Sum of electronic and thermal Free Energies=         -212.593680

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 122.196             19.119            74.351

 C,0,1.177600496,0.0431335189,-0.6958324605
 C,0,0.1130497067,0.1525947703,0.1086215945
 C,0,0.0677692581,0.0157720285,1.2925754781
 C,0,-1.0886827679,0.1602442296,1.9593857722
 C,0,1.1199103556,-0.2857803789,2.068910828
 H,0,0.9605313469,-1.1023151214,2.5432414756
 H,0,1.9313065446,-0.38436763,1.5777330915
 H,0,1.2541578864,0.3964092724,2.727487738
 H,0,-1.0187160827,0.855802618,2.6140867214
 H,0,-1.8127900914,0.3740529987,1.3742031093
 H,0,-1.3123738264,-0.6435979189,2.4296257104
 H,0,1.034497864,-0.6375171924,-1.3538027171
 H,0,1.3280369967,0.8615762072,-1.169336904
 H,0,1.9773980183,-0.1717240834,-0.2224437832
 H,0,-0.7028977048,0.3669376814,-0.3346096541
```

RHF/6-31G* (gas phase)

```
E(RHF) = -195.145768043

Zero-point correction=                           0.145810 (Hartree/Particle)
 Thermal correction to Energy=                    0.152439
 Thermal correction to Enthalpy=                  0.153384
 Thermal correction to Gibbs Free Energy=         0.116135
 Sum of electronic and zero-point Energies=           -194.999958
 Sum of electronic and thermal Energies=              -194.993329
 Sum of electronic and thermal Enthalpies=            -194.992384
 Sum of electronic and thermal Free Energies=         -195.029633

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  95.657             22.352            78.396

C,0,1.2781933496,0.0498665473,-0.9104265738
 C,0,0.0936048567,0.1686026658,0.0096627408
 C,0,0.0426565631,0.0167331275,1.324716443
 C,0,-1.2602686267,0.1799902603,2.0718329441
 C,0,1.2163064673,-0.322246434,2.2116693498
 H,0,1.0270336751,-1.247429243,2.7513571392
 H,0,2.1451389681,-0.4379458683,1.6711839031
```

```
H,0,1.3604657451,0.4535737953,2.9602527377
H,0,-1.1841536432,0.9699725791,2.8159210061
H,0,-2.0804026515,0.4224998503,1.4062880451
H,0,-1.5174579614,-0.7318603566,2.6065391992
H,0,1.1025697049,-0.7198304036,-1.6582087724
H,0,1.4356224112,0.9813594656,-1.4489364307
H,0,2.1988336736,-0.1934955086,-0.3972509436
H,0,-0.829344532,0.411430523,-0.4947547877
```

TPSSKCIS/6-31G* (gas phase)

```
E(RTPSS+HF-KCIS) = -196.532042290

Zero-point correction=                           0.137414 (Hartree/Particle)
 Thermal correction to Energy=                    0.144240
 Thermal correction to Enthalpy=                  0.145184
 Thermal correction to Gibbs Free Energy=         0.107749
 Sum of electronic and zero-point Energies=           -196.394628
 Sum of electronic and thermal Energies=              -196.387803
 Sum of electronic and thermal Enthalpies=            -196.386858
 Sum of electronic and thermal Free Energies=         -196.424293

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  90.512             23.648             78.788


 C,0,1.2786085741,0.0497641338,-0.9102088454
 C,0,0.0908838352,0.1702700981,0.0003732718
 C,0,0.0390722672,0.0163762076,1.3333884259
 C,0,-1.2647955107,0.1803902765,2.0757943542
 C,0,1.2186462731,-0.3224120165,2.2092345874
 H,0,1.0376054605,-1.2561425726,2.7566288815
 H,0,2.1501519,-0.4367081436,1.6526946508
 H,0,1.3733277404,0.4562295808,2.9669019696
 H,0,-1.1938630841,0.9763430417,2.8284079214
 H,0,-2.0887823631,0.4247854536,1.400320803
 H,0,-1.5293098485,-0.7368087159,2.6177978867
 H,0,1.1114774052,-0.7264595363,-1.6673430081
 H,0,1.4467751538,0.9862022092,-1.4565741007
 H,0,2.2016743386,-0.1960207444,-0.3813550465
 H,0,-0.8426741416,0.4154117278,-0.5062157517
```

TPSSLYP1W/6-31G* (gas phase)

```
E(RTPSS+HF-V5LYP) = -219.319217973

Zero-point correction=                           0.207054 (Hartree/Particle)
 Thermal correction to Energy=                    0.212617
 Thermal correction to Enthalpy=                  0.213561
 Thermal correction to Gibbs Free Energy=         0.178927
 Sum of electronic and zero-point Energies=           -219.112164
 Sum of electronic and thermal Energies=              -219.106601
 Sum of electronic and thermal Enthalpies=            -219.105657
 Sum of electronic and thermal Free Energies=         -219.140291

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 133.419             18.204             72.893

 C,0,1.1507153979,0.0412441608,-0.6377723334
 C,0,0.1191856411,0.147669491,0.1390934502
```

```
C,0,0.0760740129,0.015304241,1.2833833727
C,0,-1.0432279757,0.1552162929,1.9277846216
C,0,1.0957473413,-0.2765064354,2.0321128727
H,0,0.9426316318,-1.0612239628,2.485842838
H,0,1.8718339576,-0.3699391746,1.5552698515
H,0,1.2249146331,0.3795747454,2.6629601711
H,0,-0.9741788222,0.8236691413,2.5552307652
H,0,-1.7370233212,0.3604460913,1.3641245971
H,0,-1.2564359842,-0.6175926275,2.377889542
H,0,1.0117802675,-0.6131643887,-1.268152988
H,0,1.2940547687,0.8281165598,-1.0907842148
H,0,1.9158859707,-0.1651038768,-0.1787341078
H,0,-0.6631595193,0.3535107421,-0.2884024381
```

BP86/6-31G* (gas phase)

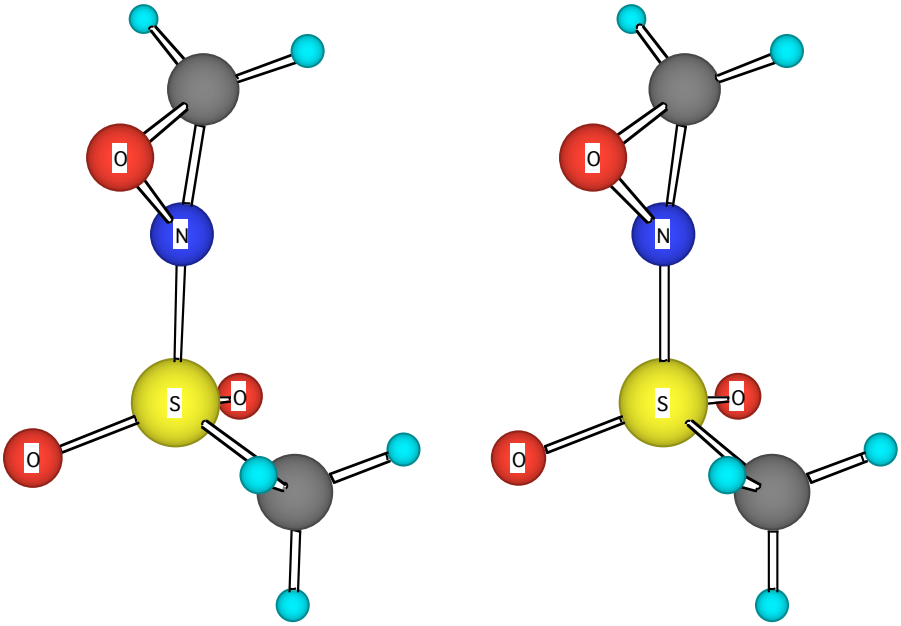
```
E(RB-P86) = -196.528002219

Zero-point correction=                           0.132948 (Hartree/Particle)
 Thermal correction to Energy=                    0.139904
 Thermal correction to Enthalpy=                  0.140849
 Thermal correction to Gibbs Free Energy=         0.103135
 Sum of electronic and zero-point Energies=           -196.395054
 Sum of electronic and thermal Energies=              -196.388098
 Sum of electronic and thermal Enthalpies=            -196.387154
 Sum of electronic and thermal Free Energies=         -196.424867

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  87.791             24.265             79.374

 C,0,1.2819616616,0.050005017,-0.9182584002
 C,0,0.0901423395,0.1712741934,-0.0063676226
 C,0,0.0369062392,0.0164948498,1.336449644
 C,0,-1.2714235648,0.1811302623,2.0804998677
 C,0,1.2213190565,-0.3233431679,2.2132858135
 H,0,1.0425366657,-1.2659505147,2.7678180305
 H,0,2.1620238797,-0.4384001989,1.6514790044
 H,0,1.3806017477,0.4604625925,2.9802689071
 H,0,-1.2026857771,0.9835444548,2.842241796
 H,0,-2.1046260643,0.428148383,1.4001688538
 H,0,-1.5409682961,-0.7434118325,2.6295074057
 H,0,1.1171701932,-0.7330053928,-1.6845073234
 H,0,1.4554347584,0.9937344136,-1.4720462193
 H,0,2.2140980887,-0.1982975725,-0.3843047544
 H,0,-0.8536929278,0.4188355128,-0.5163890027
```

*TS for Oxaziridine Inversion B3LYP/6-31G**



E(RB+HF-LYP) = -757.621010976

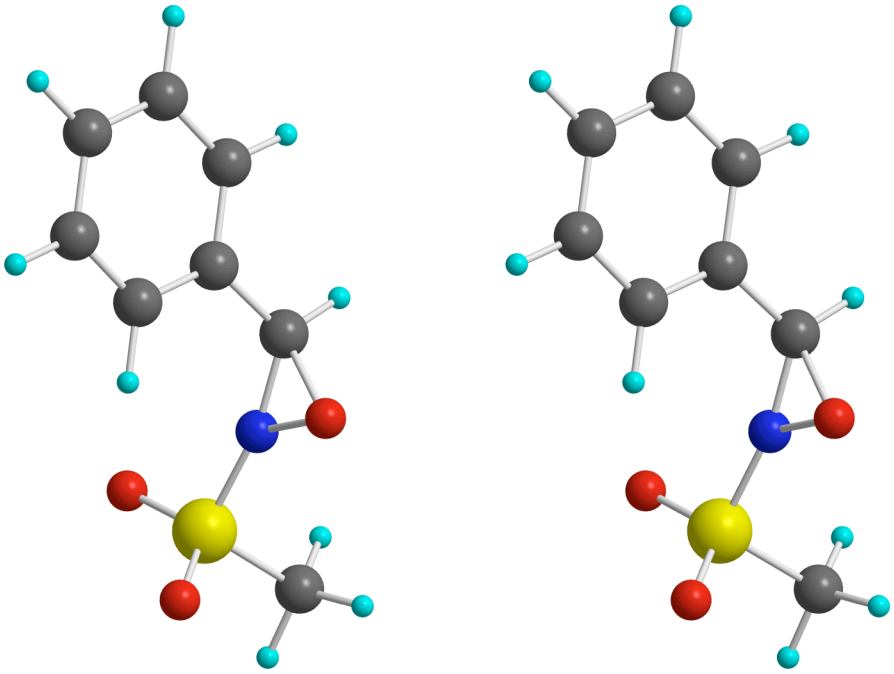
Zero-point correction= 0.083079 (Hartree/Particle)
Thermal correction to Energy= 0.090185
Thermal correction to Enthalpy= 0.091129
Thermal correction to Gibbs Free Energy= 0.051331
Sum of electronic and zero-point Energies= -757.537932
Sum of electronic and thermal Energies= -757.530826
Sum of electronic and thermal Enthalpies= -757.529882
Sum of electronic and thermal Free Energies= -757.569680

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	56.592	24.430	83.763

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.971300	-0.792031	0.349943
2	6	0	2.236374	0.435547	-0.357399
3	7	0	0.914332	0.136182	-0.057977
4	16	0	-0.721450	0.153335	0.129848
5	8	0	-1.103439	1.485113	-0.332206
6	8	0	-1.048885	-0.346694	1.457497
7	6	0	-1.308923	-1.069820	-1.056467
8	1	0	2.576818	0.319066	-1.388097
9	1	0	2.728188	1.215118	0.226013
10	1	0	-2.392823	-1.146287	-0.941270
11	1	0	-0.835355	-2.026046	-0.825289
12	1	0	-1.050479	-0.733947	-2.061764

TS for 3-phenyl-2-methanesulfonyloxaziridine Inversion



E(RB+HF-LYP) = -988.724386105

Zero-point correction=	0.163098 (Hartree/Particle)
Thermal correction to Energy=	0.174779
Thermal correction to Enthalpy=	0.175723
Thermal correction to Gibbs Free Energy=	0.123906
Sum of electronic and zero-point Energies=	-988.561288
Sum of electronic and thermal Energies=	-988.549607
Sum of electronic and thermal Enthalpies=	-988.548663
Sum of electronic and thermal Free Energies=	-988.600480

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	109.676	43.731	109.058

C,0,3.7200125257,-5.1370570039,-1.7539592083
C,0,2.8606724929,-4.2517292179,-1.107993817
C,0,3.3521857692,-3.4258415088,-0.0867226142
C,0,4.7004664613,-3.4954774845,0.2823970681
C,0,5.5597255259,-4.3870506604,-0.3652988215
C,0,5.0691773389,-5.2068975986,-1.3833670792
C,0,2.4687386203,-2.4512077415,0.602125926
N,0,1.0860612843,-2.6440693648,0.6873991792
S,0,-0.430324308,-3.196107642,1.0219260169
C,0,-1.1789589171,-1.8842515213,2.007196693
O,0,1.5841757282,-1.6203664826,-0.222922406
O,0,-0.1966981104,-4.3611289256,1.875803847
O,0,-1.1854079099,-3.2794118656,-0.2253361184
H,0,2.9321539277,-1.8926107725,1.417590582
H,0,5.0787877063,-2.8548491461,1.0752467791
H,0,6.6045557778,-4.4403646851,-0.0749766278
H,0,5.7340016176,-5.9024355227,-1.8872185332
H,0,3.3398803344,-5.7774357206,-2.5440630205
H,0,1.8124332996,-4.1939276206,-1.3835831809
H,0,-2.2108803396,-2.1804643011,2.2062741821
H,0,-0.6137190514,-1.7874268678,2.9343434186
H,0,-1.1511527736,-0.963534346,1.422239735

B3LYP/6-31+G** (PCM)

E(RB+HF-LYP) = -988.738451758

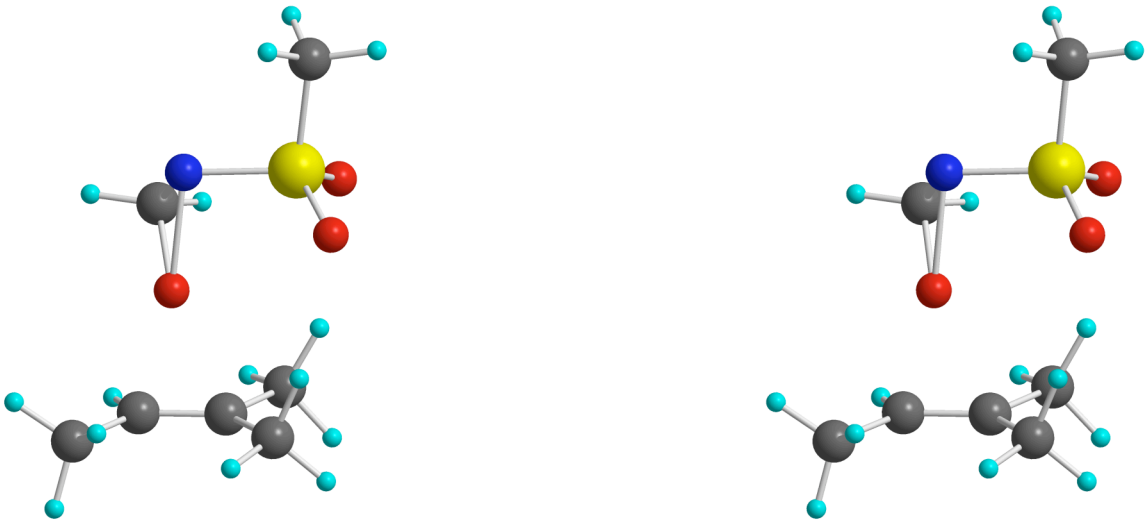
Zero-point correction=	0.162241 (Hartree/Particle)
Thermal correction to Energy=	0.173940
Thermal correction to Enthalpy=	0.174885
Thermal correction to Gibbs Free Energy=	0.122956
Sum of electronic and zero-point Energies=	-988.576210
Sum of electronic and thermal Energies=	-988.564511
Sum of electronic and thermal Enthalpies=	-988.563567
Sum of electronic and thermal Free Energies=	-988.615496

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	109.149	43.858	109.294

C,0,3.7247020027,-5.1520943098,-1.7480404856
C,0,2.8628562733,-4.2540587577,-1.1215931347
C,0,3.3475195958,-3.4178458932,-0.1042432325
C,0,4.6923746879,-3.4890657081,0.2817083296
C,0,5.5536104961,-4.3939032835,-0.3461168481
C,0,5.0699608489,-5.2242251371,-1.3603339459
C,0,2.4716913256,-2.4301547842,0.5711006629
N,0,1.0833034499,-2.6145459499,0.6740575039
S,0,-0.4236685718,-3.1664771429,1.005304792
C,0,-1.1752207111,-1.9028590709,2.0427129413
O,0,1.5697574091,-1.6148810965,-0.2628398404
O,0,-0.1950602615,-4.3726123049,1.8100507317
O,0,-1.1898094981,-3.2202290362,-0.2431894665
H,0,2.9371372066,-1.8518125785,1.373269459
H,0,5.0649959621,-2.8388632429,1.0720363857
H,0,6.5968218832,-4.4488657851,-0.0428694851
H,0,5.737952744,-5.9304694654,-1.8494116817
H,0,3.3494225241,-5.8004672164,-2.5368495267
H,0,1.8190445792,-4.1977041907,-1.4171421662
H,0,-2.1992432971,-2.2221068584,2.250756756
H,0,-0.5917684882,-1.8276281299,2.9612242608
H,0,-1.1704921604,-0.9627780574,1.4875099907

Epoxidation TS Isomer 1

B3LYP/6-31G*



E(RB+HF-LYP) = -954.183237966

Zero-point correction=	0.221013 (Hartree/Particle)
Thermal correction to Energy=	0.236268
Thermal correction to Enthalpy=	0.237212
Thermal correction to Gibbs Free Energy=	0.178334
Sum of electronic and zero-point Energies=	-953.962225
Sum of electronic and thermal Energies=	-953.946970
Sum of electronic and thermal Enthalpies=	-953.946026
Sum of electronic and thermal Free Energies=	-954.004904

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	148.260	53.729	123.920

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	2.678581	-0.569886	-0.329174
2	6	0	C	2.232722	0.723894	-0.119572
3	8	0	O	0.661504	-0.777185	-0.006249
4	6	0	C	-0.138995	-1.171253	-1.116749
5	7	0	N	-1.192441	-1.333954	-0.186565
6	16	0	S	-1.966755	0.144393	0.165154
7	8	0	O	-1.807827	1.113911	-0.941968
8	8	0	O	-1.658010	0.587565	1.533190
9	6	0	C	3.260752	-1.511483	0.680400
10	6	0	C	2.109642	1.350540	1.238147
11	6	0	C	1.842035	1.598690	-1.276294
12	6	0	C	-3.672160	-0.442364	0.161605
13	1	0	H	2.771583	-0.885112	-1.368048
14	1	0	H	0.167541	-2.130956	-1.548587
15	1	0	H	-0.240335	-0.386136	-1.875091
16	1	0	H	2.951810	-2.537666	0.458001
17	1	0	H	2.948500	-1.281372	1.700533
18	1	0	H	4.359116	-1.484681	0.639956
19	1	0	H	2.583401	2.340257	1.240182
20	1	0	H	2.555197	0.751121	2.033419
21	1	0	H	1.047173	1.491775	1.472949
22	1	0	H	0.800978	1.928259	-1.169124
23	1	0	H	1.951336	1.090211	-2.238759
24	1	0	H	2.468288	2.501041	-1.291120

25	1	0	H	-4.297365	0.405220	0.452306
26	1	0	H	-3.760792	-1.251576	0.887763
27	1	0	H	-3.932061	-0.786163	-0.840856

B3LYP/6-31G* (Onsager)

E(RB+HF-LYP) = -954.184915292

Zero-point correction= 0.220941 (Hartree/Particle)
Thermal correction to Energy= 0.236269
Thermal correction to Enthalpy= 0.237214
Thermal correction to Gibbs Free Energy= 0.177978
Sum of electronic and zero-point Energies= -953.963974
Sum of electronic and thermal Energies= -953.948646
Sum of electronic and thermal Enthalpies= -953.947702
Sum of electronic and thermal Free Energies= -954.006938

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	148.261	53.812	124.673

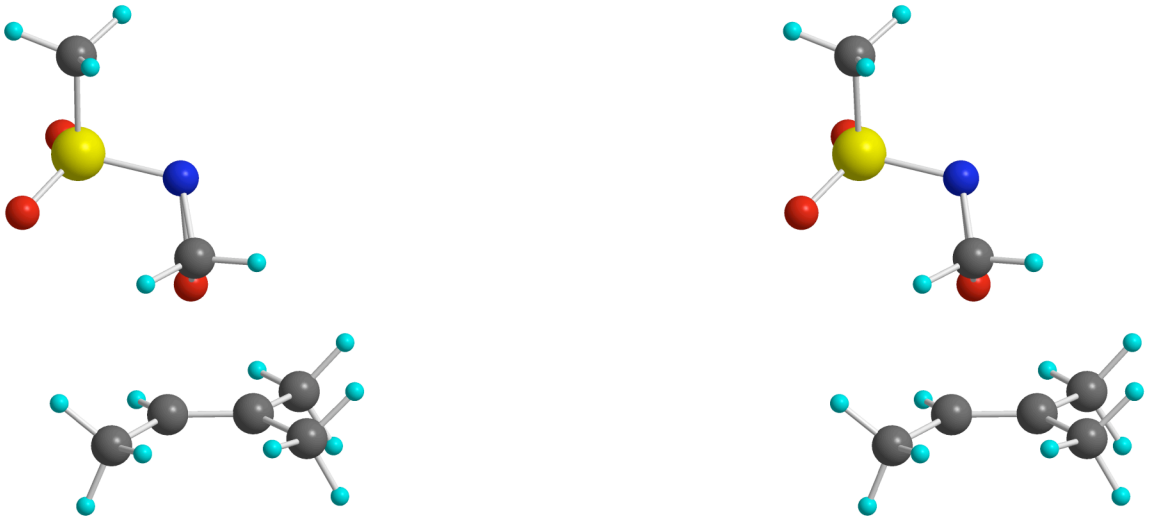
Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	2.718071	-0.558822	-0.341007
2	6	0	C	2.244016	0.720828	-0.125750
3	8	0	O	0.645135	-0.759130	0.026718
4	6	0	C	-0.132951	-1.188132	-1.078997
5	7	0	N	-1.184313	-1.328621	-0.136414
6	16	0	S	-1.984018	0.144561	0.165960
7	8	0	O	-1.803447	1.109542	-0.940657
8	8	0	O	-1.739669	0.600748	1.542689
9	6	0	C	3.318678	-1.499058	0.656898
10	6	0	C	2.129759	1.349665	1.232488
11	6	0	C	1.836901	1.593724	-1.279362
12	6	0	C	-3.682874	-0.463980	0.099308
13	1	0	H	2.795860	-0.874848	-1.381020
14	1	0	H	0.177220	-2.158985	-1.481064
15	1	0	H	-0.241086	-0.426334	-1.859278
16	1	0	H	2.998742	-2.525088	0.448646
17	1	0	H	3.043035	-1.261268	1.685801
18	1	0	H	4.415155	-1.481267	0.580054
19	1	0	H	2.661577	2.309763	1.246004
20	1	0	H	2.526690	0.723842	2.032925
21	1	0	H	1.074126	1.552344	1.449707
22	1	0	H	0.793763	1.913697	-1.166611
23	1	0	H	1.946772	1.087794	-2.243011
24	1	0	H	2.455878	2.500901	-1.298024
25	1	0	H	-4.328578	0.380243	0.353341
26	1	0	H	-3.793086	-1.266614	0.829759
27	1	0	H	-3.897337	-0.821447	-0.909163

Optimizations of this transition state structure using B3LYP/6-31+G and mPW1K/6-31+G** give isomer 3.

Epoxidation TS Isomer 2

B3LYP/6-31+G** (PCM)



filename: b3BBPCMts2
E(RB+HF-LYP) = -954.239856537

Zero-point correction=	0.218593 (Hartree/Particle)
Thermal correction to Energy=	0.234145
Thermal correction to Enthalpy=	0.235089
Thermal correction to Gibbs Free Energy=	0.174778
Sum of electronic and zero-point Energies=	-954.021264
Sum of electronic and thermal Energies=	-954.005712
Sum of electronic and thermal Enthalpies=	-954.004768
Sum of electronic and thermal Free Energies=	-954.065078

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	146.928	54.401	126.935

1	6	0	-2.171250	0.751228	-0.774462
2	6	0	-2.860575	-0.270235	-0.158704
3	8	0	-0.530281	-0.455922	-0.057943
4	6	0	0.025144	-0.138322	1.202706
5	7	0	1.123331	-0.903755	0.710056
6	16	0	2.257658	0.001947	-0.191574
7	8	0	2.035508	1.462193	-0.076676
8	8	0	2.379588	-0.576652	-1.543128
9	6	0	-1.947910	2.145349	-0.274982
10	6	0	-3.437585	-0.180349	1.225374
11	6	0	-3.153707	-1.543300	-0.900756
12	6	0	3.749843	-0.422025	0.725031
13	1	0	-1.874131	0.582505	-1.808885
14	1	0	-0.919719	2.461132	-0.479590
15	1	0	-2.147582	2.269785	0.791674
16	1	0	-2.606200	2.835454	-0.820236
17	1	0	-4.534695	-0.184017	1.163401
18	1	0	-3.136982	0.715776	1.770327
19	1	0	-3.160144	-1.061719	1.816170
20	1	0	-2.835153	-2.415411	-0.318248
21	1	0	-2.657526	-1.573316	-1.873360
22	1	0	-4.236796	-1.642525	-1.057739
23	1	0	-0.465485	-0.630990	2.048145
24	1	0	0.182253	0.933628	1.360097
25	1	0	4.579642	0.053456	0.196156

26	1	0	3.860086	-1.507136	0.723067
27	1	0	3.664301	-0.032510	1.740562

B3LYP/6-31+G** (gas phase)

Filename:b3BBgasts2
E(RB+HF-LYP) = -954.224838655

Zero-point correction=	0.219271 (Hartree/Particle)
Thermal correction to Energy=	0.234668
Thermal correction to Enthalpy=	0.235612
Thermal correction to Gibbs Free Energy=	0.175961
Sum of electronic and zero-point Energies=	-954.005568
Sum of electronic and thermal Energies=	-953.990171
Sum of electronic and thermal Enthalpies=	-953.989226
Sum of electronic and thermal Free Energies=	-954.048877

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.256	54.178	125.546

C,0,-0.3442667198,-2.5257887593,0.1249227148
C,0,1.0323156212,-2.6514179864,0.0380501049
O,0,0.2034725262,-0.5739393854,0.0416812057
C,0,0.3244453371,0.1923029956,1.2395671248
N,0,0.0450374579,1.3214367107,0.4330063251
S,0,-1.6317836538,1.5719966694,0.1972506482
O,0,-2.4316022457,0.8732736292,1.2307156552
O,0,-1.9857768873,1.3858884621,-1.2170556339
C,0,-1.2209585059,-2.7125640689,1.324948684
C,0,1.9308017566,-2.8697217753,1.22159967
C,0,1.7069312723,-2.6493001859,-1.3041095812
C,0,-1.6876906866,3.3429664776,0.5399014616
H,0,-0.8797941371,-2.4580390456,-0.8185102581
H,0,-1.9871873249,-1.9310333542,1.3530405229
H,0,-0.6774005952,-2.706893356,2.2720949654
H,0,-1.7430305921,-3.6752267956,1.2437207052
H,0,2.3910786236,-3.8651411138,1.1545393599
H,0,1.4155304128,-2.8032099424,2.1808174804
H,0,2.7559413356,-2.1475549848,1.2157797467
H,0,2.5370331827,-1.9345490782,-1.3211275981
H,0,1.0141846862,-2.3906746729,-2.1072414468
H,0,2.1314612521,-3.6415610433,-1.5127259782
H,0,1.346944658,0.2206400061,1.6308613264
H,0,-0.4148320534,-0.0852885601,1.9989472724
H,0,-2.7165402433,3.6570507317,0.3519805163
H,0,-0.9995545184,3.8446626534,-0.1407126686
H,0,-1.413759959,3.5156857721,1.5810576752

B3LYP/6-31+G** (onsager)

Filename: b3BBonsts2

E(RB+HF-LYP) = -954.228198248

Zero-point correction=	0.219132 (Hartree/Particle)
Thermal correction to Energy=	0.234626
Thermal correction to Enthalpy=	0.235570
Thermal correction to Gibbs Free Energy=	0.175316
Sum of electronic and zero-point Energies=	-954.009066
Sum of electronic and thermal Energies=	-953.993572
Sum of electronic and thermal Enthalpies=	-953.992628
Sum of electronic and thermal Free Energies=	-954.052882

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.230	54.285	126.815

C,0,-0.3390557227,-2.6246669423,0.156062536
C,0,1.0369661781,-2.6789381818,0.0546511354
O,0,0.1017905267,-0.5784590818,-0.0155803086
C,0,0.224001123,0.1866638728,1.1709912296
N,0,-0.0032051722,1.2962132226,0.3112388358
S,0,-1.6536793135,1.662027211,0.0767360611
O,0,-2.5387576464,0.9105823611,0.9942364778
O,0,-1.9639820198,1.6750534329,-1.3610853419
C,0,-1.184339423,-2.8113606006,1.3787799911
C,0,1.9603312361,-2.8224979623,1.2298571801
C,0,1.6965988304,-2.6748379724,-1.2948139882
C,0,-1.6180285961,3.3838340391,0.6304736515
H,0,-0.8901882773,-2.6066854909,-0.7808356451
H,0,-2.0040756222,-2.085873697,1.3852307763
H,0,-0.6286404024,-2.7226916314,2.3145275321
H,0,-1.6380370004,-3.8113264315,1.3577472383
H,0,2.4461490717,-3.8070948017,1.1945655328
H,0,1.4613155943,-2.7337464591,2.1955937109
H,0,2.7671922175,-2.0820133824,1.1800473766
H,0,2.4728199627,-1.9033242505,-1.3444747816
H,0,0.9798260017,-2.4968610621,-2.0991537798
H,0,2.1919337061,-3.6393648372,-1.4718905217
H,0,1.2366451466,0.1990646054,1.5865952897
H,0,-0.5434805491,-0.0445945915,1.9174537598
H,0,-2.6217875472,3.7798618499,0.4610343813
H,0,-0.8813003143,3.9221415254,0.0338617784
H,0,-1.3660119882,3.4128952562,1.6911498923

B3LYP/6-31G* (gas phase)

At this level isomer 2 is a second order saddle point (NImag=2).
E(RB+HF-LYP) = -954.179209699

Zero-point correction= 0.221052 (Hartree/Particle)
Thermal correction to Energy= 0.235483
Thermal correction to Enthalpy= 0.236427
Thermal correction to Gibbs Free Energy= 0.179535
Sum of electronic and zero-point Energies= -953.958158
Sum of electronic and thermal Energies= -953.943727
Sum of electronic and thermal Enthalpies= -953.942783
Sum of electronic and thermal Free Energies= -953.999675

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	147.768	51.694	119.740

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	-2.012648	0.642481	-0.825914
2	6	0	C	-2.855092	-0.239908	-0.166367
3	8	0	O	-0.640618	-0.526293	-0.046413
4	6	0	C	-0.014489	-0.160810	1.176354
5	7	0	N	1.113668	-0.899921	0.743928
6	16	0	S	2.253653	0.078578	-0.046356
7	8	0	O	2.776993	1.060512	0.923822

8	8	0	O	1.796153	0.577697	-1.355119
9	6	0	C	-1.698118	2.062326	-0.462217
10	6	0	C	-3.504930	0.050005	1.155644
11	6	0	C	-3.203747	-1.558128	-0.794929
12	6	0	C	3.516201	-1.171489	-0.329394
13	1	0	H	-1.715887	0.366381	-1.833570
14	1	0	H	-0.641780	2.265625	-0.665316
15	1	0	H	-1.912045	2.308650	0.581013
16	1	0	H	-2.287366	2.741247	-1.093665
17	1	0	H	-4.597101	0.074195	1.027634
18	1	0	H	-3.199926	1.001255	1.595699
19	1	0	H	-3.299389	-0.750782	1.877268
20	1	0	H	-3.022447	-2.380924	-0.093078
21	1	0	H	-2.617215	-1.744534	-1.697454
22	1	0	H	-4.271383	-1.589204	-1.056701
23	1	0	H	-0.493617	-0.612643	2.053105
24	1	0	H	0.098948	0.923479	1.302353
25	1	0	H	4.345924	-0.671606	-0.833800
26	1	0	H	3.099201	-1.958267	-0.959554
27	1	0	H	3.836680	-1.572876	0.632901

---

mPW1K/6-31+G** (PCM)

filename: mpBBPCMts2
E(RmPW+HF-PW91) = -954.047406116

Zero-point correction=	0.226233 (Hartree/Particle)
Thermal correction to Energy=	0.241133
Thermal correction to Enthalpy=	0.242077
Thermal correction to Gibbs Free Energy=	0.183642
Sum of electronic and zero-point Energies=	-953.821174
Sum of electronic and thermal Energies=	-953.806274
Sum of electronic and thermal Enthalpies=	-953.805329
Sum of electronic and thermal Free Energies=	-953.863764

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	151.313	52.543	122.987

C,0,-0.3648045373,-2.5998182339,0.1617801306
C,0,0.9987826602,-2.621485764,0.0559355198
O,0,0.1009515926,-0.583306526,0.0051552767
C,0,0.2297920084,0.1352714135,1.1970590791
N,0,0.0292194351,1.2254821215,0.3321001269
S,0,-1.5631452601,1.6059746407,0.0643076886
O,0,-2.4625201328,0.8322912844,0.9137968726
O,0,-1.8222786571,1.6109572498,-1.3655784555
C,0,-1.1872252301,-2.7785939108,1.3863515212
C,0,1.923762777,-2.7356993592,1.2179958852
C,0,1.6482211563,-2.6162894978,-1.2849228409
C,0,-1.582804543,3.2847505953,0.6175704
H,0,-0.9216776548,-2.595856151,-0.7676678129
H,0,-2.0002041726,-2.0550899822,1.4000608386
H,0,-0.6230689167,-2.6904621027,2.309848248
H,0,-1.6436142317,-3.769569639,1.3696522253
H,0,2.4101287412,-3.7127806537,1.1938413944
H,0,1.4327580396,-2.6327071391,2.1797936951
H,0,2.7189813984,-1.9938863129,1.1471244945
H,0,2.4035475086,-1.8338261033,-1.3428287126
H,0,0.9281295293,-2.4640477774,-2.0831562331
H,0,2.1576130568,-3.5672809127,-1.4517829354
H,0,1.2320719509,0.122038188,1.6167776444

```
 H,0,-0.5495716298,-0.0854452062,1.923377552
 H,0,-2.582609664,3.6657129945,0.4269053763
 H,0,-0.8478455261,3.8454515037,0.0502744154
 H,0,-1.3615906983,3.3122182804,1.6792286059
```

mPW1K/6-31+G** (gas phase)

```
filename: mpBBgasts2
E(RmPW+HF-PW91) = -954.031679331

 Zero-point correction=                           0.226873 (Hartree/Particle)
 Thermal correction to Energy=                    0.241660
 Thermal correction to Enthalpy=                  0.242604
 Thermal correction to Gibbs Free Energy=         0.184593
 Sum of electronic and zero-point Energies=           -953.804807
 Sum of electronic and thermal Energies=              -953.790019
 Sum of electronic and thermal Enthalpies=            -953.789075
 Sum of electronic and thermal Free Energies=         -953.847087

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.644             52.346            122.096

 C,0,-0.367704,-2.496616,0.136783
 C,0,0.997845,-2.597237,0.046784
 O,0,0.19677,-0.590913,0.03769
 C,0,0.337414,0.150512,1.225658
 N,0,0.072925,1.250844,0.405772
 S,0,-1.553747,1.500665,0.152756
 O,0,-2.354155,0.753776,1.117724
 O,0,-1.869917,1.371962,-1.253446
 C,0,-1.228156,-2.65423,1.337554
 C,0,1.897246,-2.783437,1.219848
 C,0,1.662017,-2.601314,-1.287192
 C,0,-1.655391,3.219521,0.563153
 H,0,-0.905054,-2.444524,-0.80015
 H,0,-1.967074,-1.854825,1.366735
 H,0,-0.676215,-2.65928,2.272389
 H,0,-1.772303,-3.596736,1.266283
 H,0,2.348235,-3.776455,1.176624
 H,0,1.39099,-2.688577,2.174384
 H,0,2.719162,-2.068893,1.18647
 H,0,2.467934,-1.87,-1.316858
 H,0,0.963602,-2.371689,-2.08559
 H,0,2.104974,-3.580331,-1.480302
 H,0,1.35513,0.15915,1.608272
 H,0,-0.405797,-0.111996,1.976805
 H,0,-2.679262,3.524746,0.368819
 H,0,-0.968926,3.765029,-0.074278
 H,0,-1.409544,3.354851,1.610313
```

mPW1K/6-31+G** (onsager)

```
filename: mpBBonsts2

E(RmPW+HF-PW91) = -954.034879393

 Zero-point correction=                           0.226752 (Hartree/Particle)
 Thermal correction to Energy=                    0.241631
 Thermal correction to Enthalpy=                  0.242576
```

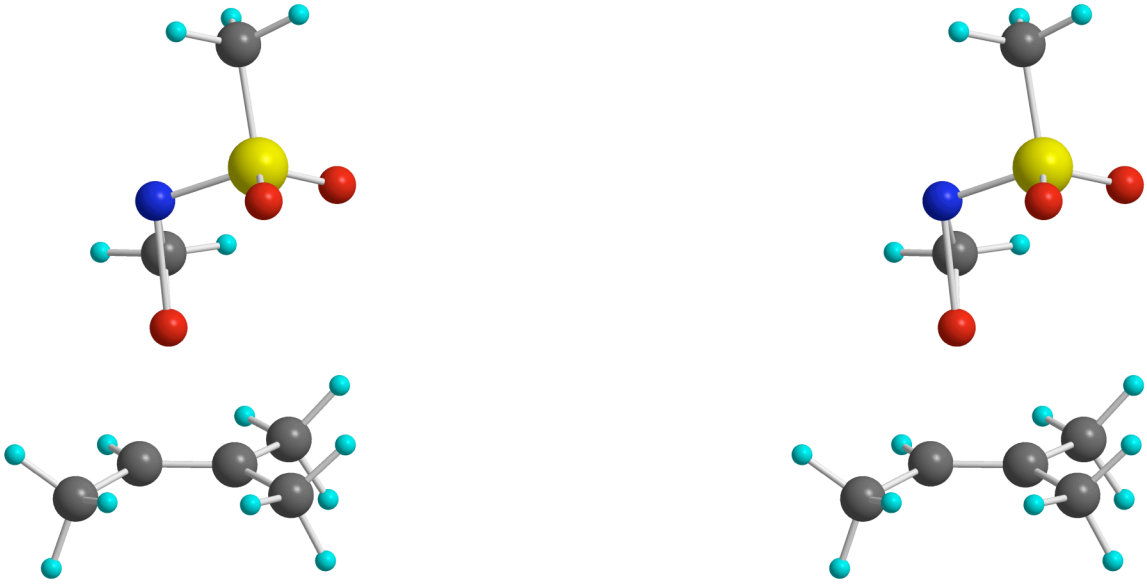
```
Thermal correction to Gibbs Free Energy=         0.183972
Sum of electronic and zero-point Energies=           -953.808128
Sum of electronic and thermal Energies=              -953.793248
Sum of electronic and thermal Enthalpies=            -953.792304
Sum of electronic and thermal Free Energies=         -953.850907

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  151.626             52.434           123.341


C,0,-0.3603389983,-2.5609804452,0.1570913209
C,0,1.0051702246,-2.6201647809,0.0615854169
O,0,0.1215868591,-0.6012161721,-0.0211406934
C,0,0.2635842781,0.1481628005,1.1536574976
N,0,0.0315864036,1.2310184064,0.2940342335
S,0,-1.5752202869,1.5722177945,0.0579388086
O,0,-2.4355586816,0.7769390464,0.9250315904
O,0,-1.8680926786,1.6156483943,-1.3598617488
C,0,-1.2028014236,-2.711278426,1.3721612693
C,0,1.9173200091,-2.7441234134,1.232294179
C,0,1.6631560498,-2.6391026975,-1.2748984641
C,0,-1.6082668876,3.243786276,0.6497449073
H,0,-0.9051968361,-2.5582517349,-0.7769983978
H,0,-1.9888201047,-1.9582652122,1.373752676
H,0,-0.6449573657,-2.6400839037,2.300618158
H,0,-1.6884346767,-3.6877880289,1.3542237048
H,0,2.3855735011,-3.7298580242,1.2210726891
H,0,1.4199424579,-2.6260086741,2.1886754241
H,0,2.7279535103,-2.0194239049,1.1646989221
H,0,2.4342922071,-1.872801132,-1.3329303806
H,0,0.9521095298,-2.4728541458,-2.0780521562
H,0,2.1529510941,-3.6014475249,-1.4335591449
H,0,1.2750371898,0.1483226468,1.5513886226
H,0,-0.4961637215,-0.0801842529,1.8989819329
H,0,-2.615288771,3.6141766892,0.4814877948
H,0,-0.8879108956,3.8235490477,0.0839734209
H,0,-1.3722129866,3.2540143716,1.7080284172
```

Epoxidation TS Isomer 3

B3LYP/6-31+G** (PCM)



filename: b3BBpcmfreqts3
E(RB+HF-LYP) = -954.240209492

Zero-point correction=	0.218465 (Hartree/Particle)
Thermal correction to Energy=	0.234124
Thermal correction to Enthalpy=	0.235068
Thermal correction to Gibbs Free Energy=	0.174414
Sum of electronic and zero-point Energies=	-954.021744
Sum of electronic and thermal Energies=	-954.006086
Sum of electronic and thermal Enthalpies=	-954.005142
Sum of electronic and thermal Free Energies=	-954.065795

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	146.915	54.448	127.656

1	6	0	2.716519	-0.683723	-0.390018
2	6	0	2.502665	0.616619	0.008441
3	8	0	0.559501	-0.663987	-0.206959
4	6	0	-0.171784	-0.517727	-1.406782
5	7	0	-1.222399	-1.057405	-0.607949
6	16	0	-2.123931	0.111729	0.254398
7	8	0	-1.805185	1.496240	-0.165479
8	8	0	-2.075349	-0.208315	1.693025
9	6	0	3.043032	-1.861097	0.476149
10	6	0	2.444788	1.054446	1.442148
11	6	0	2.385210	1.717970	-1.008466
12	6	0	-3.773003	-0.299032	-0.345304
13	1	0	2.805983	-0.856921	-1.463745
14	1	0	0.130740	-1.204889	-2.203693
15	1	0	-0.268704	0.519459	-1.742909
16	1	0	2.558894	-2.762238	0.087724
17	1	0	2.732900	-1.728108	1.514182
18	1	0	4.126569	-2.043711	0.464643
19	1	0	3.327809	1.665538	1.675844
20	1	0	2.408272	0.223637	2.146896
21	1	0	1.566473	1.688132	1.607217
22	1	0	1.463420	2.292366	-0.858878
23	1	0	2.409341	1.342208	-2.034907
24	1	0	3.216743	2.425282	-0.884771
25	1	0	-4.465965	0.350710	0.195148
26	1	0	-3.970642	-1.347954	-0.121075
27	1	0	-3.818440	-0.105571	-1.418094

B3LYP/6-31+G** (gas phase)

Filename: b3BBgasts3
E(RB+HF-LYP) = -954.226564654

Zero-point correction=	0.218975 (Hartree/Particle)
Thermal correction to Energy=	0.234559
Thermal correction to Enthalpy=	0.235503
Thermal correction to Gibbs Free Energy=	0.174774
Sum of electronic and zero-point Energies=	-954.007590
Sum of electronic and thermal Energies=	-953.992006
Sum of electronic and thermal Enthalpies=	-953.991062
Sum of electronic and thermal Free Energies=	-954.051791

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.188	54.290	127.815

C,0,-1.4789574629,-2.0771300378,-1.1689888233
C,0,-0.2462763687,-2.3223654214,-0.5894509574
O,0,-0.9233642464,-0.2325371338,-0.3889771487
C,0,-0.5331769701,0.7839849678,-1.3083193678
N,0,-0.6351592442,1.6710276821,-0.2094097196
S,0,0.7811504188,1.6977650691,0.7520477865
O,0,1.9547687788,1.1979652697,-0.0025712425
O,0,0.5099714608,1.1339065092,2.0830349405
C,0,-2.8323589566,-2.2779358795,-0.5589248971
C,0,-0.063598984,-2.7068192923,0.8481140905
C,0,1.0136038394,-2.2555610582,-1.4051232662
C,0,0.9479326752,3.4834378042,0.9436019388
H,0,-1.4751812735,-1.8685516321,-2.2383479172
H,0,-1.2942151336,0.9952823781,-2.0673066326
H,0,0.4610915776,0.6143892108,-1.7368853538
H,0,-3.522711964,-1.5065029139,-0.9121947834
H,0,-2.8142690653,-2.2383130308,0.5309818607
H,0,-3.2442923108,-3.2503451518,-0.8624365415
H,0,0.3734397246,-3.712711521,0.9070813912
H,0,-0.9909222902,-2.698513893,1.4200298249
H,0,0.6390577985,-2.0171167929,1.3280231132
H,0,1.713726093,-1.5339574026,-0.9678631739
H,0,0.8229760649,-1.9798673314,-2.4457433654
H,0,1.5135080497,-3.2331083611,-1.3957753153
H,0,1.7984530716,3.6409918231,1.6101187447
H,0,0.0299332163,3.866371439,1.3898318315
H,0,1.1321845012,3.9318327006,-0.0330990166

B3LYP/6-31+G** (onsager)

Filename: b3BBonsts3
E(RB+HF-LYP) = -954.228622521

Zero-point correction=	0.219019 (Hartree/Particle)
Thermal correction to Energy=	0.234595
Thermal correction to Enthalpy=	0.235539
Thermal correction to Gibbs Free Energy=	0.174989
Sum of electronic and zero-point Energies=	-954.009603
Sum of electronic and thermal Energies=	-953.994027
Sum of electronic and thermal Enthalpies=	-953.993083
Sum of electronic and thermal Free Energies=	-954.053634

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.211	54.330	127.439

C,0,-1.4812220564,-2.0781914159,-1.171300172
C,0,-0.2462225242,-2.3636150654,-0.6254689063
O,0,-0.87861155,-0.2253681534,-0.315431978
C,0,-0.4733512278,0.7786432044,-1.2304901218
N,0,-0.6455506175,1.6545480572,-0.1254681876
S,0,0.7366438042,1.7736706429,0.8731209566
O,0,1.9384196994,1.1865875171,0.2390326061
O,0,0.39615278,1.3819325212,2.2492889413
C,0,-2.8275205708,-2.269818903,-0.5452022938
C,0,-0.0468845265,-2.8140577225,0.7915620642
C,0,0.9990948479,-2.302923828,-1.4647846849
C,0,0.9213958436,3.5716303472,0.8580049774
H,0,-1.4932560338,-1.8241075978,-2.2306731943
H,0,-1.2056063354,0.9759546053,-2.0203491694
H,0,0.5424949726,0.63252749,-1.6133044604
H,0,-3.4996585127,-1.4579956945,-0.8381159437
H,0,-2.7889759757,-2.3012429847,0.5446174828

```
 H,0,-3.2756806066,-3.2075537056,-0.9010873828
 H,0,0.254447795,-3.8706529113,0.8020824359
 H,0,-0.9394640643,-2.7053680777,1.4073147788
 H,0,0.7623174613,-2.2401682418,1.2549016783
 H,0,1.7327364782,-1.6235146004,-1.0155269099
 H,0,0.7972384345,-1.9828239018,-2.4902852968
 H,0,1.4664070151,-3.2957607171,-1.5053775777
 H,0,1.7463183172,3.7993202919,1.5366966907
 H,0,-0.0086521551,4.0154821405,1.2137114528
 H,0,1.1543053078,3.8984857032,-0.1560187856
```

mPW1K/6-31+G** (PCM)

```
Filename: mpBBgasPCMts3 (PCM)

E(RmPW+HF-PW91) = -954.048055898

Zero-point correction=                           0.225993 (Hartree/Particle)
 Thermal correction to Energy=                    0.241063
 Thermal correction to Enthalpy=                  0.242007
 Thermal correction to Gibbs Free Energy=         0.182748
 Sum of electronic and zero-point Energies=           -953.822063
 Sum of electronic and thermal Energies=              -953.806993
 Sum of electronic and thermal Enthalpies=            -953.806049
 Sum of electronic and thermal Free Energies=         -953.865307

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.269             52.629            124.721


 C,0,-1.4696444824,-2.0320408714,-1.1599846283
 C,0,-0.2379759161,-2.3249206181,-0.643359173
 O,0,-0.8561408374,-0.227617262,-0.3088080686
 C,0,-0.4166242129,0.7355705226,-1.2204798873
 N,0,-0.6579222863,1.5864819655,-0.1282603569
 S,0,0.6202871139,1.7458658412,0.918356476
 O,0,1.8143330888,1.0599694294,0.4359094494
 O,0,0.1674274226,1.4521478216,2.2670413878
 C,0,-2.7892114047,-2.2127029058,-0.5012698505
 C,0,-0.0129808884,-2.786298569,0.7528367119
 C,0,0.9808968651,-2.2619279915,-1.4995137036
 C,0,0.9028030152,3.4881567137,0.8163307102
 H,0,-1.5038766062,-1.7715393595,-2.2133132269
 H,0,-1.1049110725,0.910215945,-2.0436011893
 H,0,0.6147720539,0.5952820777,-1.5367267067
 H,0,-3.4601018355,-1.4023667216,-0.7769992353
 H,0,-2.7209996427,-2.2414307981,0.581058663
 H,0,-3.2481933903,-3.1435715647,-0.838914454
 H,0,0.2897432814,-3.8350959168,0.7435348036
 H,0,-0.8891324272,-2.6895642468,1.3831342951
 H,0,0.8008171213,-2.2205203842,1.2029637226
 H,0,1.7307131632,-1.6116407195,-1.0498520388
 H,0,0.7632625532,-1.9155373408,-2.5065357715
 H,0,1.4274031508,-3.2551707372,-1.5707733658
 H,0,1.6932111698,3.7195271527,1.5255131085
 H,0,-0.0124736152,4.0039779608,1.0856846383
 H,0,1.2118316189,3.7403685767,-0.1925243099
```

mPW1K/6-31+G** (gas phase)

```
filename: mpBBgasPCMts3

E(RmPW+HF-PW91) = -954.033662090

Zero-point correction=                           0.226465 (Hartree/Particle)
 Thermal correction to Energy=                    0.241491
 Thermal correction to Enthalpy=                  0.242435
 Thermal correction to Gibbs Free Energy=         0.183229
 Sum of electronic and zero-point Energies=           -953.807197
 Sum of electronic and thermal Energies=              -953.792171
 Sum of electronic and thermal Enthalpies=            -953.791227
 Sum of electronic and thermal Free Energies=         -953.850433

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.538             52.496            124.611

C,0,-1.4583224934,-2.0430998243,-1.1719626385
 C,0,-0.2361382697,-2.255142651,-0.5855751647
 O,0,-0.9217289286,-0.2478451096,-0.375299529
 C,0,-0.5671946393,0.75582441,-1.2930063972
 N,0,-0.6600379814,1.5998101382,-0.1826665594
 S,0,0.7199646909,1.6033210804,0.7482925564
 O,0,1.8491765164,1.0398098233,0.0146457462
 O,0,0.436178432,1.0844856134,2.0701522152
 C,0,-2.7997453772,-2.2560792103,-0.5680439866
 C,0,-0.0581692763,-2.624186407,0.8439645884
 C,0,1.0208372581,-2.1522470549,-1.3789373881
 C,0,0.9740185823,3.3470095614,0.905738104
 H,0,-1.4493994243,-1.8373720996,-2.2360811139
 H,0,-1.3424452659,0.9586371249,-2.0280996363
 H,0,0.4166130659,0.5985454819,-1.7327784661
 H,0,-3.4952737361,-1.501400744,-0.9268831757
 H,0,-2.7824299555,-2.2024318665,0.5147856742
 H,0,-3.1950997164,-3.230577584,-0.8595257091
 H,0,0.4310030933,-3.5968479511,0.9101309863
 H,0,-0.9888882895,-2.6671694731,1.3963302727
 H,0,0.5910528263,-1.8960015413,1.3277120071
 H,0,1.6761020253,-1.3980431889,-0.9422932441
 H,0,0.8342228695,-1.903101266,-2.4203077631
 H,0,1.5546797214,-3.1026677953,-1.3454199065
 H,0,1.8282395176,3.4790902428,1.5630407071
 H,0,0.0845387877,3.7835110465,1.3455336657
 H,0,1.1755589668,3.7697872442,-0.0719978449
```

mPW1K/6-31+G** (onsager)

```
Filename: mpBBonsts3

E(RmPW+HF-PW91) = -954.035816188

 Zero-point correction=                           0.226570 (Hartree/Particle)
 Thermal correction to Energy=                    0.241575
 Thermal correction to Enthalpy=                  0.242520
 Thermal correction to Gibbs Free Energy=         0.183333
 Sum of electronic and zero-point Energies=           -953.809246
 Sum of electronic and thermal Energies=              -953.794241
 Sum of electronic and thermal Enthalpies=            -953.793297
 Sum of electronic and thermal Free Energies=         -953.852483
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	151.591	52.512	124.568

```
C,0,-1.4649886457,-2.0383082998,-1.1736755729
C,0,-0.2339717406,-2.2817584861,-0.6249742165
O,0,-0.8959905812,-0.2492845877,-0.3184290865
C,0,-0.4987248665,0.7463469111,-1.2195346013
N,0,-0.6789265183,1.5835400614,-0.1106054165
S,0,0.6484535331,1.6727903655,0.88362992
O,0,1.8045223899,0.9966956901,0.3074663244
O,0,0.2655360222,1.3524578387,2.2432399028
C,0,-2.7946269047,-2.2530411369,-0.5471611064
C,0,-0.0272845083,-2.7078983691,0.7854205933
C,0,1.0036840617,-2.1898368217,-1.4504191688
C,0,0.9534059387,3.4179106782,0.8224665697
H,0,-1.479756292,-1.7953838957,-2.2297650786
H,0,-1.2268346585,0.9388827478,-2.0034851355
H,0,0.5141121317,0.6040428834,-1.5921163578
H,0,-3.4792350649,-1.4607573627,-0.8398320558
H,0,-2.7493973575,-2.2740933331,0.5361066575
H,0,-3.2212128977,-3.1960681482,-0.8923996757
H,0,0.3074224413,-3.7464936557,0.8049081773
H,0,-0.9205574771,-2.6230440759,1.3924519539
H,0,0.7545556322,-2.1022381358,1.2395200308
H,0,1.7027423164,-1.4837508033,-1.0028933985
H,0,0.7990903022,-1.892717307,-2.4755443457
H,0,1.4994354733,-3.1612333608,-1.4734861536
H,0,1.7754077703,3.6148796301,1.5044474431
H,0,0.0566982788,3.9344892797,1.1452784891
H,0,1.2237572213,3.6994886933,-0.1891656919
```

B3LYP/6-31G* (gas phase)

```
E(RB+HF-LYP) =  -954.180726424
```

Zero-point correction=	0.220947 (Hartree/Particle)
Thermal correction to Energy=	0.236352
Thermal correction to Enthalpy=	0.237297
Thermal correction to Gibbs Free Energy=	0.177298
Sum of electronic and zero-point Energies=	-953.959780
Sum of electronic and thermal Energies=	-953.944374
Sum of electronic and thermal Enthalpies=	-953.943430
Sum of electronic and thermal Free Energies=	-954.003428

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	148.313	53.710	126.278

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	-2.581460	0.585001	-0.448706
2	6	0	C	-2.296543	-0.740626	-0.165825
3	8	0	O	-0.669640	0.672881	0.224500
4	6	0	C	0.138627	1.374663	-0.714499
5	7	0	N	1.191240	1.305888	0.222886
6	16	0	S	2.022385	-0.179402	0.145407
7	8	0	O	1.664574	-0.951126	-1.066351
8	8	0	O	1.977506	-0.850177	1.450373

9	6	0	C	-3.276636	1.595425	0.411134
10	6	0	C	-2.468479	-1.346347	1.193402
11	6	0	C	-1.768471	-1.658155	-1.229358
12	6	0	C	3.695407	0.457461	-0.096474
13	1	0	H	-2.451825	0.882202	-1.489393
14	1	0	H	-0.193533	2.409577	-0.862392
15	1	0	H	0.248992	0.833136	-1.661591
16	1	0	H	-2.801581	2.574932	0.291876
17	1	0	H	-3.257616	1.339422	1.471617
18	1	0	H	-4.324302	1.703024	0.097473
19	1	0	H	-3.206382	-2.159016	1.148400
20	1	0	H	-2.789128	-0.627886	1.948443
21	1	0	H	-1.518805	-1.787230	1.518542
22	1	0	H	-0.739864	-1.957471	-0.992381
23	1	0	H	-1.765504	-1.191894	-2.218489
24	1	0	H	-2.376735	-2.571390	-1.275634
25	1	0	H	4.361904	-0.407688	-0.134605
26	1	0	H	3.950790	1.104511	0.743660
27	1	0	H	3.732556	1.007823	-1.038452

MPW1K/6-31+G* (gas phase)

E(RmPW+HF-PW91) = -954.006577465

Zero-point correction= 0.227643 (Hartree/Particle)
Thermal correction to Energy= 0.242616
Thermal correction to Enthalpy= 0.243561
Thermal correction to Gibbs Free Energy= 0.184629
Sum of electronic and zero-point Energies= -953.778934
Sum of electronic and thermal Energies= -953.763961
Sum of electronic and thermal Enthalpies= -953.763017
Sum of electronic and thermal Free Energies= -953.821948

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	152.244	52.298	124.032

C,0,-1.4023970111,-2.0217591272,-1.1683400356
C,0,-0.1771919187,-2.2445870456,-0.5930514701
O,0,-0.8555991996,-0.2320767101,-0.3765780343
C,0,-0.4841516712,0.7663617243,-1.2921261424
N,0,-0.5996065289,1.616692741,-0.1893700063
S,0,0.7624016453,1.6344362259,0.7673597929
O,0,1.9067385524,1.0639409367,0.0641417011
O,0,0.4525351007,1.1356432278,2.0906623998
C,0,-2.7413636337,-2.2242164618,-0.5546051243
C,0,0.0121833308,-2.6157806251,0.834835958
C,0,1.0732279543,-2.1580105044,-1.3994435167
C,0,1.0098631008,3.3819521095,0.9040121362
H,0,-1.4025336348,-1.8157406703,-2.2327789119
H,0,-1.2451640571,0.9630580835,-2.0434996395
H,0,0.5075813762,0.6068475575,-1.712136272
H,0,-3.4326460021,-1.4598067231,-0.9033795533
H,0,-2.716322113,-2.1784593419,0.5290972759
H,0,-3.1497072798,-3.1934660213,-0.8490370085
H,0,0.4438777127,-3.6168661083,0.8970543965
H,0,-0.9064484731,-2.6009829149,1.4098959879
H,0,0.7148579938,-1.9265754097,1.3015954152
H,0,1.7473551696,-1.4168418313,-0.9684806759
H,0,0.8808541582,-1.9024770973,-2.439172059
H,0,1.5934765834,-3.1174186305,-1.3757344675
H,0,1.8529290333,3.5280253241,1.5740146778

```
H,0,0.1126820911,3.8252277862,1.3226140739
H,0,1.2276102849,3.7938271425,-0.0757192466
```

MPW1K/6-31+G* (Onsager)

```
E(RmPW+HF-PW91) =  -954.008495653

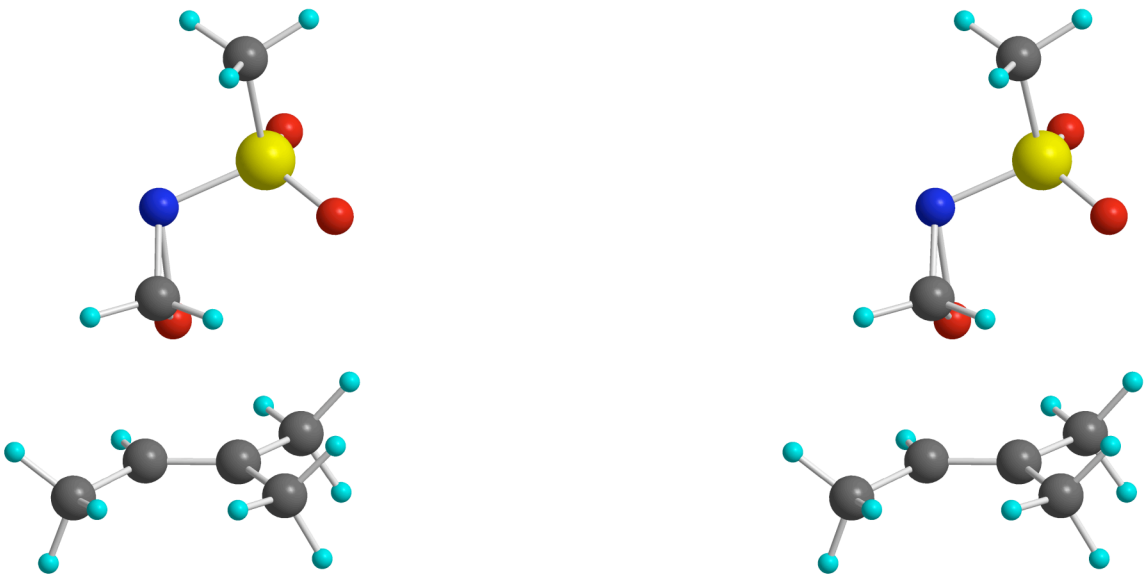
 Zero-point correction=                           0.227753 (Hartree/Particle)
 Thermal correction to Energy=                    0.242689
 Thermal correction to Enthalpy=                  0.243633
 Thermal correction to Gibbs Free Energy=         0.184741
 Sum of electronic and zero-point Energies=           -953.780743
 Sum of electronic and thermal Energies=              -953.765807
 Sum of electronic and thermal Enthalpies=            -953.764863
 Sum of electronic and thermal Free Energies=         -953.823755

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 152.290             52.297           123.950

 C,0,-1.3892963971,-2.0345192647,-1.2110365569
 C,0,-0.1572333407,-2.2819329314,-0.6662988682
 O,0,-0.8180661374,-0.2465990264,-0.37240611
 C,0,-0.4136451189,0.7450614854,-1.2744565337
 N,0,-0.5980331493,1.588635929,-0.1720581473
 S,0,0.7203628747,1.6720195185,0.835028612
 O,0,1.8837412311,1.0077787235,0.2602892337
 O,0,0.3281362413,1.3344869089,2.187494475
 C,0,-2.7183295786,-2.2384421243,-0.5782011673
 C,0,0.0552591439,-2.6970623903,0.7467742252
 C,0,1.077183055,-2.2025992759,-1.4985344675
 C,0,1.0162343539,3.4198041773,0.795501268
 H,0,-1.4087505392,-1.7990117798,-2.269060751
 H,0,-1.1373504338,0.9345032543,-2.0631501543
 H,0,0.6001952558,0.5982635373,-1.6419321841
 H,0,-3.4024390867,-1.447543499,-0.8786461141
 H,0,-2.6712853136,-2.2459983352,0.5058502886
 H,0,-3.1492813892,-3.185314875,-0.9101557452
 H,0,0.3906190225,-3.7362431254,0.7748456878
 H,0,-0.835217883,-2.6076177828,1.3585521389
 H,0,0.8391229675,-2.087938758,1.1946094459
 H,0,1.7864678583,-1.5011712026,-1.0584543121
 H,0,0.8705356654,-1.9064122439,-2.5244956424
 H,0,1.5659687428,-3.1785831167,-1.5221785248
 H,0,1.8327859496,3.6160143619,1.4855112182
 H,0,0.1151748167,3.9304148438,1.1180902819
 H,0,1.2923570322,3.7166840168,-0.2109445812
```

Epoxidation TS Isomer 4

B3LYP/6-31+G** (PCM)



Filename: b3BBgasPCMts4

E(RB+HF-LYP) = -954.240143389

Zero-point correction=	0.218672 (Hartree/Particle)
Thermal correction to Energy=	0.234179
Thermal correction to Enthalpy=	0.235124
Thermal correction to Gibbs Free Energy=	0.175155
Sum of electronic and zero-point Energies=	-954.021471
Sum of electronic and thermal Energies=	-954.005964
Sum of electronic and thermal Enthalpies=	-954.005020
Sum of electronic and thermal Free Energies=	-954.064988

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	146.950	54.393	126.214

C,0,2.6764215717,-0.302790058,-0.6468396567
C,0,2.3127254885,0.811556606,0.076774785
O,0,0.4997681317,-0.4543703974,-0.621962522
C,0,-0.0651452356,-1.32251885,0.3401197528
N,0,-1.2104212791,-1.2195790508,-0.5034899528
S,0,-2.2227490177,0.1111978546,-0.1484075351
O,0,-2.3580516921,0.9510799027,-1.3530500859
O,0,-1.8603534855,0.7709933968,1.1275484097
C,0,3.2311579625,-1.5944510247,-0.1289607524
C,0,2.323529078,0.8839593866,1.5769615927
C,0,1.9574688507,2.089116836,-0.628778496
C,0,-3.7786596277,-0.7672771859,0.0860885745
H,0,2.6974297562,-0.1939588911,-1.730646403
H,0,-0.1309165151,-0.8881065327,1.3426859636
H,0,0.3521685922,-2.3340224824,0.3338205646
H,0,2.8003906775,-2.442482706,-0.6724569456
H,0,3.0709045762,-1.7469853772,0.9407485004
H,0,4.3143144151,-1.6254809066,-0.31051334
H,0,3.1125569966,1.5765476375,1.9009428513
H,0,2.5011540885,-0.0766349091,2.0629913502
H,0,1.3770697751,1.2964943892,1.9445420916
H,0,0.9906640858,2.4674756269,-0.2791083338
H,0,1.9108379207,1.95949161,-1.7123677424
H,0,2.7064826404,2.8600817889,-0.4007880539
H,0,-4.5396491189,-0.0012453736,0.2549050196
H,0,-3.6897426906,-1.421993208,0.9543016835
H,0,-3.9948789451,-1.3348200814,-0.8198993198

B3LYP/6-31+G** (gas phase)

```
Filename: b3BBgasPCMts4 (gas)

E(RB+HF-LYP) = -954.225688536

Zero-point correction=                           0.219055 (Hartree/Particle)
 Thermal correction to Energy=                    0.234520
 Thermal correction to Enthalpy=                  0.235464
 Thermal correction to Gibbs Free Energy=         0.175711
 Sum of electronic and zero-point Energies=           -954.006634
 Sum of electronic and thermal Energies=              -953.991169
 Sum of electronic and thermal Enthalpies=            -953.990225
 Sum of electronic and thermal Free Energies=         -954.049977

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 147.163             54.320            125.760

 C,0,2.7035315681,-0.3300777255,-0.6222471285
 C,0,2.1968045312,0.7883707721,0.0190745177
 O,0,0.6049067689,-0.4988386928,-0.6713387014
 C,0,0.0108261367,-1.4982172037,0.1553611859
 N,0,-1.1943667735,-1.2232522044,-0.5354324772
 S,0,-2.0233202993,0.1285487389,0.1041125827
 O,0,-2.0161755361,1.2463917895,-0.8524483324
 O,0,-1.6130388656,0.3975009854,1.5035570037
 C,0,3.2929653143,-1.558649126,0.0007650914
 C,0,2.055499177,0.9219914004,1.5073941477
 C,0,1.8208326719,2.0042244569,-0.7785901301
 C,0,-3.6911843676,-0.55719894,0.1211893084
 H,0,2.8174329682,-0.2578119556,-1.7008214288
 H,0,0.0533947651,-1.2512255748,1.2224471011
 H,0,0.3737511143,-2.5079106026,-0.0623338375
 H,0,2.966539544,-2.4559075484,-0.5358152207
 H,0,3.0430154291,-1.6754180601,1.0572013513
 H,0,4.3879503607,-1.5261271322,-0.0821481224
 H,0,2.6756409967,1.7571934358,1.8579806083
 H,0,2.3498765677,0.0273523865,2.058000979
 H,0,1.0167354973,1.1644867515,1.760679277
 H,0,0.7928931828,2.3050646312,-0.5521756815
 H,0,1.8968490774,1.8279735199,-1.8535480693
 H,0,2.4796273562,2.8413345783,-0.5110377521
 H,0,-4.3499217894,0.2490965577,0.4503011071
 H,0,-3.7259017173,-1.3956637508,0.8173617768
 H,0,-3.9406866787,-0.8719534874,-0.8923271563
```

B3LYP/6-31+G** (onsager)

```
Filename: b3BBonsts4

E(RB+HF-LYP) = -954.228302223

 Zero-point correction=                           0.219204 (Hartree/Particle)
 Thermal correction to Energy=                    0.234655
 Thermal correction to Enthalpy=                  0.235599
 Thermal correction to Gibbs Free Energy=         0.175626
 Sum of electronic and zero-point Energies=           -954.009099
 Sum of electronic and thermal Energies=              -953.993647
 Sum of electronic and thermal Enthalpies=            -953.992703
 Sum of electronic and thermal Free Energies=         -954.052676
```

```
                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 147.248             54.274           126.223

 C,0,2.6859756649,-0.3139906923,-0.6344025502
 C,0,2.2694727686,0.7937214946,0.0774190543
 O,0,0.5545967862,-0.4495048102,-0.6518498856
 C,0,-0.04571177,-1.3458191361,0.2679109428
 N,0,-1.1970931567,-1.204945725,-0.5535641473
 S,0,-2.1599223703,0.1464649681,-0.1530550527
 O,0,-2.3452492628,0.9965330881,-1.3393674419
 O,0,-1.747238513,0.7771280591,1.1209852196
 C,0,3.2518049673,-1.5935886814,-0.1006847414
 C,0,2.2217624575,0.8654984365,1.576551653
 C,0,1.9134206448,2.0635278915,-0.6421063345
 C,0,-3.723947474,-0.7140504219,0.1360479417
 H,0,2.7425682694,-0.2007032456,-1.71414142
 H,0,-0.0953900713,-0.9494148971,1.2877150153
 H,0,0.3583197862,-2.3618520057,0.2212367243
 H,0,2.8551386105,-2.4498016453,-0.6563794573
 H,0,3.0625008445,-1.7492487286,0.9632973164
 H,0,4.3401078388,-1.6036337958,-0.2479746725
 H,0,2.9572008302,1.6009888961,1.9291139994
 H,0,2.4379919876,-0.0835193159,2.0688568479
 H,0,1.2376619954,1.2186708408,1.9045729657
 H,0,0.9338933652,2.4271923678,-0.3145886078
 H,0,1.88770305,1.9261901203,-1.7251949097
 H,0,2.6500982858,2.8433354729,-0.4046565149
 H,0,-4.467510153,0.0616108708,0.332185158
 H,0,-3.6162775776,-1.3717827055,0.9993062238
 H,0,-3.9774018044,-1.2777287002,-0.7620703265
```

mPW1K/6-31+G** (PCM)

```
Filename: mpBBgasPCMts4

E(RmPW+HF-PW91) = -954.047890663

Zero-point correction=                           0.226238 (Hartree/Particle)
 Thermal correction to Energy=                    0.241122
 Thermal correction to Enthalpy=                  0.242066
 Thermal correction to Gibbs Free Energy=         0.183615
 Sum of electronic and zero-point Energies=           -953.821653
 Sum of electronic and thermal Energies=              -953.806769
 Sum of electronic and thermal Enthalpies=            -953.805825
 Sum of electronic and thermal Free Energies=         -953.864276

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.306             52.547           123.021

C,0,2.6346615244,-0.3083831031,-0.6383393953
 C,0,2.2361325261,0.781914862,0.0854329423
 O,0,0.5429579214,-0.441825777,-0.636448107
 C,0,-0.0189646435,-1.3053991179,0.3076257003
 N,0,-1.1347131559,-1.1891407902,-0.5398958966
 S,0,-2.108054657,0.1164120141,-0.2197873408
 O,0,-2.3014382522,0.8738939178,-1.444263922
 O,0,-1.6785920521,0.8421472552,0.9708431737
 C,0,3.1799923137,-1.5906047204,-0.1210028206
 C,0,2.2011045288,0.833640155,1.5735527217
 C,0,1.8771720182,2.0513805921,-0.605823949
```

```
 C,0,-3.6310099041,-0.7024434334,0.1489703523
 H,0,2.690626066,-0.1817208664,-1.7130925519
 H,0,-0.0895735918,-0.871855145,1.3027591918
 H,0,0.4013119347,-2.3072313074,0.2979999126
 H,0,2.7758491734,-2.4303879025,-0.6839169825
 H,0,2.987027972,-1.7542249095,0.9350060225
 H,0,4.2613722696,-1.609221557,-0.2665215239
 H,0,2.9533070663,1.5431672459,1.9229611517
 H,0,2.3964654661,-0.1209749606,2.050382827
 H,0,1.2359245878,1.2083788045,1.9119440212
 H,0,0.8972192147,2.3951328703,-0.2788960788
 H,0,1.863882178,1.9364510085,-1.6854808209
 H,0,2.5978422632,2.8287678712,-0.3459282031
 H,0,-4.3730673734,0.0746828105,0.3121555126
 H,0,-3.5057164512,-1.3020673166,1.0443298086
 H,0,-3.9072419432,-1.3192105001,-0.6994037459
```

mPW1K/6-31+G** (gas phase)

```
Filename: mpBBgasPCMts4

E(RmPW+HF-PW91) = -954.032906119

Zero-point correction=                           0.226722 (Hartree/Particle)
 Thermal correction to Energy=                    0.241521
 Thermal correction to Enthalpy=                  0.242465
 Thermal correction to Gibbs Free Energy=         0.184565
 Sum of electronic and zero-point Energies=           -953.806184
 Sum of electronic and thermal Energies=              -953.791385
 Sum of electronic and thermal Enthalpies=            -953.790441
 Sum of electronic and thermal Free Energies=         -953.848341

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.557             52.439            121.861

C,0,2.658124324,-0.329132619,-0.6182625616
 C,0,2.1500852044,0.7688873138,0.0299171263
 O,0,0.6061402297,-0.4827319748,-0.6668940213
 C,0,0.042103169,-1.4703670297,0.1593147453
 N,0,-1.1315191739,-1.1940124234,-0.5492672185
 S,0,-1.9408737276,0.1378219716,0.0326062241
 O,0,-1.9777202162,1.1874750787,-0.9645660532
 O,0,-1.4834542472,0.4822895929,1.3759937129
 C,0,3.2317957171,-1.5577067611,-0.0078662391
 C,0,1.9947102277,0.8808485405,1.506216741
 C,0,1.7658210779,1.9805234941,-0.7469138181
 C,0,-3.5727858791,-0.5338899689,0.1561352359
 H,0,2.7799093071,-0.2416066132,-1.6890002229
 H,0,0.0718582822,-1.2064041722,1.2157488813
 H,0,0.4167174839,-2.4694417875,-0.0475504718
 H,0,2.9193116286,-2.4409770168,-0.5619761635
 H,0,2.9598879164,-1.6899432602,1.0347347797
 H,0,4.320926568,-1.5224799445,-0.0651991085
 H,0,2.5796105563,1.7283090093,1.8651074622
 H,0,2.3152596875,-0.0031543854,2.0470939003
 H,0,0.950702254,1.0844116519,1.7463795509
 H,0,0.737726068,2.2583102763,-0.5221259537
 H,0,1.8481228063,1.8194014723,-1.8172206137
 H,0,2.4072188547,2.8170686426,-0.4659742679
 H,0,-4.2214946376,0.2792583931,0.4677279573
 H,0,-3.5779555602,-1.3301839509,0.8917778621
 H,0,-3.8657509212,-0.9012955296,-0.8207754655
```

mPW1K/6-31+G** (onsager)

```
Filename: mpBBonsts4

E(RmPW+HF-PW91) = -954.035584179

 Zero-point correction=                           0.226770 (Hartree/Particle)
 Thermal correction to Energy=                    0.241609
 Thermal correction to Enthalpy=                  0.242553
 Thermal correction to Gibbs Free Energy=         0.184026
 Sum of electronic and zero-point Energies=           -953.808814
 Sum of electronic and thermal Energies=              -953.793975
 Sum of electronic and thermal Enthalpies=            -953.793031
 Sum of electronic and thermal Free Energies=         -953.851559

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.612             52.439            123.182

 C,0,2.648778929,-0.3188130711,-0.6226289913
 C,0,2.199946434,0.7681087647,0.0802598214
 O,0,0.580269922,-0.4406647715,-0.66874732
 C,0,-0.0055722744,-1.3416685798,0.2282627869
 N,0,-1.1289800139,-1.1714954599,-0.5935321345
 S,0,-2.050940741,0.1517474518,-0.203606779
 O,0,-2.2857755974,0.9507716314,-1.388882826
 O,0,-1.5706035194,0.8168277243,1.0016144037
 C,0,3.1999460148,-1.5880030615,-0.0807019969
 C,0,2.1055664415,0.828548387,1.5651844373
 C,0,1.8402002427,2.025659067,-0.6329545515
 C,0,-3.5802870381,-0.6521390529,0.1960358361
 H,0,2.7396624023,-0.1947984681,-1.6929857515
 H,0,-0.054544462,-0.9576497212,1.2455529308
 H,0,0.3992637415,-2.3478980369,0.1634919304
 H,0,2.8347771343,-2.4379315857,-0.6541768279
 H,0,2.9696439559,-1.751055813,0.9674370452
 H,0,4.2861166015,-1.5874277663,-0.1823757391
 H,0,2.8027901479,1.5805746773,1.9374541561
 H,0,2.3375769881,-0.1098504095,2.0569006608
 H,0,1.1059009055,1.1474037671,1.8578282789
 H,0,0.8475331,2.3551564518,-0.3317078326
 H,0,1.8494835772,1.8971922756,-1.7109220547
 H,0,2.5462986106,2.8142008327,-0.3674316193
 H,0,-4.300690421,0.1334010397,0.4047766983
 H,0,-3.4387560084,-1.2783007018,1.0699932002
 H,0,-3.8931290731,-1.2406185711,-0.6589737616
```

B3LYP/6-31G* (gas phase)

```
E(RB+HF-LYP) =  -954.181279558

 Zero-point correction=                           0.220961 (Hartree/Particle)
 Thermal correction to Energy=                    0.236239
 Thermal correction to Enthalpy=                  0.237183
 Thermal correction to Gibbs Free Energy=         0.177626
 Sum of electronic and zero-point Energies=           -953.960318
 Sum of electronic and thermal Energies=              -953.945041
 Sum of electronic and thermal Enthalpies=            -953.944097
 Sum of electronic and thermal Free Energies=         -954.003654
```

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	148.242	53.789	125.348

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	2.723630	-0.362510	-0.584189
2	6	0	C	2.206344	0.782318	0.004218
3	8	0	O	0.665285	-0.484933	-0.688017
4	6	0	C	0.005891	-1.516247	0.054517
5	7	0	N	-1.175742	-1.171220	-0.638911
6	16	0	S	-1.997486	0.123090	0.099147
7	8	0	O	-1.730170	1.409116	-0.567648
8	8	0	O	-1.853944	0.063087	1.570491
9	6	0	C	3.300962	-1.563571	0.100259
10	6	0	C	2.048370	0.978944	1.483774
11	6	0	C	1.834839	1.960551	-0.850488
12	6	0	C	-3.677010	-0.358005	-0.343980
13	1	0	H	2.871883	-0.328729	-1.660319
14	1	0	H	0.028246	-1.353958	1.138891
15	1	0	H	0.352934	-2.519096	-0.219353
16	1	0	H	2.949171	-2.485493	-0.376523
17	1	0	H	3.063901	-1.614202	1.165355
18	1	0	H	4.395539	-1.556834	-0.001062
19	1	0	H	2.626300	1.859154	1.796481
20	1	0	H	2.381263	0.127102	2.079733
21	1	0	H	0.998053	1.184177	1.723524
22	1	0	H	0.791751	2.239505	-0.666173
23	1	0	H	1.945608	1.741003	-1.915286
24	1	0	H	2.468526	2.822574	-0.600424
25	1	0	H	-4.340324	0.411733	0.057231
26	1	0	H	-3.905142	-1.331218	0.092918
27	1	0	H	-3.745264	-0.393655	-1.432228

mPW1K/6-31+G** (gas phase)

E(RmPW+HF-PW91) = -954.005797625

Zero-point correction=	0.227819 (Hartree/Particle)
Thermal correction to Energy=	0.242619
Thermal correction to Enthalpy=	0.243564
Thermal correction to Gibbs Free Energy=	0.185440
Sum of electronic and zero-point Energies=	-953.777979
Sum of electronic and thermal Energies=	-953.763178
Sum of electronic and thermal Enthalpies=	-953.762234
Sum of electronic and thermal Free Energies=	-953.820357

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	152.246	52.267	122.331

C,0,-1.4152299006,-2.244391407,-0.6886026638
C,0,-0.0460824983,-2.2097576057,-0.6021471662
O,0,-0.8883334337,-0.2835204031,-0.3999066043
C,0,-1.152621734,0.2524081816,0.8718683453
N,0,-0.8699361871,1.477732944,0.2612002063
S,0,0.759710825,1.7978898713,0.1681388136
O,0,1.1843599068,1.8730713641,-1.2140724727
O,0,1.5157974609,0.9396694128,1.0752052341
C,0,-2.3824130743,-2.6533369219,0.3648517532

C,0,0.7297800838,-2.4955575535,0.6362289128
C,0,0.7705132176,-1.9278326522,-1.816091186
C,0,0.7768004403,3.4442759043,0.8181814117
H,0,-1.8399455281,-2.0885033092,-1.6708522825
H,0,-0.463427971,-0.1079693068,1.6341599079
H,0,-2.1969418139,0.1736795166,1.1621805439
H,0,-3.2562974475,-2.003182841,0.3538101461
H,0,-1.9613354353,-2.6474087055,1.3662291345
H,0,-2.7426159876,-3.6642927704,0.1626644076
H,0,1.3809197353,-3.3542620643,0.4625450148
H,0,0.1104569069,-2.7140627083,1.5006372279
H,0,1.3737947163,-1.6465684734,0.8684790087
H,0,1.4549989574,-1.1024229428,-1.6259222564
H,0,0.1529910579,-1.6663501038,-2.6707123223
H,0,1.3695220211,-2.8045751456,-2.0707738902
H,0,1.8014078555,3.7993154096,0.7470266105
H,0,0.4515716288,3.4272933329,1.8529991026
H,0,0.1200107334,4.0603308989,0.2133614848

mPW1K/6-31+G** (onsager)

E(RmPW+HF-PW91) = -954.008165436

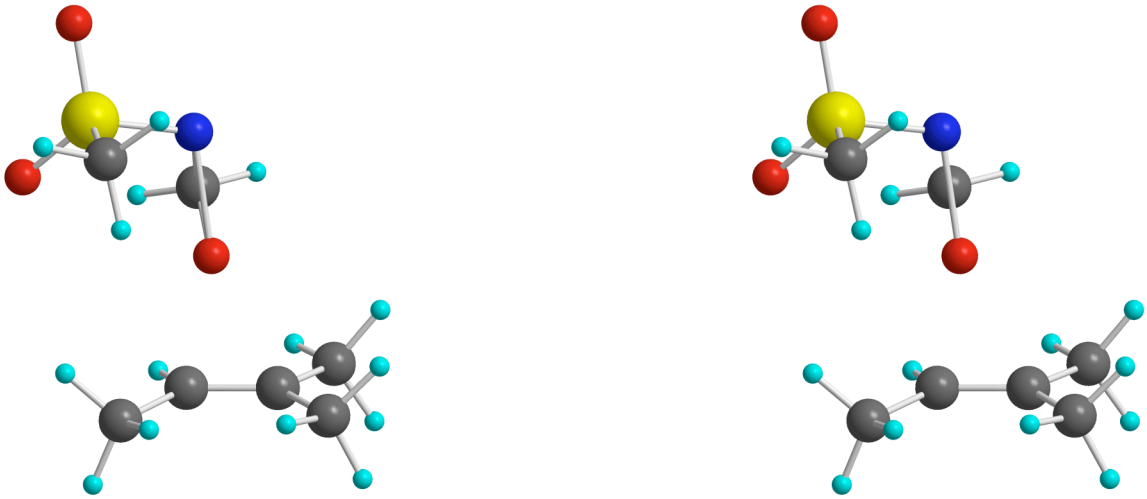
Zero-point correction= 0.227946 (Hartree/Particle)
Thermal correction to Energy= 0.242723
Thermal correction to Enthalpy= 0.243668
Thermal correction to Gibbs Free Energy= 0.185443
Sum of electronic and zero-point Energies= -953.780219
Sum of electronic and thermal Energies= -953.765442
Sum of electronic and thermal Enthalpies= -953.764498
Sum of electronic and thermal Free Energies= -953.822723

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	152.311	52.228	122.545

C,0,-1.3957302161,-2.28226092,-0.6389462508
C,0,-0.031400523,-2.3026276419,-0.514598334
O,0,-0.8422529515,-0.31304615,-0.3599620916
C,0,-1.0165725014,0.2068072256,0.9281412618
N,0,-0.8604191267,1.4377588628,0.2770305077
S,0,0.7230336986,1.8867122091,0.0633365917
O,0,0.9616046946,2.1988439412,-1.3306218203
O,0,1.6423336042,0.9813608383,0.7420401877
C,0,-2.4094851039,-2.6505534796,0.384214854
C,0,0.6944273885,-2.6261461409,0.7451007646
C,0,0.8330987895,-2.061993074,-1.7041525825
C,0,0.7210881736,3.4226517196,0.9503866666
H,0,-1.7861260768,-2.1098533952,-1.6327487089
H,0,-0.2388353586,-0.1069375345,1.6216899986
H,0,-2.0223963901,0.0759637778,1.3175694288
H,0,-3.2516240175,-1.9605484715,0.3522997976
H,0,-2.0190520414,-2.6738591022,1.3975806728
H,0,-2.8102621133,-3.6418863339,0.1635120083
H,0,1.2554899264,-3.5529061242,0.608422938
H,0,0.0447088851,-2.7572856147,1.6045677703
H,0,1.4208929174,-1.8440187051,0.9654158075
H,0,1.5674710981,-1.288118405,-1.4849091037
H,0,0.2556392437,-1.7524584691,-2.570824953
H,0,1.3789845011,-2.9740962846,-1.9551500133
H,0,1.7080607526,3.8600834603,0.8241625774
H,0,0.5238011685,3.2331450103,2.0004269303
H,0,-0.0383966083,4.0685336365,0.5228573425

Epoxidation TS Isomer 5

B3LYP/6-31+G** (PCM)



Filename: b3BBgasPCMts5

E(RB+HF-LYP) = -954.242998697

Zero-point correction=	0.218724 (Hartree/Particle)
Thermal correction to Energy=	0.234261
Thermal correction to Enthalpy=	0.235205
Thermal correction to Gibbs Free Energy=	0.175171
Sum of electronic and zero-point Energies=	-954.024275
Sum of electronic and thermal Energies=	-954.008738
Sum of electronic and thermal Enthalpies=	-954.007794
Sum of electronic and thermal Free Energies=	-954.067828

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.001	54.342	126.352

C,0,0.1108120154,-2.3054608131,0.2337770058
C,0,1.4871808984,-2.3299871963,0.2997817695
O,0,0.5853582784,-0.2361418914,-0.1081486489
C,0,0.3902072652,0.1924042233,-1.4409811288
N,0,0.3986514147,1.4920979415,-0.8504667037
S,0,-1.1302607713,2.0439940159,-0.3493607514
O,0,-2.1993182785,1.029752722,-0.4851120101
O,0,-1.3193619968,3.3379877992,-1.0427265788
C,0,-0.8631982324,-2.1787255197,1.3620929244
C,0,2.2690121541,-2.1144373783,1.5619387702
C,0,2.3041189586,-2.653965012,-0.9195951607
C,0,-0.8673172415,2.3767289234,1.3956671488
H,0,-0.3351625223,-2.5466058134,-0.7323575846
H,0,-0.5466051242,-0.1635357901,-1.8829728964
H,0,1.2547943955,0.0394377572,-2.0939448212
H,0,-1.6669962996,-1.4902721378,1.0810271993
H,0,-0.4078903809,-1.8220969125,2.2879863146
H,0,-1.3255623526,-3.1542897396,1.564870034
H,0,2.7443239018,-3.0574341654,1.8659219454
H,0,1.6609643463,-1.7573515587,2.3935545031
H,0,3.0768276416,-1.3947908199,1.3874840657

```
 H,0,3.0418718092,-1.8664165299,-1.1165194872
 H,0,1.6868762022,-2.7931292925,-1.8111563021
 H,0,2.8734075302,-3.5780256218,-0.7504541589
 H,0,-1.7818050172,2.8443130942,1.7675054407
 H,0,-0.0177153421,3.0545515548,1.4879368771
 H,0,-0.6742362522,1.4293041612,1.8979442342
```

B3LYP/6-31+G** (gas phase)

```
Filename: b3BBgasPCMts5

E(RB+HF-LYP) = -954.227845538

 Zero-point correction=                           0.219272 (Hartree/Particle)
 Thermal correction to Energy=                    0.234710
 Thermal correction to Enthalpy=                  0.235654
 Thermal correction to Gibbs Free Energy=         0.175914
 Sum of electronic and zero-point Energies=           -954.008573
 Sum of electronic and thermal Energies=              -953.993136
 Sum of electronic and thermal Enthalpies=            -953.992191
 Sum of electronic and thermal Free Energies=         -954.051931

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 147.283             54.122            125.733

 C,0,0.131908584,-2.2345190426,0.1912259126
 C,0,1.509866642,-2.3634996096,0.276097853
 O,0,0.6411132347,-0.3210048176,-0.0515762454
 C,0,0.4324508683,0.2171776336,-1.3593354031
 N,0,0.3685179708,1.4937439248,-0.7537876542
 S,0,-1.2019002715,1.9511990518,-0.2922660929
 O,0,-2.1383713364,0.8093895773,-0.2052774299
 O,0,-1.5683596076,3.0947293842,-1.1467186134
 C,0,-0.8590397553,-2.1408329299,1.3086706674
 C,0,2.2777468182,-2.240329006,1.5576354855
 C,0,2.324794059,-2.6829180148,-0.9446584964
 C,0,-0.9017761963,2.5724129074,1.3691052308
 H,0,-0.3073089816,-2.4313041731,-0.7858158789
 H,0,-0.4781260666,-0.1764595583,-1.8269515584
 H,0,1.309008098,0.1188555773,-2.0078025587
 H,0,-1.623523594,-1.4012822506,1.0499016375
 H,0,-0.4056330073,-1.8542931492,2.2594660435
 H,0,-1.3572358617,-3.1097423234,1.445512569
 H,0,2.6955881153,-3.2180734928,1.8362670252
 H,0,1.6718862075,-1.8796531616,2.3887979289
 H,0,3.1252978453,-1.5584303534,1.4265882045
 H,0,3.1061834475,-1.9293499207,-1.1008509884
 H,0,1.714800285,-2.7500791442,-1.8491032222
 H,0,2.8403689761,-3.6434987112,-0.8090898144
 H,0,-1.8461843496,2.9908003358,1.722405814
 H,0,-0.1334648507,3.3434613303,1.3088366672
 H,0,-0.5796302731,1.7414059366,1.9964149172
```

B3LYP/6-31+G** (onsager)

```
Filename: b3BBonsts5
E(RB+HF-LYP) = -954.234256412
```

```
 Zero-point correction=                           0.219069 (Hartree/Particle)
 Thermal correction to Energy=                    0.234629
 Thermal correction to Enthalpy=                  0.235573
 Thermal correction to Gibbs Free Energy=         0.175341
 Sum of electronic and zero-point Energies=           -954.015187
 Sum of electronic and thermal Energies=              -953.999627
 Sum of electronic and thermal Enthalpies=            -953.998683
 Sum of electronic and thermal Free Energies=         -954.058915

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 147.232             54.291            126.768

 C,0,0.1230589575,-2.2761485955,0.228550411
 C,0,1.4989341223,-2.3228592835,0.3100927535
 O,0,0.5741314673,-0.2238634011,-0.1336967285
 C,0,0.3518270107,0.1998597304,-1.4625419675
 N,0,0.3696331505,1.508061536,-0.8967904038
 S,0,-1.1511755239,2.0542355788,-0.3582019184
 O,0,-2.2220281868,1.0447879901,-0.4947047933
 O,0,-1.3460375006,3.3741849497,-0.9915886135
 C,0,-0.8643554327,-2.1461838386,1.345160717
 C,0,2.2679406489,-2.1112317014,1.5794000169
 C,0,2.3238645444,-2.6627214241,-0.8986024558
 C,0,-0.8413345172,2.324613073,1.3946961281
 H,0,-0.3113851819,-2.5235813189,-0.7392071301
 H,0,-0.5943674989,-0.1617692611,-1.8808395861
 H,0,1.2032846184,0.0371129528,-2.1309013397
 H,0,-1.6730148146,-1.4708104287,1.0471477268
 H,0,-0.4190950975,-1.7715925557,2.2687580853
 H,0,-1.3130592945,-3.1247709621,1.561466978
 H,0,2.7252300139,-3.0586726348,1.8955168141
 H,0,1.6553890016,-1.7417432097,2.4018418407
 H,0,3.0893949702,-1.4059136068,1.4121821421
 H,0,3.0743512664,-1.8863327739,-1.090116664
 H,0,1.7153444455,-2.7991967869,-1.7963942091
 H,0,2.8792840643,-3.5928962628,-0.7205622217
 H,0,-1.7408003877,2.7874303927,1.8054946575
 H,0,0.0184422789,2.9884093522,1.4876068144
 H,0,-0.6444801245,1.35949949,1.8599259462
```

mPW1K/6-31+G** (PCM)

```
Filename:  mpBBgasPCMts5

E(RmPW+HF-PW91) = -954.050491961

Zero-point correction=                           0.226284 (Hartree/Particle)
 Thermal correction to Energy=                    0.241215
 Thermal correction to Enthalpy=                  0.242159
 Thermal correction to Gibbs Free Energy=         0.183728
 Sum of electronic and zero-point Energies=           -953.824208
 Sum of electronic and thermal Energies=              -953.809277
 Sum of electronic and thermal Enthalpies=            -953.808333
 Sum of electronic and thermal Free Energies=         -953.866764

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.365             52.521            122.980

 C,0,0.0858908911,-2.2458389567,0.2279766731
 C,0,1.4524581792,-2.2586880371,0.2955072873
 O,0,0.5838047492,-0.2642849699,-0.1090109986
```

```
 C,0,0.4052578401,0.1438320592,-1.433850518
 N,0,0.4151321632,1.4222941162,-0.8481537414
 S,0,-1.0670392238,1.9561028724,-0.3353484795
 O,0,-2.1146928131,0.9559584684,-0.50294184
 O,0,-1.2732471735,3.2536148687,-0.9649028919
 C,0,-0.8797516545,-2.0967380866,1.3449762896
 C,0,2.2247369676,-2.0168836848,1.5439228413
 C,0,2.2657699367,-2.5949205038,-0.907438387
 C,0,-0.8120873111,2.2217371491,1.388371377
 H,0,-0.3541764246,-2.5083505353,-0.72886483
 H,0,-0.5263893271,-0.2107203488,-1.8706612324
 H,0,1.2701267291,-0.0233895285,-2.0699526364
 H,0,-1.665754519,-1.4012893448,1.0556868686
 H,0,-0.4217348671,-1.741002365,2.2621635451
 H,0,-1.353322823,-3.056993926,1.5540247085
 H,0,2.696343582,-2.9475789855,1.8649359225
 H,0,1.6171337721,-1.6456137637,2.3610784811
 H,0,3.0250985576,-1.3030929391,1.3553171102
 H,0,2.9965584685,-1.8122034527,-1.111641544
 H,0,1.6537179323,-2.7496326296,-1.7920750179
 H,0,2.8326991941,-3.5087678974,-0.72204711
 H,0,-1.7210501085,2.6694632282,1.7797363737
 H,0,0.0289985735,2.8958044999,1.5095382203
 H,0,-0.6155042911,1.2650886934,1.8573455288
```

mPW1K/6-31+G** (gas phase)

```
Filename:  mpBBgasPCMts5

E(RmPW+HF-PW91) = -954.033993454

Zero-point correction=                           0.226828 (Hartree/Particle)
 Thermal correction to Energy=                    0.241693
 Thermal correction to Enthalpy=                  0.242638
 Thermal correction to Gibbs Free Energy=         0.184343
 Sum of electronic and zero-point Energies=           -953.807166
 Sum of electronic and thermal Energies=              -953.792300
 Sum of electronic and thermal Enthalpies=            -953.791356
 Sum of electronic and thermal Free Energies=         -953.849650

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.665             52.353            122.691

C,0,0.0960920267,-2.2128138404,0.1936093736
 C,0,1.4652167278,-2.2826882169,0.2783591771
 O,0,0.6249717018,-0.3340297778,-0.0683471735
 C,0,0.4317872638,0.1584987107,-1.3760650171
 N,0,0.3955418523,1.4177654696,-0.777569488
 S,0,-1.1209587135,1.881671132,-0.2898510648
 O,0,-2.0570260801,0.764699922,-0.2687519311
 O,0,-1.478327358,3.061417254,-1.0526890807
 C,0,-0.8890472808,-2.0884666945,1.2960102246
 C,0,2.2240717375,-2.1012093456,1.5446342932
 C,0,2.2837592862,-2.6074322999,-0.9240555428
 C,0,-0.8133121466,2.3848097879,1.3744112879
 H,0,-0.3340591338,-2.4380681865,-0.7749733249
 H,0,-0.4845849039,-0.2230260632,-1.8252806226
 H,0,1.3021661128,0.0278162628,-2.0141715309
 H,0,-1.6282452207,-1.3362076255,1.0246512668
 H,0,-0.4359882561,-1.8063970858,2.2406669074
 H,0,-1.4078579408,-3.0372150218,1.4367139013
 H,0,2.6733329354,-3.0503036114,1.8429572604
```

```
 H,0,1.6094298092,-1.7437467472,2.3622104977
 H,0,3.0380290282,-1.3944685612,1.3927943164
 H,0,3.0419363499,-1.8432104289,-1.0933136406
 H,0,1.6798474954,-2.709340435,-1.821549083
 H,0,2.8159576235,-3.5467136661,-0.7649650654
 H,0,-1.7430904172,2.7917900866,1.7594063577
 H,0,-0.0404790417,3.1448605198,1.3616772267
 H,0,-0.5001864573,1.5199144623,1.9471724746
```

mPW1K/6-31+G** (onsager)

```
Filename: mpBBonsts5
E(RmPW+HF-PW91) = -954.039594722

 Zero-point correction=                           0.226727 (Hartree/Particle)
 Thermal correction to Energy=                    0.241653
 Thermal correction to Enthalpy=                  0.242597
 Thermal correction to Gibbs Free Energy=         0.184108
 Sum of electronic and zero-point Energies=           -953.812868
 Sum of electronic and thermal Energies=              -953.797941
 Sum of electronic and thermal Enthalpies=            -953.796997
 Sum of electronic and thermal Free Energies=         -953.855487

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.640             52.434           123.101

 C,0,0.0974254632,-2.2186958761,0.2125859998
 C,0,1.4640428506,-2.2552215396,0.300917556
 O,0,0.5835612894,-0.2698348835,-0.1224547507
 C,0,0.3726670496,0.1478209906,-1.441458603
 N,0,0.3828763194,1.4306586968,-0.8765958244
 S,0,-1.0961686826,1.9443564982,-0.3288190534
 O,0,-2.1225642552,0.9179069933,-0.447978053
 O,0,-1.3462040049,3.2379543099,-0.940666198
 C,0,-0.8883494574,-2.073229243,1.3123758706
 C,0,2.2185695311,-2.0240638512,1.5610091198
 C,0,2.2900220414,-2.5996127681,-0.8903016102
 C,0,-0.7764992873,2.2156595141,1.3875130425
 H,0,-0.3270577483,-2.4804852116,-0.7493590534
 H,0,-0.5658350407,-0.2189160189,-1.8545722863
 H,0,1.2247605136,-0.0212444307,-2.0947474238
 H,0,-1.664006816,-1.3707973754,1.011658067
 H,0,-0.4422809876,-1.7250123625,2.2381526317
 H,0,-1.365986535,-3.0333256057,1.5104788529
 H,0,2.6761017593,-2.9592243897,1.8882002138
 H,0,1.601269172,-1.6498346047,2.3690157663
 H,0,3.0286808754,-1.3178822804,1.3879633019
 H,0,3.0341249726,-1.8266867158,-1.0812164798
 H,0,1.6897859333,-2.7446281901,-1.7843453001
 H,0,2.8415719498,-3.5214422868,-0.7005265322
 H,0,-1.6749379954,2.6503545853,1.8144060114
 H,0,0.0598187055,2.9000467949,1.4728909625
 H,0,-0.5464086156,1.2632842506,1.8495617721
```

B3LYP/6-31G* (gas phase)

```
E(RB+HF-LYP) =  -954.182691841

 Zero-point correction=                           0.221188 (Hartree/Particle)
 Thermal correction to Energy=                    0.236491
```

```
 Thermal correction to Enthalpy=                  0.237435
 Thermal correction to Gibbs Free Energy=         0.177442
 Sum of electronic and zero-point Energies=           -953.961503
 Sum of electronic and thermal Energies=              -953.946201
 Sum of electronic and thermal Enthalpies=            -953.945256
 Sum of electronic and thermal Free Energies=         -954.005250

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                148.401             53.568            126.267

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0    C   -1.960999    0.585401   -0.781160
    2          6             0    C   -2.883078   -0.092111   -0.001880
    3          8             0    O   -0.619763   -0.249275    0.398056
    4          6             0    C    0.061087   -1.346267   -0.186802
    5          7             0    N    1.148107   -1.030666    0.666045
    6         16             0    S    2.284823   -0.020991   -0.083546
    7          8             0    O    1.679249    1.020512   -0.934726
    8          8             0    O    3.307829   -0.894765   -0.683779
    9          6             0    C   -1.564695    2.027216   -0.695500
   10          6             0    C   -3.532618    0.493734    1.215785
   11          6             0    C   -3.320306   -1.481963   -0.369610
   12          6             0    C    2.997723    0.764392    1.366860
   13          1             0    H   -1.660150    0.093853   -1.705241
   14          1             0    H    0.198980   -1.231976   -1.270596
   15          1             0    H   -0.383773   -2.317815    0.057175
   16          1             0    H   -0.485914    2.105973   -0.861014
   17          1             0    H   -1.804401    2.479487    0.269469
   18          1             0    H   -2.075894    2.601433   -1.479982
   19          1             0    H   -4.604181    0.653093    1.022807
   20          1             0    H   -3.099046    1.447969    1.517396
   21          1             0    H   -3.466552   -0.200396    2.062177
   22          1             0    H   -3.152383   -2.179114    0.461588
   23          1             0    H   -2.800413   -1.862340   -1.253344
   24          1             0    H   -4.400196   -1.499412   -0.575682
   25          1             0    H    3.798048    1.417423    1.011924
   26          1             0    H    3.397117   -0.012703    2.019952
   27          1             0    H    2.223635    1.340851    1.875212
 ---------------------------------------------------------------------
```

B3LYP/6-31G* (Onsager)

```
E(RB+HF-LYP) =  -954.188848791

 Zero-point correction=                           0.221157 (Hartree/Particle)
 Thermal correction to Energy=                    0.236431
 Thermal correction to Enthalpy=                  0.237375
 Thermal correction to Gibbs Free Energy=         0.178220
 Sum of electronic and zero-point Energies=           -953.967691
 Sum of electronic and thermal Energies=              -953.952418
 Sum of electronic and thermal Enthalpies=            -953.951474
 Sum of electronic and thermal Free Energies=         -954.010629

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                148.363             53.662            124.502

    1          6             0    C   -2.038785    0.563913   -0.882810
```

2	6	0	C	-2.811827	-0.070151	0.070358
3	8	0	O	-0.561826	-0.348965	0.223142
4	6	0	C	0.098264	-1.404796	-0.451084
5	7	0	N	1.153138	-1.198548	0.477747
6	16	0	S	2.283660	-0.038804	-0.023227
7	8	0	O	1.890318	0.677629	-1.253116
8	8	0	O	3.596996	-0.706010	0.009697
9	6	0	C	-1.549510	1.977730	-0.893352
10	6	0	C	-3.181531	0.543002	1.387357
11	6	0	C	-3.381886	-1.434090	-0.195907
12	6	0	C	2.220502	1.124325	1.349903
13	1	0	H	-1.909870	0.034258	-1.826034
14	1	0	H	0.292219	-1.183288	-1.507079
15	1	0	H	-0.377437	-2.381938	-0.312211
16	1	0	H	-0.507658	1.997947	-1.231377
17	1	0	H	-1.608415	2.458625	0.085725
18	1	0	H	-2.144259	2.573750	-1.598864
19	1	0	H	-4.262964	0.736811	1.417554
20	1	0	H	-2.663979	1.481932	1.588367
21	1	0	H	-2.963366	-0.154846	2.204172
22	1	0	H	-3.095100	-2.138917	0.594508
23	1	0	H	-3.065424	-1.838639	-1.161640
24	1	0	H	-4.479735	-1.389820	-0.189472
25	1	0	H	3.000643	1.869789	1.178511
26	1	0	H	2.405715	0.576546	2.274941
27	1	0	H	1.233832	1.587656	1.365740

HF/6-31G* (gas phase)

E(RHF) = -950.073474341

Zero-point correction= 0.237797 (Hartree/Particle)
Thermal correction to Energy= 0.252040
Thermal correction to Enthalpy= 0.252984
Thermal correction to Gibbs Free Energy= 0.196042
Sum of electronic and zero-point Energies= -949.835677
Sum of electronic and thermal Energies= -949.821434
Sum of electronic and thermal Enthalpies= -949.820490
Sum of electronic and thermal Free Energies= -949.877432

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	158.158	50.161	119.844

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.982067	0.649585	-0.853506
2	6	0	-2.723884	-0.085141	0.025062
3	8	0	-0.617693	-0.250602	0.281346
4	6	0	0.066399	-1.410792	-0.232488
5	7	0	1.099499	-1.063986	0.605220
6	16	0	2.230522	-0.073611	-0.047774
7	8	0	1.736634	0.580999	-1.237159
8	8	0	3.471696	-0.788134	-0.151230
9	6	0	-1.540372	2.076264	-0.737192
10	6	0	-3.179292	0.404801	1.370256
11	6	0	-3.248016	-1.440600	-0.369304
12	6	0	2.425756	1.149581	1.212994
13	1	0	-1.792923	0.205081	-1.815143
14	1	0	0.197787	-1.330744	-1.300040

15	1	0	-0.436269	-2.316346	0.065977
16	1	0	-0.507978	2.150863	-1.055382
17	1	0	-1.623408	2.463552	0.268209
18	1	0	-2.143139	2.698836	-1.393257
19	1	0	-4.251381	0.586104	1.345521
20	1	0	-2.686709	1.313500	1.679228
21	1	0	-2.994819	-0.354391	2.122023
22	1	0	-3.011100	-2.183730	0.384805
23	1	0	-2.856175	-1.771653	-1.322865
24	1	0	-4.331764	-1.400100	-0.446507
25	1	0	3.213667	1.816900	0.890166
26	1	0	2.705200	0.659072	2.133604
27	1	0	1.497916	1.688448	1.332913

BP86/6-31G* (gas phase)

E(RB-P86) = -954.232449721

Zero-point correction= 0.214083 (Hartree/Particle)
Thermal correction to Energy= 0.229789
Thermal correction to Enthalpy= 0.230733
Thermal correction to Gibbs Free Energy= 0.170236
Sum of electronic and zero-point Energies= -954.018366
Sum of electronic and thermal Energies= -954.002660
Sum of electronic and thermal Enthalpies= -954.001716
Sum of electronic and thermal Free Energies= -954.062214

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	144.195	55.177	127.328

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.968122	0.571492	-0.836760
2	6	0	-2.870049	-0.067606	0.008702
3	8	0	-0.582914	-0.300166	0.354820
4	6	0	0.075635	-1.423247	-0.213835
5	7	0	1.148087	-1.093317	0.681311
6	16	0	2.295466	-0.045687	-0.064412
7	8	0	1.764806	0.699674	-1.241782
8	8	0	3.525469	-0.867059	-0.225823
9	6	0	-1.506122	1.997971	-0.785465
10	6	0	-3.401529	0.545011	1.274589
11	6	0	-3.393132	-1.439011	-0.330188
12	6	0	2.567627	1.137362	1.278912
13	1	0	-1.726805	0.047591	-1.772521
14	1	0	0.254741	-1.322944	-1.302608
15	1	0	-0.382248	-2.397232	0.042586
16	1	0	-0.436228	2.039279	-1.053679
17	1	0	-1.640576	2.458474	0.206563
18	1	0	-2.065972	2.606248	-1.522768
19	1	0	-4.483440	0.764175	1.168442
20	1	0	-2.890862	1.479998	1.548902
21	1	0	-3.305503	-0.162941	2.118240
22	1	0	-3.187849	-2.157971	0.485772
23	1	0	-2.960877	-1.835289	-1.264257
24	1	0	-4.495120	-1.412421	-0.448889
25	1	0	3.375551	1.811748	0.954993
26	1	0	2.862211	0.580529	2.180132

```
  27          1              0        1.634170    1.693553    1.447060
 -------------------------------------------------------------------
```

MPW1K/6-31+G* (gas phase)

```
E(RmPW+HF-PW91) =  -954.006944332

 Zero-point correction=                           0.227969 (Hartree/Particle)
 Thermal correction to Energy=                    0.242801
 Thermal correction to Enthalpy=                  0.243745
 Thermal correction to Gibbs Free Energy=         0.185520
 Sum of electronic and zero-point Energies=           -953.778975
 Sum of electronic and thermal Energies=              -953.764143
 Sum of electronic and thermal Enthalpies=            -953.763199
 Sum of electronic and thermal Free Energies=         -953.821424

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 152.360             52.162            122.545

 C,0,0.094803248,-2.2105402933,0.1977319831
 C,0,1.463745754,-2.2861068245,0.2775874953
 O,0,0.6212287647,-0.3330134284,-0.0615588268
 C,0,0.4412794812,0.1605290005,-1.3696887539
 N,0,0.4002017734,1.4191818076,-0.7706661233
 S,0,-1.1198975917,1.8866921505,-0.2978975553
 O,0,-2.0598573026,0.7734831778,-0.2866055683
 O,0,-1.4648693255,3.0688388642,-1.0624799149
 C,0,-0.8861416696,-2.0894449586,1.3051345371
 C,0,2.229551829,-2.1096183169,1.5407229168
 C,0,2.2773121594,-2.6077820334,-0.9293990036
 C,0,-0.8259985995,2.3872558432,1.3705661231
 H,0,-0.3412149197,-2.4322365353,-0.7692964313
 H,0,-0.4697456594,-0.2207479697,-1.8293475709
 H,0,1.3181864825,0.0294445398,-1.9985148655
 H,0,-1.6401191262,-1.3520961967,1.0325813939
 H,0,-0.4324094708,-1.7901291041,2.2449948815
 H,0,-1.3899509149,-3.0452233116,1.4599828906
 H,0,2.6814265103,-3.0600479289,1.8342019514
 H,0,1.6203108327,-1.755219261,2.3646564306
 H,0,3.0436154288,-1.4018071466,1.3883195681
 H,0,3.0352464454,-1.8427496287,-1.1015127109
 H,0,1.6699477789,-2.707725203,-1.8258888694
 H,0,2.8115482404,-3.5479443175,-0.7763602012
 H,0,-1.7577934611,2.7973440174,1.7497291946
 H,0,-0.0505593162,3.1457943351,1.3686090031
 H,0,-0.5208701037,1.5217732392,1.9480917757
```

MPW1K/6-31+G* (Onsager)

```
E(RmPW+HF-PW91) =  -954.013090273

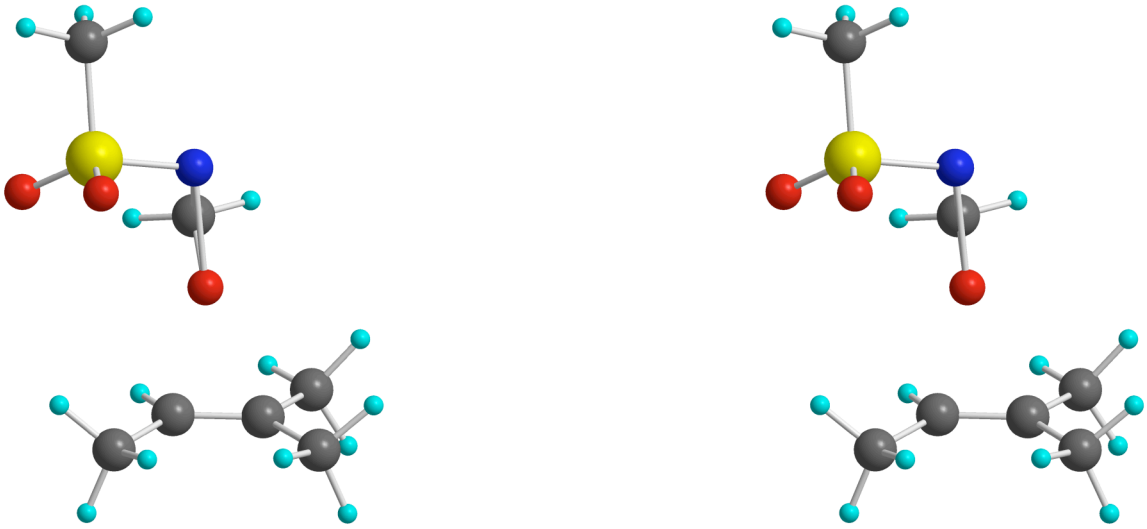
 Zero-point correction=                           0.227852 (Hartree/Particle)
 Thermal correction to Energy=                    0.242746
 Thermal correction to Enthalpy=                  0.243690
 Thermal correction to Gibbs Free Energy=         0.185301
 Sum of electronic and zero-point Energies=           -953.785238
 Sum of electronic and thermal Energies=              -953.770344
 Sum of electronic and thermal Enthalpies=            -953.769400
 Sum of electronic and thermal Free Energies=         -953.827790
```

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	152.325	52.254	122.891

C,0,0.0919871522,-2.2584282026,0.2359217998
C,0,1.4583222077,-2.2946141877,0.3192702559
O,0,0.5713237483,-0.3011744846,-0.1016027724
C,0,0.3709976379,0.1116020504,-1.4216586243
N,0,0.3833716912,1.3951811815,-0.8572893151
S,0,-1.0956216478,1.9207446945,-0.3211589094
O,0,-2.133675648,0.9092807852,-0.4596473023
O,0,-1.3221686733,3.2227370524,-0.9247322738
C,0,-0.8896046423,-2.1160335607,1.3407084288
C,0,2.2191642621,-2.0638174698,1.5760042597
C,0,2.2805630677,-2.6357469456,-0.8758718723
C,0,-0.7917493485,2.1753916029,1.4015695543
H,0,-0.3377729555,-2.5195289861,-0.7241934765
H,0,-0.5655845765,-0.2519085635,-1.8412256463
H,0,1.2270137831,-0.0619369941,-2.06838277
H,0,-1.6810278797,-1.4311102413,1.0390352396
H,0,-0.4441759599,-1.7489385966,2.2603386867
H,0,-1.350122638,-3.0822142843,1.554583267
H,0,2.6800516152,-2.9990194264,1.9013113426
H,0,1.6066631034,-1.6907449801,2.3892365274
H,0,3.0288237961,-1.3564022702,1.4005445857
H,0,3.0214793469,-1.8596871647,-1.0713019592
H,0,1.6773759936,-2.7832991888,-1.7686474873
H,0,2.837714394,-3.5559903574,-0.6900087119
H,0,-1.6881752203,2.6215292567,1.8230846684
H,0,0.0541301999,2.8467146725,1.5040777867
H,0,-0.5819659131,1.2174871961,1.8633116778

Epoxidation TS Isomer 6

B3LYP/6-31+G** (PCM)



Filename: b3BBgasPCMts6 (PCM)

E(RB+HF-LYP) = -954.240463788

Zero-point correction= 0.218506 (Hartree/Particle)
Thermal correction to Energy= 0.234125

```
 Thermal correction to Enthalpy=                  0.235069
 Thermal correction to Gibbs Free Energy=         0.174589
 Sum of electronic and zero-point Energies=           -954.021958
 Sum of electronic and thermal Energies=              -954.006339
 Sum of electronic and thermal Enthalpies=            -954.005395
 Sum of electronic and thermal Free Energies=         -954.065875

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 146.915             54.434            127.290

 C,0,0.6398449124,-2.2670126429,-0.2721608932
 C,0,1.9804781418,-1.9909381082,-0.1282854494
 O,0,0.605195674,-0.1100532856,-0.0064619684
 C,0,0.3909080899,0.6309895408,-1.1898166179
 N,0,0.0407687076,1.6513502233,-0.2576619711
 S,0,-1.597416172,1.6226616076,0.2329043102
 O,0,-1.6560779127,1.5334055303,1.7033366229
 O,0,-2.4109133922,0.6723732809,-0.5600427705
 C,0,-0.3282307175,-2.6851328678,0.7901589614
 C,0,2.6910988556,-1.9638798116,1.1934410562
 C,0,2.84903635,-1.7722295393,-1.3363017095
 C,0,-2.0636822209,3.2988943139,-0.2369952001
 H,0,0.2600814457,-2.3267843531,-1.2934172198
 H,0,-0.4015239256,0.2241022576,-1.8271380861
 H,0,1.3041581492,0.8790492155,-1.7395460224
 H,0,-1.2941712807,-2.1968931676,0.6303524693
 H,0,0.011998474,-2.4485032563,1.7997846557
 H,0,-0.4964259418,-3.7694873927,0.7319979174
 H,0,3.3418871632,-2.8453546378,1.2800890433
 H,0,2.0126444475,-1.9564197714,2.0468408893
 H,0,3.3395238309,-1.0831166464,1.2586629779
 H,0,3.3861577412,-0.8182955552,-1.2660979374
 H,0,2.2777910632,-1.7914162011,-2.2682788255
 H,0,3.6161740033,-2.5567166133,-1.3898097648
 H,0,-3.0973644589,3.4323444509,0.0918392573
 H,0,-1.9871721515,3.3979730205,-1.3208607084
 H,0,-1.4011818758,3.9983014091,0.2744139834
```

B3LYP/6-31+G** (gas phase)

```
Filename: b3BBgasPCMts6 (gas)

E(RB+HF-LYP) = -954.226181066

 Zero-point correction=                           0.219050 (Hartree/Particle)
 Thermal correction to Energy=                    0.234576
 Thermal correction to Enthalpy=                  0.235520
 Thermal correction to Gibbs Free Energy=         0.175268
 Sum of electronic and zero-point Energies=           -954.007131
 Sum of electronic and thermal Energies=              -953.991605
 Sum of electronic and thermal Enthalpies=            -953.990661
 Sum of electronic and thermal Free Energies=         -954.050913

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 147.199             54.247            126.813

 C,0,0.6235330199,-2.1735661367,-0.2821284312
 C,0,1.982066789,-1.9693288856,-0.1254848462
 O,0,0.6980173822,-0.1312872258,-0.081814653
 C,0,0.4263674608,0.63356962,-1.2529415136
 N,0,0.0636242624,1.6671049282,-0.3571243736
```

S,0,-1.5455716066,1.5295134544,0.2144191882
O,0,-1.5454825657,1.3645723418,1.6743673296
O,0,-2.3401691959,0.5938057819,-0.6134594163
C,0,-0.3815788523,-2.5252152502,0.7696981827
C,0,2.6665959764,-1.9308184281,1.2086492406
C,0,2.877809501,-1.834211614,-1.3251703607
C,0,-2.1027002195,3.2094839329,-0.1405115069
H,0,0.2638480594,-2.2545943239,-1.3073867471
H,0,-0.3636757533,0.1918167567,-1.8717550988
H,0,1.3250610258,0.8909675024,-1.8235261931
H,0,-1.3246583453,-2.0100442,0.5671765346
H,0,-0.0578518346,-2.2543485508,1.7754953071
H,0,-0.5785898034,-3.6058908668,0.7482481633
H,0,3.259273285,-2.8459585531,1.3487268518
H,0,1.970321985,-1.8427099605,2.0423625745
H,0,3.3637168669,-1.087355724,1.2527625993
H,0,3.4524153452,-0.901235503,-1.2804375525
H,0,2.3211925241,-1.8618475,-2.2656531433
H,0,3.6111275011,-2.6519969508,-1.3393105966
H,0,-3.118918334,3.2820472322,0.2527759587
H,0,-2.0931283705,3.3705202612,-1.2189620072
H,0,-1.4390591031,3.9062188618,0.3719315097

B3LYP/6-31+G** (Onsager)

b3BBonsts6
E(RB+HF-LYP) = -954.228987424

Zero-point correction=	0.218981 (Hartree/Particle)
Thermal correction to Energy=	0.234575
Thermal correction to Enthalpy=	0.235520
Thermal correction to Gibbs Free Energy=	0.174923
Sum of electronic and zero-point Energies=	-954.010007
Sum of electronic and thermal Energies=	-953.994412
Sum of electronic and thermal Enthalpies=	-953.993468
Sum of electronic and thermal Free Energies=	-954.054065

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.198	54.331	127.537

C,0,0.6347865109,-2.2251905115,-0.2742281536
C,0,1.9857332411,-1.9862061092,-0.133800452
O,0,0.6278336261,-0.1306129363,-0.0048227781
C,0,0.4026474982,0.6375155738,-1.1726166409
N,0,0.0417721532,1.6532486459,-0.2462912111
S,0,-1.593600932,1.5886069461,0.2469622791
O,0,-1.6666827204,1.5201023269,1.7140156946
O,0,-2.3909353928,0.6362013892,-0.5565915418
C,0,-0.3436581192,-2.6284665966,0.7850374824
C,0,2.6951837404,-1.9702265331,1.1880174409
C,0,2.8563914528,-1.7890240996,-1.3430591013
C,0,-2.0762670038,3.2629420798,-0.2365609197
H,0,0.2572233592,-2.2813535441,-1.2945454693
H,0,-0.3845600984,0.2272035903,-1.8153438164
H,0,1.3157507102,0.8938556438,-1.7190714954
H,0,-1.2987793742,-2.1216032654,0.6201645635
H,0,-0.0016258769,-2.390186462,1.7934246303
H,0,-0.5256302549,-3.7105325145,0.7301175628
H,0,3.3286776772,-2.8635264667,1.2782416769
H,0,2.0144458245,-1.944930202,2.0388752243
H,0,3.3593401334,-1.1016837733,1.2512831268
H,0,3.4130778798,-0.8465498367,-1.2764435241

```
 H,0,2.2855698643,-1.7994501838,-2.2750398104
 H,0,3.6075776377,-2.5881711868,-1.3972859523
 H,0,-3.1090853739,3.3902942264,0.0952389016
 H,0,-2.0054384474,3.3568534234,-1.3208200315
 H,0,-1.4161607151,3.9701003759,0.2660893146
```

mPW1K/6-31+G** (PCM)

```
Filename: mpBBgasPCMts6

E(RmPW+HF-PW91) = -954.048261701

Zero-point correction=                           0.226045 (Hartree/Particle)
 Thermal correction to Energy=                    0.241079
 Thermal correction to Enthalpy=                  0.242023
 Thermal correction to Gibbs Free Energy=         0.182983
 Sum of electronic and zero-point Energies=           -953.822217
 Sum of electronic and thermal Energies=              -953.807182
 Sum of electronic and thermal Enthalpies=            -953.806238
 Sum of electronic and thermal Free Energies=         -953.865279

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.279             52.606           124.262

C,0,0.6054638376,-2.2104448343,-0.293192748
 C,0,1.9362254208,-1.9378424686,-0.1388571494
 O,0,0.6244118264,-0.1493433824,-0.0030500281
 C,0,0.4172712582,0.5955334411,-1.1663288607
 N,0,0.0882964263,1.5891723269,-0.228965875
 S,0,-1.4933269245,1.5675853522,0.2744720344
 O,0,-1.5276906609,1.5418741861,1.7263537666
 O,0,-2.2867512961,0.5772531126,-0.4448873293
 C,0,-0.3625576494,-2.6197340844,0.7556168556
 C,0,2.6295763245,-1.9137246654,1.1777663289
 C,0,2.8070475442,-1.7184989978,-1.3291252899
 C,0,-2.012360533,3.175754153,-0.2456169312
 H,0,0.2371538883,-2.2697696373,-1.3126364019
 H,0,-0.3790208442,0.2004534519,-1.7947903324
 H,0,1.3270656501,0.8296026553,-1.7124941485
 H,0,-1.309170224,-2.106655157,0.6031708956
 H,0,-0.0170325167,-2.4043666695,1.7610547487
 H,0,-0.5528526236,-3.6917743477,0.6824139483
 H,0,3.2616542817,-2.7989874373,1.2720154764
 H,0,1.9467820833,-1.8916543705,2.0191150097
 H,0,3.2838419574,-1.0459843616,1.241926506
 H,0,3.3425709963,-0.7722821294,-1.2493738486
 H,0,2.2468780078,-1.7339759211,-2.2604071495
 H,0,3.566237842,-2.5011409035,-1.3765125273
 H,0,-3.0371200116,3.2992044812,0.0947129489
 H,0,-1.9620838105,3.2340142489,-1.3277451824
 H,0,-1.3669232507,3.9149429586,0.2163122833
```

mPW1K/6-31+G** (gas phase)

```
Filename: mpBBgasPCMts6

E(RmPW+HF-PW91) = -954.033081677

Zero-point correction=                           0.226524 (Hartree/Particle)
 Thermal correction to Energy=                    0.241537
 Thermal correction to Enthalpy=                  0.242481
```

```
 Thermal correction to Gibbs Free Energy=         0.183394
 Sum of electronic and zero-point Energies=           -953.806558
 Sum of electronic and thermal Energies=              -953.791544
 Sum of electronic and thermal Enthalpies=            -953.790600
 Sum of electronic and thermal Free Energies=         -953.849687

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.567             52.477            124.359

 C,0,0.5948565742,-2.1479575631,-0.3041629011
 C,0,1.9357581503,-1.9183967355,-0.1337656344
 O,0,0.7044013123,-0.1545456348,-0.0864450559
 C,0,0.443342206,0.5947891259,-1.2476751912
 N,0,0.1111844368,1.6047847206,-0.3429434468
 S,0,-1.4394467472,1.4784811229,0.251102486
 O,0,-1.4060987708,1.3619774245,1.6928848348
 O,0,-2.2200400608,0.5107023672,-0.5109394664
 C,0,-0.412926731,-2.4840764742,0.7325089332
 C,0,2.5979266427,-1.8627786396,1.1977174532
 C,0,2.8368430195,-1.7772234738,-1.3133919061
 C,0,-2.0404142059,3.0981040688,-0.1362133392
 H,0,0.2497782603,-2.2345879123,-1.3279620033
 H,0,-0.3564284262,0.1643720758,-1.8496961918
 H,0,1.3374517038,0.8324390045,-1.8190377287
 H,0,-1.336292116,-1.9466529655,0.5297104495
 H,0,-0.0887220462,-2.2276027365,1.734852927
 H,0,-0.631345523,-3.5526762194,0.7019825039
 H,0,3.1709174519,-2.7775679947,1.3619198585
 H,0,1.894018474,-1.7480909229,2.0133601856
 H,0,3.2987344746,-1.0311972395,1.2333621272
 H,0,3.3930141959,-0.8413267613,-1.2641836578
 H,0,2.295810643,-1.8180075159,-2.2551114231
 H,0,3.5757991081,-2.5801656184,-1.3120804197
 H,0,-3.0436759283,3.1629390156,0.2743832236
 H,0,-2.0608835234,3.2263138079,-1.2125894059
 H,0,-1.3899755744,3.8271626738,0.3333597889
```

mPW1K/6-31+G** (onsager)

```
Filename: mpBBonsts6
E(RmPW+HF-PW91) = -954.036022137

 Zero-point correction=                           0.226533 (Hartree/Particle)
 Thermal correction to Energy=                    0.241557
 Thermal correction to Enthalpy=                  0.242501
 Thermal correction to Gibbs Free Energy=         0.183376
 Sum of electronic and zero-point Energies=           -953.809489
 Sum of electronic and thermal Energies=              -953.794465
 Sum of electronic and thermal Enthalpies=            -953.793521
 Sum of electronic and thermal Free Energies=         -953.852646

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.579             52.519            124.439

 C,0,0.6007163854,-2.1738401941,-0.2946110698
 C,0,1.9401699492,-1.9348817527,-0.1431670608
 O,0,0.6501289667,-0.1570224552,-0.0043927316
 C,0,0.4304344969,0.6070361119,-1.1562232423
 N,0,0.0938867202,1.5964980035,-0.223424999
 S,0,-1.4840253349,1.5355212113,0.2901797563
 O,0,-1.5265033881,1.5292501634,1.7377165195
```

O,0,-2.2583752653,0.538157458,-0.4368909944
C,0,-0.3799131978,-2.563641109,0.7503642799
C,0,2.6322184588,-1.9204071417,1.1738843381
C,0,2.8138027965,-1.7364134717,-1.3345560325
C,0,-2.0275457187,3.1371284662,-0.2430866376
H,0,0.2348961433,-2.2288289334,-1.3132014685
H,0,-0.3630249134,0.2056543875,-1.7853197048
H,0,1.3385907068,0.8479221219,-1.7024324527
H,0,-1.3143872639,-2.0313182262,0.5895256936
H,0,-0.0343427454,-2.3442952621,1.7547071783
H,0,-0.5854189751,-3.6330245597,0.6829085312
H,0,3.2488895515,-2.8157371746,1.2718379015
H,0,1.9468976392,-1.882090299,2.0122343828
H,0,3.2997485617,-1.0632663172,1.236802276
H,0,3.3672629813,-0.8006937093,-1.2586632312
H,0,2.2544830698,-1.7441678499,-2.2660650617
H,0,3.5581147005,-2.5326104513,-1.3826872581
H,0,-3.0508042888,3.2499155641,0.1030990095
H,0,-1.9857802925,3.1883090518,-1.3254544363
H,0,-1.3865357438,3.8860553675,0.2078645145

B3LYP/6-31G* (gas phase)

E(RB+HF-LYP) = -954.181440932

Zero-point correction= 0.220966 (Hartree/Particle)
Thermal correction to Energy= 0.236356
Thermal correction to Enthalpy= 0.237300
Thermal correction to Gibbs Free Energy= 0.177177
Sum of electronic and zero-point Energies= -953.960475
Sum of electronic and thermal Energies= -953.945085
Sum of electronic and thermal Enthalpies= -953.944141
Sum of electronic and thermal Free Energies= -954.004263

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	148.316	53.682	126.539

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	1.898459	0.696101	0.715720
2	6	0	C	2.818584	-0.113575	0.074144
3	8	0	O	0.590016	-0.231573	-0.447230
4	6	0	C	-0.058653	-1.414659	-0.005735
5	7	0	N	-1.154886	-0.983422	-0.793261
6	16	0	S	-2.153045	0.121812	0.049404
7	8	0	O	-1.999913	1.483588	-0.482745
8	8	0	O	-2.063127	-0.083237	1.509456
9	6	0	C	1.557208	2.119600	0.393212
10	6	0	C	3.510120	0.259923	-1.203869
11	6	0	C	3.221592	-1.431990	0.673716
12	6	0	C	-3.748303	-0.501564	-0.515329
13	1	0	H	1.533900	0.349833	1.681743
14	1	0	H	-0.194626	-1.455432	1.081789
15	1	0	H	0.390357	-2.330816	-0.406080
16	1	0	H	0.476554	2.268121	0.471838
17	1	0	H	1.865583	2.414339	-0.611937
18	1	0	H	2.049096	2.788154	1.112740
19	1	0	H	4.565224	0.499803	-1.004154
20	1	0	H	3.054820	1.117012	-1.701281

21	1	0	H	3.506608	-0.584376	-1.903271
22	1	0	H	3.054498	-2.257635	-0.030404
23	1	0	H	2.685953	-1.650469	1.602150
24	1	0	H	4.298739	-1.430615	0.895264
25	1	0	H	-4.507706	0.161084	-0.093326
26	1	0	H	-3.886300	-1.521992	-0.154472
27	1	0	H	-3.769622	-0.465296	-1.605243

MPW1K/6-31+G* (gas phase)

```
E(RmPW+HF-PW91) =  -954.006055041

 Zero-point correction=                           0.227694 (Hartree/Particle)
 Thermal correction to Energy=                    0.242650
 Thermal correction to Enthalpy=                  0.243594
 Thermal correction to Gibbs Free Energy=         0.184754
 Sum of electronic and zero-point Energies=           -953.778361
 Sum of electronic and thermal Energies=              -953.763405
 Sum of electronic and thermal Enthalpies=            -953.762461
 Sum of electronic and thermal Free Energies=         -953.821301

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 152.265             52.281            123.840

 C,0,0.5927342553,-2.1475392776,-0.2981227551
 C,0,1.9348246251,-1.9213349157,-0.133825654
 O,0,0.6979291027,-0.156473712,-0.0794502728
 C,0,0.4495715887,0.5960582697,-1.2402701017
 N,0,0.1073474234,1.6031877938,-0.3364498298
 S,0,-1.4497772587,1.476502139,0.2401061167
 O,0,-1.4325214856,1.3466832466,1.6809064035
 O,0,-2.2265863847,0.5202553596,-0.5394156732
 C,0,-0.4105675183,-2.4859165349,0.7431465678
 C,0,2.6053270665,-1.8682749633,1.1938685644
 C,0,2.8300681855,-1.77634753,-1.3178358409
 C,0,-2.0385103888,3.1035298514,-0.1385853359
 H,0,0.2410758159,-2.232743911,-1.320080499
 H,0,-0.3422106813,0.1672316167,-1.8534219682
 H,0,1.3501640881,0.8350886352,-1.8005043942
 H,0,-1.342728865,-1.9647523255,0.5356691469
 H,0,-0.0905660473,-2.2129355693,1.7432557021
 H,0,-0.6144798574,-3.5586757231,0.7261834606
 H,0,3.1917065566,-2.777434452,1.3478617507
 H,0,1.9068615633,-1.7690511923,2.0171255051
 H,0,3.2970672716,-1.0280895013,1.2324543395
 H,0,3.3870331156,-0.8398760304,-1.2700593789
 H,0,2.284417868,-1.813826933,-2.2580748244
 H,0,3.5703084963,-2.5792885317,-1.324516275
 H,0,-3.0474838183,3.1713428777,0.2595204137
 H,0,-2.0457523898,3.2447132032,-1.2142448197
 H,0,-1.3916656838,3.8271805048,0.3457064554
```

MPW1K/6-31+G* (gas phase)

```
E(RmPW+HF-PW91) =  -954.009042478

 Zero-point correction=                           0.227673 (Hartree/Particle)
 Thermal correction to Energy=                    0.242653
 Thermal correction to Enthalpy=                  0.243597
```

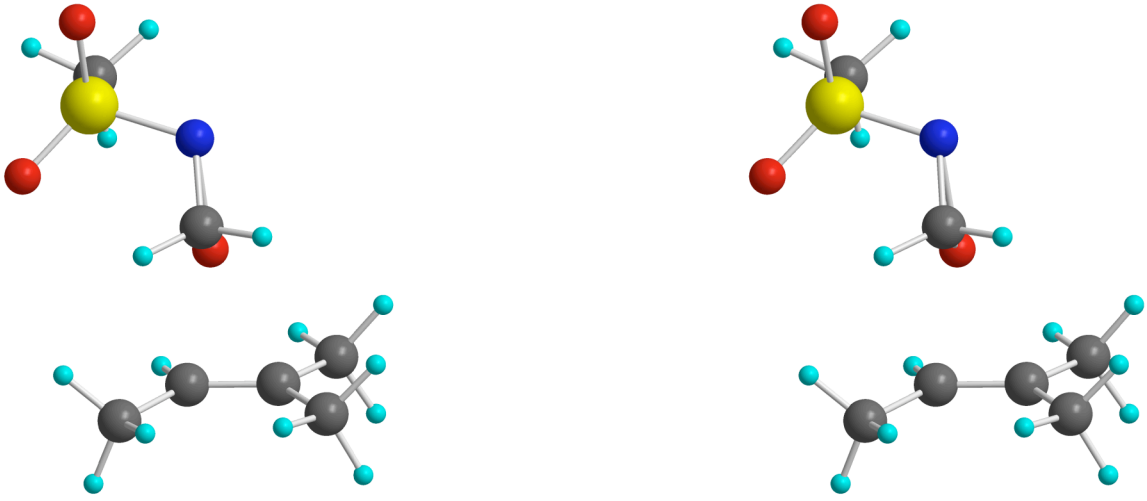
```
 Thermal correction to Gibbs Free Energy=         0.184608
 Sum of electronic and zero-point Energies=           -953.781370
 Sum of electronic and thermal Energies=              -953.766390
 Sum of electronic and thermal Enthalpies=            -953.765446
 Sum of electronic and thermal Free Energies=         -953.824434

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 152.267             52.325           124.152

 C,0,0.6174844469,-2.1906087897,-0.3173255402
 C,0,1.957509763,-1.9539359498,-0.1695508458
 O,0,0.662860715,-0.1748918815,-0.0246883465
 C,0,0.4523615288,0.5915625972,-1.1754824734
 N,0,0.1084557115,1.5783254824,-0.2427839532
 S,0,-1.472946685,1.5171328866,0.2594638113
 O,0,-1.5255975024,1.5057545394,1.7065004077
 O,0,-2.2447236296,0.5251718922,-0.4769851809
 C,0,-0.3610466592,-2.5819084889,0.729915748
 C,0,2.6548810374,-1.9406999353,1.14504687
 C,0,2.8276893604,-1.752558816,-1.3633897348
 C,0,-2.0085735131,3.1230122243,-0.2716569868
 H,0,0.247160529,-2.2444356298,-1.3346455993
 H,0,-0.3347813179,0.1914544511,-1.812845204
 H,0,1.3650503236,0.8337092781,-1.7132108619
 H,0,-1.3019750501,-2.0613319045,0.5642054844
 H,0,-0.0200695303,-2.3505428443,1.7339199259
 H,0,-0.5560053796,-3.6548127454,0.6720056464
 H,0,3.2785689346,-2.8327905559,1.2380676889
 H,0,1.9737084889,-1.9102912555,1.9880733459
 H,0,3.3181119499,-1.079267559,1.2099525381
 H,0,3.3815728127,-0.8160565896,-1.2884751366
 H,0,2.2656717074,-1.7578947015,-2.2943451091
 H,0,3.5732437814,-2.548417525,-1.4171375353
 H,0,-3.0356714911,3.2385982882,0.0647750671
 H,0,-1.9574749264,3.1812154894,-1.3540074138
 H,0,-1.3713063019,3.8710057902,0.1877765895
```

Epoxidation TS Isomer 7

B3LYP/6-31+G** (PCM)



```
E(RB+HF-LYP) = -954.241944716
```

```
Zero-point correction=                           0.218847 (Hartree/Particle)
 Thermal correction to Energy=                    0.234302
 Thermal correction to Enthalpy=                  0.235246
 Thermal correction to Gibbs Free Energy=         0.175485
 Sum of electronic and zero-point Energies=           -954.023098
 Sum of electronic and thermal Energies=              -954.007643
 Sum of electronic and thermal Enthalpies=            -954.006699
 Sum of electronic and thermal Free Energies=         -954.066459

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 147.027             54.323           125.777

 C,0,-0.4895952753,-2.2218947131,-0.4372953307
 C,0,-0.5879424653,-2.0212805135,-1.7985631526
 O,0,-0.2635314754,-0.0935625837,-0.5694456964
 C,0,1.0534144206,0.4216019311,-0.5964804526
 N,0,0.4201126659,1.6484071031,-0.2299805913
 S,0,0.2886310797,1.891507829,1.4471116109
 O,0,0.9088551598,3.2127549071,1.6947041539
 O,0,0.7730050988,0.7451484929,2.2489279556
 C,0,0.6807873148,-2.7390242858,0.3388353681
 C,0,0.5538711817,-2.1939838157,-2.7580708075
 C,0,-1.9129781697,-1.6876262546,-2.4221957411
 C,0,-1.4841784663,2.054733743,1.6862911764
 H,0,-1.4144920303,-2.1397491611,0.1318084261
 H,0,0.8116246559,-2.1568215833,1.2574408243
 H,0,1.6196176506,-2.7290960753,-0.2191390433
 H,0,0.4838348518,-3.7753472964,0.6451201435
 H,0,0.3596489813,-3.0627821651,-3.4020867851
 H,0,1.5184588386,-2.3470379441,-2.2718276432
 H,0,0.6288375615,-1.3267157164,-3.4250041616
 H,0,-1.8330124234,-0.7903464838,-3.0464128597
 H,0,-2.690927832,-1.5242903433,-1.6728738096
 H,0,-2.2315387128,-2.5073231673,-3.0810097265
 H,0,1.4917778694,0.4780308665,-1.5974243218
 H,0,1.7211929942,-0.0431953205,0.1352418958
 H,0,-1.6351616617,2.3344202196,2.7314494191
 H,0,-1.949394653,1.0954985607,1.4612074513
 H,0,-1.8462241593,2.8370877699,1.017974698
```

B3LYPL/6-31+G** (gas phase)

```
Filename: b3BBgasPCMts7

E(RB+HF-LYP) = -954.226584967

Zero-point correction=                           0.219518 (Hartree/Particle)
 Thermal correction to Energy=                    0.234800
 Thermal correction to Enthalpy=                  0.235744
 Thermal correction to Gibbs Free Energy=         0.176660
 Sum of electronic and zero-point Energies=           -954.007067
 Sum of electronic and thermal Energies=              -953.991785
 Sum of electronic and thermal Enthalpies=            -953.990841
 Sum of electronic and thermal Free Energies=         -954.049925

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 147.339             54.057           124.353

C,0,-0.4960099758,-2.1322472109,-0.4655997185
 C,0,-0.5628425871,-2.0499438051,-1.85033308
 O,0,-0.3721907363,-0.1672366338,-0.6554822555
```

C,0,0.9064864284,0.4742760403,-0.694996348
N,0,0.2840260375,1.6423906273,-0.1927463954
S,0,0.3032268343,1.743316075,1.5015629237
O,0,1.1330773225,2.9135442303,1.8398772794
O,0,0.6109227249,0.4516633663,2.1559893451
C,0,0.6527460391,-2.5768237775,0.3852304312
C,0,0.6205325876,-2.2312730154,-2.7554515071
C,0,-1.8807635802,-1.8273283358,-2.5333284039
C,0,-1.4119165926,2.1631616543,1.8470336891
H,0,-1.4466914592,-2.0812374139,0.0589340371
H,0,0.7409377175,-1.9166646693,1.2547748079
H,0,1.6087638583,-2.5958262571,-0.1423384748
H,0,0.4545460949,-3.5901274673,0.7580396203
H,0,0.4976098023,-3.1549036085,-3.3383341296
H,0,1.571622731,-2.2951867182,-2.2252449088
H,0,0.678884736,-1.4132121072,-3.4830674545
H,0,-1.8238048932,-0.9749791451,-3.2196700915
H,0,-2.6863798951,-1.6424565022,-1.8197449106
H,0,-2.1442054614,-2.7074872599,-3.1367899272
H,0,1.2734262891,0.6207371709,-1.7158216998
H,0,1.6428292184,-0.0271812651,-0.0576365522
H,0,-1.4772000555,2.3556536481,2.9196384547
H,0,-2.0405331304,1.3211712911,1.5580353543
H,0,-1.6624070549,3.0573150888,1.2757729147

B3LYP/6-31+G** (Onsager)

Filename: b3BBonsts7

E(RB+HF-LYP) = -954.233368444

Zero-point correction=	0.219129 (Hartree/Particle)
Thermal correction to Energy=	0.234636
Thermal correction to Enthalpy=	0.235581
Thermal correction to Gibbs Free Energy=	0.175521
Sum of electronic and zero-point Energies=	-954.014239
Sum of electronic and thermal Energies=	-953.998732
Sum of electronic and thermal Enthalpies=	-953.997788
Sum of electronic and thermal Free Energies=	-954.057847

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.237	54.307	126.406

C,0,-0.4913165428,-2.176866237,-0.4375468195
C,0,-0.5968144293,-2.0093912785,-1.8037388954
O,0,-0.2431987255,-0.0689598402,-0.5646105784
C,0,1.0745916256,0.441202434,-0.5836032184
N,0,0.4620946048,1.6776147645,-0.2198083679
S,0,0.3108425817,1.9077605645,1.4597459099
O,0,0.8489835629,3.2574178567,1.7261543759
O,0,0.828643688,0.7752158706,2.2568305623
C,0,0.6696171165,-2.7080091832,0.3444421555
C,0,0.5375613831,-2.2209567198,-2.7634214259
C,0,-1.9200447317,-1.6718498783,-2.4266082185
C,0,-1.476663223,1.9811357727,1.6708755651
H,0,-1.4128264262,-2.0739301413,0.1301685134
H,0,0.811694596,-2.1191776936,1.2571307389
H,0,1.6069186567,-2.7203538731,-0.2160123376
H,0,0.4561904819,-3.7389920166,0.6561668418
H,0,0.337625897,-3.1122716136,-3.3733978822
H,0,1.5044187067,-2.360511101,-2.2779275551
H,0,0.6102774338,-1.3806182288,-3.4636524722
H,0,-1.8325822684,-0.7913188048,-3.0728197464

```
 H,0,-2.6918764312,-1.4805904551,-1.6781153992
 H,0,-2.2548509357,-2.5016326424,-3.0635749492
 H,0,1.5165520419,0.4906590861,-1.5837393232
 H,0,1.7341781333,-0.0319747053,0.1509662491
 H,0,-1.6591664519,2.2476784217,2.7138845744
 H,0,-1.8910318164,1.0023548572,1.4329981479
 H,0,-1.8651255277,2.7454787847,0.9975165549
```

mPW1K/6-31+G** (PCM)

```
Filename: mpBBgasPCMts7 (pcm)

E(RmPW+HF-PW91) = -954.049191479

Zero-point correction=                           0.226491 (Hartree/Particle)
 Thermal correction to Energy=                    0.241287
 Thermal correction to Enthalpy=                  0.242231
 Thermal correction to Gibbs Free Energy=         0.184258
 Sum of electronic and zero-point Energies=           -953.822701
 Sum of electronic and thermal Energies=              -953.807905
 Sum of electronic and thermal Enthalpies=            -953.806960
 Sum of electronic and thermal Free Energies=         -953.864934

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.410             52.446           122.015

 C,0,-0.5258470447,-2.120683923,-0.4109141781
 C,0,-0.5860279264,-1.9660668387,-1.7699272043
 O,0,-0.2923914505,-0.0882418594,-0.591153754
 C,0,1.0090563769,0.4125833207,-0.6872498039
 N,0,0.3927109422,1.606726756,-0.2672403764
 S,0,0.3133731279,1.7920741247,1.3767188554
 O,0,0.894875458,3.0958310665,1.6681570295
 O,0,0.8500019144,0.6428394924,2.0969243858
 C,0,0.6162836969,-2.6006628447,0.4075745847
 C,0,0.5735053805,-2.166227823,-2.6824610956
 C,0,-1.8808382815,-1.6509964315,-2.4350453323
 C,0,-1.419834613,1.8903914028,1.6844396891
 H,0,-1.4636043645,-2.0298800462,0.1239077014
 H,0,0.7469155664,-1.9542252062,1.2745680394
 H,0,1.5546711769,-2.6496660698,-0.1363243665
 H,0,0.3951679802,-3.6008705116,0.7823455633
 H,0,0.4058876734,-3.0635248263,-3.2814109833
 H,0,1.5213532255,-2.2825202966,-2.1678686621
 H,0,0.6536266789,-1.3375668048,-3.3856945952
 H,0,-1.7814177209,-0.772221084,-3.0709133875
 H,0,-2.6756684273,-1.4732698201,-1.7168823241
 H,0,-2.1752471099,-2.4805747084,-3.0805771703
 H,0,1.3825514712,0.481940614,-1.7051038966
 H,0,1.7074833596,-0.0652616844,-0.0041721172
 H,0,-1.5433097182,2.1191712916,2.7391023833
 H,0,-1.8674413441,0.9354576153,1.436780896
 H,0,-1.8311430279,2.6845590947,1.0707231195
```

mPW1K/6-31+G** (gas phase)

```
Filename: mpBBgasPCMts7 (gas)

E(RmPW+HF-PW91) = -954.032784970
```

```
Zero-point correction=                           0.227049 (Hartree/Particle)
 Thermal correction to Energy=                    0.241741
 Thermal correction to Enthalpy=                  0.242685
 Thermal correction to Gibbs Free Energy=         0.185193
 Sum of electronic and zero-point Energies=           -953.805736
 Sum of electronic and thermal Energies=              -953.791044
 Sum of electronic and thermal Enthalpies=            -953.790100
 Sum of electronic and thermal Free Energies=         -953.847592

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.695             52.287            121.004

C,0,-0.4939114335,-2.104967064,-0.4204555096
 C,0,-0.5686807482,-1.9813434893,-1.787435435
 O,0,-0.3349453096,-0.1662223163,-0.6399244925
 C,0,0.9478962133,0.417222911,-0.7020854264
 N,0,0.3297374496,1.5801688063,-0.2370182708
 S,0,0.2952818347,1.6971265626,1.4166980819
 O,0,1.0388426048,2.8871169808,1.7808916246
 O,0,0.649230687,0.438981147,2.0632946087
 C,0,0.6556282165,-2.550538699,0.4067415069
 C,0,0.5939334064,-2.1586532349,-2.700855308
 C,0,-1.8778317252,-1.722862593,-2.4488647328
 C,0,-1.4154681151,2.0161783771,1.7170328056
 H,0,-1.432699594,-2.0422686024,0.1125435435
 H,0,0.7775982476,-1.8709531049,1.2498337832
 H,0,1.5914375796,-2.6068061784,-0.1406897742
 H,0,0.4442350369,-3.5410946242,0.8103140006
 H,0,0.4542978155,-3.0665944223,-3.2906682189
 H,0,1.5440338897,-2.2400924477,-2.1842712008
 H,0,0.6509398169,-1.3342928651,-3.4108426758
 H,0,-1.8110494286,-0.8571992542,-3.1058901849
 H,0,-2.6691487993,-1.5456507885,-1.7272081341
 H,0,-2.1571897456,-2.5773430587,-3.0681891283
 H,0,1.3148811312,0.5253796275,-1.7194815187
 H,0,1.6603984967,-0.080251344,-0.0467318529
 H,0,-1.5213837094,2.1985187893,2.7818624333
 H,0,-1.9908489598,1.1509708323,1.4103997989
 H,0,-1.7005218581,2.8945840532,1.1493026766
```

mPW1K/6-31+G** (Onsager)

```
Filename: mpBBonsts7
E(RmPW+HF-PW91) = -954.039004265

 Zero-point correction=                           0.226817 (Hartree/Particle)
 Thermal correction to Energy=                    0.241652
 Thermal correction to Enthalpy=                  0.242596
 Thermal correction to Gibbs Free Energy=         0.184432
 Sum of electronic and zero-point Energies=           -953.812187
 Sum of electronic and thermal Energies=              -953.797353
 Sum of electronic and thermal Enthalpies=            -953.796409
 Sum of electronic and thermal Free Energies=         -953.854572

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.639             52.425            122.415

 C,0,-0.511056762,-2.0968547466,-0.4093572945
 C,0,-0.5913074931,-1.9565326974,-1.7702096415
 O,0,-0.2728041754,-0.0877202596,-0.5881357884
 C,0,1.0308527289,0.4133024526,-0.6593567662
```

N,0,0.4309981442,1.6163166206,-0.2519302443
S,0,0.3200759567,1.7935054,1.3928533524
O,0,0.8654459477,3.1018285366,1.712619196
O,0,0.837926177,0.6383813044,2.114104722
C,0,0.6326644974,-2.5892266619,0.400261234
C,0,0.5543301967,-2.1718739776,-2.6959400324
C,0,-1.8936065419,-1.6407079145,-2.4185777994
C,0,-1.427359584,1.8687455201,1.64810134
H,0,-1.4417877458,-1.9999830452,0.1329211
H,0,0.7734720612,-1.9476476416,1.2694249597
H,0,1.5656414675,-2.6425776307,-0.1523890288
H,0,0.4083695679,-3.5911961428,0.7674135497
H,0,0.3760595113,-3.0745766352,-3.2828554789
H,0,1.5077622894,-2.2877235204,-2.1920788306
H,0,0.6280769252,-1.3520770179,-3.4096421911
H,0,-1.7991529719,-0.7718548095,-3.0680173522
H,0,-2.6759352269,-1.447189999,-1.6914247811
H,0,-2.2060008142,-2.476314943,-3.046961194
H,0,1.4205332735,0.4732703036,-1.6720676631
H,0,1.7123020634,-0.0730692854,0.0353523735
H,0,-1.5860172204,2.0901028129,2.6989834662
H,0,-1.8572766401,0.9112393364,1.3813408444
H,0,-1.8275136322,2.6595506413,1.0238739486

B3LYP/6-31G* (gas phase)

E(RB+HF-LYP) = -954.182500320

Zero-point correction= 0.221367 (Hartree/Particle)
Thermal correction to Energy= 0.236491
Thermal correction to Enthalpy= 0.237436
Thermal correction to Gibbs Free Energy= 0.178811
Sum of electronic and zero-point Energies= -953.961134
Sum of electronic and thermal Energies= -953.946009
Sum of electronic and thermal Enthalpies= -953.945065
Sum of electronic and thermal Free Energies= -954.003689

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	148.401	53.545	123.386

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	-1.916300	0.556289	-0.891507
2	6	0	C	-2.805853	-0.211902	-0.150519
3	8	0	O	-0.604248	-0.524697	0.035108
4	6	0	C	-0.018045	-0.078088	1.261019
5	7	0	N	1.131057	-0.838428	0.939653
6	16	0	S	2.283716	0.034688	0.059400
7	8	0	O	3.507500	0.058074	0.874768
8	8	0	O	1.764860	1.314649	-0.467856
9	6	0	C	-1.545085	1.994322	-0.698466
10	6	0	C	-3.419624	0.237855	1.142626
11	6	0	C	-3.246364	-1.555608	-0.653599
12	6	0	C	2.565872	-1.067689	-1.335180
13	1	0	H	-1.644817	0.155930	-1.865178
14	1	0	H	-0.464457	2.110934	-0.836398
15	1	0	H	-1.818446	2.389377	0.283041
16	1	0	H	-2.049631	2.604564	-1.459421
17	1	0	H	-4.504026	0.366203	1.009966

18	1	0	H	-3.015376	1.181166	1.514348
19	1	0	H	-3.293644	-0.526482	1.919692
20	1	0	H	-3.091999	-2.328212	0.109116
21	1	0	H	-2.708076	-1.851842	-1.557181
22	1	0	H	-4.323000	-1.542070	-0.878917
23	1	0	H	-0.531883	-0.477119	2.142375
24	1	0	H	0.080924	1.011864	1.304084
25	1	0	H	3.373995	-0.633793	-1.928697
26	1	0	H	1.646541	-1.135466	-1.917828
27	1	0	H	2.854525	-2.046346	-0.949378

B3LYLP/6-31G* (Onsager)

Key Distances: N-O 1.936; O-Csec 2.045; O-Ctert 2.305
E(RB+HF-LYP) = -954.188519323

Zero-point correction=	0.221315 (Hartree/Particle)
Thermal correction to Energy=	0.236465
Thermal correction to Enthalpy=	0.237409
Thermal correction to Gibbs Free Energy=	0.178865
Sum of electronic and zero-point Energies=	-953.967205
Sum of electronic and thermal Energies=	-953.952054
Sum of electronic and thermal Enthalpies=	-953.951110
Sum of electronic and thermal Free Energies=	-954.009655

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	148.384	53.620	123.217

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	1.978853	0.588047	0.895510
2	6	0	C	2.806659	-0.232831	0.152294
3	8	0	O	0.525378	-0.495844	-0.050112
4	6	0	C	0.002173	-0.037456	-1.282189
5	7	0	N	-1.148167	-0.816393	-0.968757
6	16	0	S	-2.303989	0.024004	-0.058228
7	8	0	O	-3.587298	-0.157167	-0.759570
8	8	0	O	-1.888191	1.395409	0.301084
9	6	0	C	1.643659	2.029112	0.667185
10	6	0	C	3.427293	0.167763	-1.153701
11	6	0	C	3.189961	-1.589136	0.667960
12	6	0	C	-2.361494	-0.955049	1.452830
13	1	0	H	1.682523	0.206953	1.869906
14	1	0	H	0.567483	2.183742	0.806677
15	1	0	H	1.923926	2.391461	-0.325036
16	1	0	H	2.166631	2.647708	1.408766
17	1	0	H	4.515129	0.263515	-1.027281
18	1	0	H	3.053444	1.115431	-1.545961
19	1	0	H	3.275025	-0.611883	-1.910302
20	1	0	H	2.974674	-2.364226	-0.077116
21	1	0	H	2.666642	-1.842147	1.593250
22	1	0	H	4.271371	-1.627070	0.860747
23	1	0	H	0.527806	-0.434608	-2.157478
24	1	0	H	-0.114826	1.050481	-1.326039
25	1	0	H	-3.168572	-0.551416	2.068936
26	1	0	H	-1.400413	-0.865875	1.959043
27	1	0	H	-2.561581	-1.993279	1.184279

BP86 (gas phase)

E(RB-P86) = -954.231678674

Zero-point correction=	0.214234 (Hartree/Particle)
Thermal correction to Energy=	0.229821
Thermal correction to Enthalpy=	0.230766
Thermal correction to Gibbs Free Energy=	0.171111
Sum of electronic and zero-point Energies=	-954.017444
Sum of electronic and thermal Energies=	-954.001857
Sum of electronic and thermal Enthalpies=	-954.000913
Sum of electronic and thermal Free Energies=	-954.060568

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	144.215	55.131	125.554

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.955910	0.538809	-0.909630
2	6	0	-2.839180	-0.230326	-0.149516
3	8	0	-0.587313	-0.524339	0.073351
4	6	0	-0.012913	0.021250	1.258693
5	7	0	1.132024	-0.795710	0.976028
6	16	0	2.303805	0.045984	0.042934
7	8	0	3.505368	0.143863	0.914741
8	8	0	1.787256	1.283054	-0.612642
9	6	0	-1.598238	1.985562	-0.738277
10	6	0	-3.464777	0.239346	1.135234
11	6	0	-3.249716	-1.599093	-0.622458
12	6	0	2.636790	-1.180541	-1.248272
13	1	0	-1.662187	0.112555	-1.876964
14	1	0	-0.510189	2.113769	-0.883889
15	1	0	-1.875030	2.395205	0.246742
16	1	0	-2.112155	2.589404	-1.511289
17	1	0	-4.563117	0.325481	1.008947
18	1	0	-3.089688	1.215993	1.478175
19	1	0	-3.306877	-0.499988	1.943121
20	1	0	-3.076134	-2.357898	0.162545
21	1	0	-2.699930	-1.905800	-1.526643
22	1	0	-4.334952	-1.620077	-0.850284
23	1	0	-0.518230	-0.301857	2.188247
24	1	0	0.111269	1.120297	1.218000
25	1	0	3.473678	-0.796213	-1.851837
26	1	0	1.730460	-1.298314	-1.859257
27	1	0	2.909203	-2.128997	-0.762992

MPW1K/6-31+G* (gas phase)

E(RmPW+HF-PW91) = -954.005743621

Zero-point correction=	0.228189 (Hartree/Particle)
Thermal correction to Energy=	0.242851
Thermal correction to Enthalpy=	0.243795
Thermal correction to Gibbs Free Energy=	0.186324
Sum of electronic and zero-point Energies=	-953.777555
Sum of electronic and thermal Energies=	-953.762893
Sum of electronic and thermal Enthalpies=	-953.761948

```
 Sum of electronic and thermal Free Energies=         -953.819420

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 152.391             52.094           120.959

 C,0,-0.4878654963,-2.1093250204,-0.4194506759
 C,0,-0.5682640088,-1.9826658054,-1.7856679556
 O,0,-0.3295551195,-0.1704865136,-0.6348478806
 C,0,0.952805767,0.4122359019,-0.6938691716
 N,0,0.3334770295,1.5763304938,-0.2342284182
 S,0,0.2913950136,1.6998141027,1.4187066418
 O,0,1.0365594549,2.889125338,1.7814331341
 O,0,0.6363826999,0.4437836623,2.0731457934
 C,0,0.6641302476,-2.5608522424,0.402154669
 C,0,0.5899277536,-2.1568324262,-2.7057336112
 C,0,-1.8799316223,-1.7195033496,-2.4409456161
 C,0,-1.4208404851,2.0266893231,1.7071825023
 H,0,-1.4237964942,-2.0467969916,0.1189029057
 H,0,0.7844897117,-1.8940601493,1.2560090944
 H,0,1.6014226222,-2.6057087743,-0.1452465618
 H,0,0.4578654669,-3.5590278489,0.7921747079
 H,0,0.4489906988,-3.0633650881,-3.2990568521
 H,0,1.5439900875,-2.2395459372,-2.1949880827
 H,0,0.6442667639,-1.3295138252,-3.413742503
 H,0,-1.8162929289,-0.8489310475,-3.0931036066
 H,0,-2.6701515006,-1.5465936862,-1.715709422
 H,0,-2.1631962175,-2.5698917411,-3.0656893576
 H,0,1.3227074054,0.5172734239,-1.7104523117
 H,0,1.6633842264,-0.0845070295,-0.0362418567
 H,0,-1.5349851869,2.214751264,2.771028161
 H,0,-2.0002747107,1.1627132097,1.4020957206
 H,0,-1.7019485839,2.9040069419,1.1344434034
```

MPW1K/6-31+G* (Onsager)

```
E(RmPW+HF-PW91) =  -954.012815112

 Zero-point correction=                           0.227855 (Hartree/Particle)
 Thermal correction to Energy=                    0.242708
 Thermal correction to Enthalpy=                  0.243652
 Thermal correction to Gibbs Free Energy=         0.185265
 Sum of electronic and zero-point Energies=           -953.784960
 Sum of electronic and thermal Energies=              -953.770107
 Sum of electronic and thermal Enthalpies=            -953.769163
 Sum of electronic and thermal Free Energies=         -953.827550

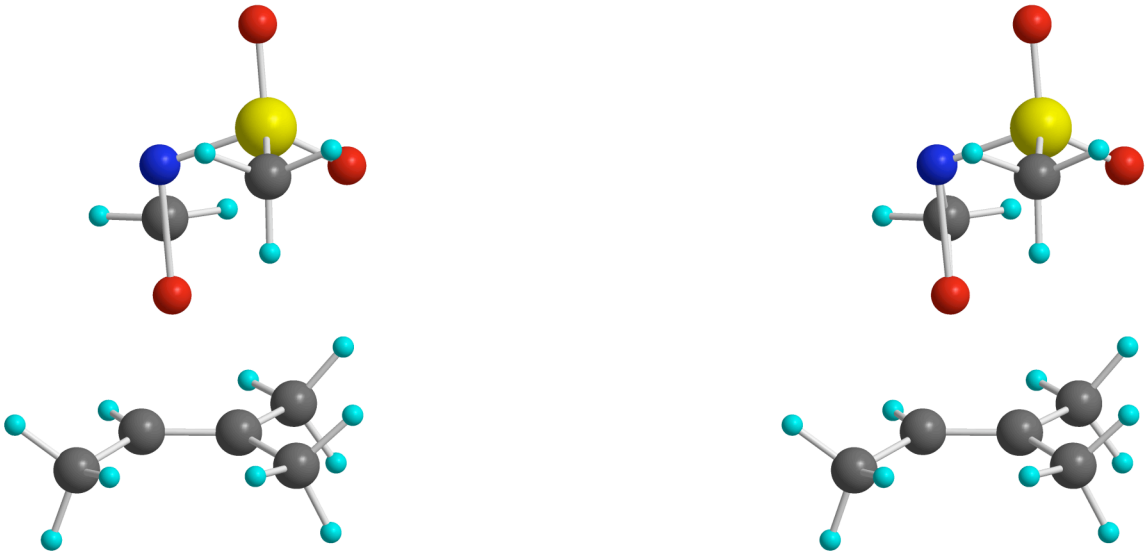
                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 152.301             52.288           122.886

 C,0,-0.5089461672,-2.1663866265,-0.4067121395
 C,0,-0.6050476904,-2.0065752968,-1.763519022
 O,0,-0.2620605481,-0.1413649036,-0.5713319216
 C,0,1.0453621858,0.3452927157,-0.6245344706
 N,0,0.4419963911,1.5573360586,-0.2477072968
 S,0,0.2966120117,1.7656736224,1.3906719775
 O,0,0.8185232449,3.0883357428,1.6918393608
 O,0,0.8146673979,0.6344804321,2.1474803779
 C,0,0.6419358372,-2.6795056564,0.3807783019
 C,0,0.5262991196,-2.2160948365,-2.7084270743
 C,0,-1.913307962,-1.6718327057,-2.3908831627
 C,0,-1.4571460844,1.8249558927,1.6113549925
```

H,0,-1.4309015799,-2.0689740332,0.1507849959
H,0,0.7876198892,-2.0680295289,1.2711146572
H,0,1.5729734988,-2.7126932242,-0.1781455877
H,0,0.4243177439,-3.6946626498,0.7176185163
H,0,0.3342819111,-3.1084800026,-3.3081594068
H,0,1.4869397424,-2.3472434586,-2.2205276216
H,0,0.5975209841,-1.3850795148,-3.4105839921
H,0,-1.8221163589,-0.7926685304,-3.028134236
H,0,-2.6870714653,-1.4852327834,-1.6514764606
H,0,-2.240231824,-2.4952332909,-3.0293195572
H,0,1.4554213873,0.3875360663,-1.6299439885
H,0,1.709423972,-0.1339540009,0.0911267789
H,0,-1.6403640225,2.0731167943,2.6531377731
H,0,-1.8735991225,0.8554752318,1.364639328
H,0,-1.8579178697,2.5932614676,0.9588211499

Epoxidation TS Isomer 8

B3LYP/6-31+G**



E(RB+HF-LYP) = -954.243234987

Zero-point correction= 0.218584 (Hartree/Particle)
Thermal correction to Energy= 0.234177
Thermal correction to Enthalpy= 0.235121
Thermal correction to Gibbs Free Energy= 0.174801
Sum of electronic and zero-point Energies= -954.024651
Sum of electronic and thermal Energies= -954.009058
Sum of electronic and thermal Enthalpies= -954.008114
Sum of electronic and thermal Free Energies= -954.068434

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	146.948	54.405	126.955

C,0,0.5740735795,-2.2518025688,-1.5020188522
C,0,0.7922193379,-2.360339925,-0.1453852558
O,0,-0.0051268404,-0.2950543231,-0.8240529196
C,0,0.9425457041,0.7357070804,-1.0137166151
N,0,-0.1912772977,1.5856730217,-0.8347593396
S,0,-0.4740652055,2.0429071604,0.7790258773

O,0,-0.4915198557,3.5230508872,0.7667901213
O,0,0.4226785809,1.3744113592,1.7482643685
C,0,-0.6472896177,-2.6607286171,-2.2657110293
C,0,-0.251346524,-2.8060277815,0.8354611604
C,0,2.1501967748,-2.0899032084,0.4369675321
C,0,-2.1524849257,1.4658166843,1.0529445207
H,0,1.4362305835,-1.9829305635,-2.1144492562
H,0,1.3391800779,0.7962086812,-2.0320383115
H,0,1.7244690941,0.7611699295,-0.2485866522
H,0,-0.842101695,-1.9509243574,-3.0754292252
H,0,-1.5417754691,-2.724933985,-1.6435115728
H,0,-0.4841322744,-3.6438551611,-2.7285549679
H,0,0.004332945,-3.8041173069,1.2175395326
H,0,-1.2542659113,-2.8535678384,0.4099603594
H,0,-0.2666005726,-2.1316785741,1.6992492746
H,0,2.0908910453,-1.3233973521,1.2194817554
H,0,2.8731676795,-1.7727551979,-0.3192451499
H,0,2.5346683877,-2.9990789405,0.918681736
H,0,-2.4476622145,1.816852188,2.0443398189
H,0,-2.1514241479,0.3774322057,1.002117415
H,0,-2.7905982386,1.8975325033,0.2808066751

B3LYP/6-31+G** (gas phase)

Filename: b3BBgasPCMts8 (gas)

E(RB+HF-LYP) = -954.228554512

Zero-point correction= 0.219200 (Hartree/Particle)
Thermal correction to Energy= 0.234652
Thermal correction to Enthalpy= 0.235596
Thermal correction to Gibbs Free Energy= 0.175596
Sum of electronic and zero-point Energies= -954.009354
Sum of electronic and thermal Energies= -953.993902
Sum of electronic and thermal Enthalpies= -953.992958
Sum of electronic and thermal Free Energies= -954.052959

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.247	54.180	126.282

C,0,0.6257572951,-2.2532371157,-1.5285588231
C,0,0.807690378,-2.3398359348,-0.1565136431
O,0,-0.0477197066,-0.4515369702,-0.8748864898
C,0,0.7918910068,0.6813644041,-1.0992349479
N,0,-0.3240865051,1.4949658916,-0.788594611
S,0,-0.4197931626,1.9007984378,0.8570516493
O,0,-0.1288301634,3.3424917768,0.9586714804
O,0,0.3340332517,0.9724762999,1.730017897
C,0,-0.5323777033,-2.7643347505,-2.3298668144
C,0,-0.2484353845,-2.8139879566,0.7945351401
C,0,2.1186986862,-1.9723898516,0.4739438069
C,0,-2.1776625108,1.6671867042,1.158002286
H,0,1.496838244,-1.954636573,-2.1103487993
H,0,1.0903201865,0.7877638079,-2.1476586572
H,0,1.6521714437,0.7050099625,-0.4207873513
H,0,-0.7287555522,-2.0969052144,-3.1737242616
H,0,-1.4491755321,-2.8468528435,-1.7441348108
H,0,-0.2978084311,-3.7554678653,-2.7415310274
H,0,0.0665025652,-3.7583487782,1.2586733409
H,0,-1.2178310655,-2.970692877,0.3215279174
H,0,-0.3633747157,-2.0802359468,1.6003748199
H,0,1.9713014186,-1.1563622579,1.1924647428
H,0,2.868933623,-1.6714579327,-0.2618378617
H,0,2.5134979695,-2.8276664768,1.0377059716

```
 H,0,-2.3675905056,1.9976382373,2.1809019865
 H,0,-2.4137970504,0.6102387554,1.0349365264
 H,0,-2.7274150795,2.2796810678,0.4430415335
```

B3LYP/6-31+G** (Onsager)

```
Filename: b3BBonsts8
E(RB+HF-LYP) = -954.233541612

 Zero-point correction=                           0.219081 (Hartree/Particle)
 Thermal correction to Energy=                    0.234626
 Thermal correction to Enthalpy=                  0.235570
 Thermal correction to Gibbs Free Energy=         0.175300
 Sum of electronic and zero-point Energies=           -954.014461
 Sum of electronic and thermal Energies=              -953.998916
 Sum of electronic and thermal Enthalpies=            -953.997972
 Sum of electronic and thermal Free Energies=         -954.058241

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 147.230             54.289           126.848

 C,0,0.5759466859,-2.2357151907,-1.4919001263
 C,0,0.7592311654,-2.3500486576,-0.1290575778
 O,0,-0.0164095873,-0.2992355403,-0.8300270341
 C,0,0.9067217474,0.7450539087,-1.0688042548
 N,0,-0.2126260236,1.6031623832,-0.8664402389
 S,0,-0.433292301,2.0806673686,0.7536956607
 O,0,-0.5495985879,3.5522979189,0.7240975415
 O,0,0.5420225921,1.4697157758,1.6817983726
 C,0,-0.6134927445,-2.6618664939,-2.2943479516
 C,0,-0.3074627436,-2.8167487022,0.8153639105
 C,0,2.0937029441,-2.0615382729,0.4963346165
 C,0,-2.0622068539,1.4050524308,1.1167555173
 H,0,1.4544835222,-1.9617475992,-2.0749066111
 H,0,1.2668074298,0.7873458534,-2.1020752029
 H,0,1.7172345843,0.7855089893,-0.3334463436
 H,0,-0.7872621342,-1.9607423965,-3.1157708721
 H,0,-1.5279953387,-2.7278989774,-1.7028464078
 H,0,-0.4272962065,-3.6475933181,-2.7413392962
 H,0,-0.0608818252,-3.8230576309,1.1806633197
 H,0,-1.298016987,-2.858356076,0.3620950636
 H,0,-0.3451276309,-2.1619518425,1.693235344
 H,0,1.9995064806,-1.2717950749,1.2521463482
 H,0,2.8442150227,-1.7628742254,-0.2400934698
 H,0,2.4630975178,-2.9556030505,1.0153602521
 H,0,-2.3329477851,1.7543528848,2.1151111282
 H,0,-1.9961568308,0.3182527004,1.0809828101
 H,0,-2.7592161122,1.7810278349,0.3675865017
```

mPW1K/6-31+G** (PCM)

```
Filename: mpBBPCMts8
E(RmPW+HF-PW91) = -954.050296352

 Zero-point correction=                           0.226064 (Hartree/Particle)
 Thermal correction to Energy=                    0.241090
 Thermal correction to Enthalpy=                  0.242034
 Thermal correction to Gibbs Free Energy=         0.182854
 Sum of electronic and zero-point Energies=           -953.824232
 Sum of electronic and thermal Energies=              -953.809206
```

```
 Sum of electronic and thermal Enthalpies=            -953.808262
 Sum of electronic and thermal Free Energies=         -953.867442

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.286             52.611           124.555

    1          6             0        2.614950   -0.593593   -0.404407
    2          6             0        2.299589    0.651044    0.068812
    3          8             0        0.543006   -0.640132   -0.268409
    4          6             0       -0.133829   -0.502840   -1.483023
    5          7             0       -1.197393   -1.047031   -0.739730
    6         16             0       -2.130810    0.075069    0.043293
    7          8             0       -3.502405   -0.151243   -0.393141
    8          8             0       -1.604072    1.429360   -0.079816
    9          6             0        2.985442   -1.793839    0.388620
   10          6             0        2.155345    0.976642    1.513010
   11          6             0        2.131222    1.800961   -0.862793
   12          6             0       -2.006088   -0.428033    1.727861
   13          1             0        2.753845   -0.682690   -1.477281
   14          1             0        0.215602   -1.177594   -2.260097
   15          1             0       -0.221882    0.528697   -1.815541
   16          1             0        2.555684   -2.686541   -0.060023
   17          1             0        2.656054   -1.739903    1.420872
   18          1             0        4.069594   -1.918443    0.384589
   19          1             0        2.991469    1.602412    1.830387
   20          1             0        2.127806    0.100623    2.151099
   21          1             0        1.246959    1.556734    1.670089
   22          1             0        1.147691    2.253373   -0.732916
   23          1             0        2.259802    1.514511   -1.903264
   24          1             0        2.865989    2.572641   -0.627772
   25          1             0       -2.669111    0.212590    2.302165
   26          1             0       -0.977345   -0.310227    2.046771
   27          1             0       -2.319474   -1.463994    1.798787
```

mPW1K/6-31+G** (gas phase)

```
Filename: mpBBgasts8
E(RmPW+HF-PW91) = -954.034604333

 Zero-point correction=                           0.226816 (Hartree/Particle)
 Thermal correction to Energy=                    0.241637
 Thermal correction to Enthalpy=                  0.242581
 Thermal correction to Gibbs Free Energy=         0.184417
 Sum of electronic and zero-point Energies=           -953.807788
 Sum of electronic and thermal Energies=              -953.792967
 Sum of electronic and thermal Enthalpies=            -953.792023
 Sum of electronic and thermal Free Energies=         -953.850187

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.630             52.366           122.417

 C,0,0.5935214157,-2.1490446328,-1.5366227989
 C,0,0.7589458837,-2.1916792965,-0.1736418786
 O,0,-0.0373774427,-0.3604581049,-0.8880771596
 C,0,0.8251353753,0.7278596767,-1.1198114084
 N,0,-0.2808955772,1.5230320304,-0.811231821
 S,0,-0.4041146056,1.8811164758,0.8029165596
 O,0,-0.1976246118,3.3079628722,0.9568539031
 O,0,0.3927450543,0.9806567103,1.6290445313
 C,0,-0.571750281,-2.6316742688,-2.3224907016
 C,0,-0.3064118832,-2.602504768,0.777969138
```

```
C,0,2.0618090813,-1.8395531483,0.4541231932
C,0,-2.111834092,1.543981556,1.0966136863
H,0,1.4701597193,-1.8852381593,-2.1163294329
H,0,1.1228394909,0.8195639444,-2.1616412784
H,0,1.6736954767,0.7394595272,-0.4379419924
H,0,-0.7585701021,-1.9646091867,-3.1603936875
H,0,-1.4799933432,-2.6904882652,-1.7328448806
H,0,-0.3642688086,-3.6219240999,-2.7308635385
H,0,-0.0200362981,-3.5327659719,1.2706313016
H,0,-1.2714002202,-2.7476847097,0.3067312939
H,0,-0.400547495,-1.840413876,1.5506745055
H,0,1.9206641134,-1.0066482511,1.1444441671
H,0,2.8208648931,-1.5781223641,-0.2783250994
H,0,2.4276949645,-2.6839873065,1.0393766548
H,0,-2.3193595138,1.8252078026,2.1242451895
H,0,-2.2911152087,0.4871044853,0.9379059474
H,0,-2.6981059848,2.1447013286,0.4106366065
```

mPW1K/6-31+G** (Onsager)

```
Filename: mpBBonsts8blowest
E(RmPW+HF-PW91) = -954.040141440

 Zero-point correction=                           0.226519 (Hartree/Particle)
 Thermal correction to Energy=                    0.241548
 Thermal correction to Enthalpy=                  0.242492
 Thermal correction to Gibbs Free Energy=         0.182811
 Sum of electronic and zero-point Energies=           -953.813623
 Sum of electronic and thermal Energies=              -953.798594
 Sum of electronic and thermal Enthalpies=            -953.797650
 Sum of electronic and thermal Free Energies=         -953.857330

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.573             52.523            125.608

 C,0,0.5625721558,-2.1977205321,-1.4858175434
 C,0,0.7415886171,-2.2729018204,-0.1302950214
 O,0,-0.0044345658,-0.3277011229,-0.8235095613
 C,0,0.9201163349,0.6940606902,-1.0590690685
 N,0,-0.1850872162,1.5302636757,-0.8385154729
 S,0,-0.4109920023,1.9506857751,0.750085452
 O,0,-0.5020485452,3.4001504554,0.7955809706
 O,0,0.5360427231,1.2935225133,1.640713342
 C,0,-0.6264612013,-2.6222839949,-2.2673514372
 C,0,-0.3226871096,-2.6917386803,0.8197754903
 C,0,2.0668396111,-1.9840475443,0.484622878
 C,0,-2.0216149057,1.3014312157,1.0744483395
 H,0,1.4399598328,-1.9497295067,-2.0715544955
 H,0,1.2693010564,0.7354500178,-2.0878621874
 H,0,1.7270884512,0.7166411703,-0.3296420607
 H,0,-0.8003986446,-1.9339985979,-3.0907543313
 H,0,-1.5305682585,-2.6715470722,-1.6704601398
 H,0,-0.4522203739,-3.6087771813,-2.6990007572
 H,0,-0.0932306044,-3.68514536,1.2087058765
 H,0,-1.3082502075,-2.7279052174,0.3702639694
 H,0,-0.3440920508,-2.0122632717,1.6705541384
 H,0,1.9756333845,-1.1761584558,1.2115701906
 H,0,2.8186167313,-1.7199824319,-0.2543175887
 H,0,2.4191613701,-2.8626472924,1.026415185
 H,0,-2.2932136934,1.6085876537,2.0795707266
 H,0,-1.9804470847,0.2219360347,0.9939752075
 H,0,-2.7081898046,1.7174838804,0.3460388993
```

B3LYP/6-31G* (gas phase)

```
E(RB+HF-LYP) =  -954.184431488

 Zero-point correction=                           0.221284 (Hartree/Particle)
 Thermal correction to Energy=                    0.236453
 Thermal correction to Enthalpy=                  0.237397
 Thermal correction to Gibbs Free Energy=         0.178438
 Sum of electronic and zero-point Energies=           -953.963147
 Sum of electronic and thermal Energies=              -953.947978
 Sum of electronic and thermal Enthalpies=            -953.947034
 Sum of electronic and thermal Free Energies=         -954.005994

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                148.377             53.588            124.091

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0    C    2.660307   -0.567334   -0.368579
    2          6             0    C    2.275124    0.707788    0.018020
    3          8             0    O    0.670029   -0.727558   -0.173250
    4          6             0    C   -0.110279   -0.767682   -1.367202
    5          7             0    N   -1.202656   -1.195554   -0.577454
    6         16             0    S   -2.127224    0.091506    0.015358
    7          8             0    O   -3.425962    0.052092   -0.675771
    8          8             0    O   -1.390685    1.374296    0.046403
    9          6             0    C    3.162402   -1.676110    0.504735
   10          6             0    C    2.108242    1.135253    1.444422
   11          6             0    C    1.996761    1.772405   -1.002056
   12          6             0    C   -2.382952   -0.447326    1.712735
   13          1             0    H    2.795759   -0.724461   -1.438015
   14          1             0    H    0.217564   -1.549621   -2.061656
   15          1             0    H   -0.173772    0.209266   -1.859542
   16          1             0    H    2.799927   -2.639094    0.132142
   17          1             0    H    2.843292   -1.574278    1.543777
   18          1             0    H    4.260882   -1.707271    0.485030
   19          1             0    H    2.807016    1.950192    1.677547
   20          1             0    H    2.268729    0.328664    2.161098
   21          1             0    H    1.092811    1.528172    1.577104
   22          1             0    H    0.962449    2.123961   -0.895390
   23          1             0    H    2.153616    1.424012   -2.027065
   24          1             0    H    2.651116    2.637751   -0.829448
   25          1             0    H   -3.055031    0.274796    2.181917
   26          1             0    H   -1.418674   -0.470451    2.222056
   27          1             0    H   -2.836186   -1.439455    1.695393
 ---------------------------------------------------------------------
```

B3LYP/6-31G* (Onsager)

```
SCF Done:  E(RB+HF-LYP) =  -954.189597504

 Zero-point correction=                           0.221137 (Hartree/Particle)
 Thermal correction to Energy=                    0.236399
 Thermal correction to Enthalpy=                  0.237343
 Thermal correction to Gibbs Free Energy=         0.178108
 Sum of electronic and zero-point Energies=           -953.968461
```

```
 Sum of electronic and thermal Energies=             -953.953199
 Sum of electronic and thermal Enthalpies=           -953.952255
 Sum of electronic and thermal Free Energies=        -954.011489

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 148.342             53.712            124.670

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0    C     2.671026   -0.606148   -0.349722
    2          6             0    C     2.318662    0.692331   -0.039708
    3          8             0    O     0.583211   -0.712825   -0.126561
    4          6             0    C    -0.144278   -0.849428   -1.330951
    5          7             0    N    -1.235019   -1.230821   -0.501037
    6         16             0    S    -2.173830    0.081900    0.018780
    7          8             0    O    -3.560766   -0.218105   -0.379491
    8          8             0    O    -1.606187    1.395138   -0.349221
    9          6             0    C     3.146817   -1.677541    0.580379
   10          6             0    C     2.222050    1.216602    1.361729
   11          6             0    C     2.041292    1.697314   -1.120032
   12          6             0    C    -2.063211   -0.096142    1.807117
   13          1             0    H     2.770503   -0.837659   -1.409807
   14          1             0    H     0.195958   -1.682021   -1.956940
   15          1             0    H    -0.230510    0.085290   -1.895117
   16          1             0    H     2.733152   -2.646383    0.282982
   17          1             0    H     2.872734   -1.494757    1.621121
   18          1             0    H     4.241134   -1.760822    0.527337
   19          1             0    H     3.033544    1.933837    1.547329
   20          1             0    H     2.282374    0.436060    2.121448
   21          1             0    H     1.278713    1.761283    1.487395
   22          1             0    H     1.011931    2.068487   -1.029524
   23          1             0    H     2.184788    1.284106   -2.122755
   24          1             0    H     2.707498    2.563209   -1.008881
   25          1             0    H    -2.723664    0.653769    2.248906
   26          1             0    H    -1.028397    0.068212    2.108264
   27          1             0    H    -2.387562   -1.102853    2.074321
 ---------------------------------------------------------------------
```

B3LYP/6-311+G** (gas phase)

```
E(RB+HF-LYP) =  -954.376511508

 Zero-point correction=                           0.218433 (Hartree/Particle)
 Thermal correction to Energy=                    0.233864
 Thermal correction to Enthalpy=                  0.234808
 Thermal correction to Gibbs Free Energy=         0.174905
 Sum of electronic and zero-point Energies=           -954.158078
 Sum of electronic and thermal Energies=              -954.142648
 Sum of electronic and thermal Enthalpies=            -954.141704
 Sum of electronic and thermal Free Energies=         -954.201607

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 146.752             54.218            126.077

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
```

1	6	0	2.690185	-0.573978	-0.365235
2	6	0	2.307169	0.704696	-0.004588
3	8	0	0.665498	-0.736147	-0.144862
4	6	0	-0.125347	-0.822596	-1.327784
5	7	0	-1.211575	-1.209240	-0.510274
6	16	0	-2.153359	0.095753	0.015637
7	8	0	-3.429641	0.021438	-0.704559
8	8	0	-1.424739	1.377647	0.005156
9	6	0	3.206312	-1.655930	0.529105
10	6	0	2.178639	1.164924	1.412743
11	6	0	2.009309	1.743449	-1.041864
12	6	0	-2.449069	-0.377934	1.723498
13	1	0	2.805794	-0.757674	-1.430679
14	1	0	0.189201	-1.632713	-1.991073
15	1	0	-0.194343	0.134730	-1.853102
16	1	0	2.867355	-2.631434	0.174254
17	1	0	2.882967	-1.541036	1.562758
18	1	0	4.303188	-1.665147	0.512456
19	1	0	2.937284	1.928338	1.623930
20	1	0	2.288021	0.362664	2.139587
21	1	0	1.200472	1.635721	1.548929
22	1	0	0.977213	2.093248	-0.928813
23	1	0	2.156482	1.375347	-2.058454
24	1	0	2.659514	2.613302	-0.893269
25	1	0	-3.132088	0.362830	2.138533
26	1	0	-1.497764	-0.376899	2.251362
27	1	0	-2.900651	-1.367945	1.724182

BP86/6-31G* (gas phase)

E(RB-P86) = -954.232792909

Zero-point correction= 0.214126 (Hartree/Particle)
Thermal correction to Energy= 0.229789
Thermal correction to Enthalpy= 0.230733
Thermal correction to Gibbs Free Energy= 0.170489
Sum of electronic and zero-point Energies= -954.018667
Sum of electronic and thermal Energies= -954.003004
Sum of electronic and thermal Enthalpies= -954.002060
Sum of electronic and thermal Free Energies= -954.062304

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	144.195	55.210	126.794

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.710752	-0.564635	-0.374551
2	6	0	2.298213	0.708754	0.014317
3	8	0	0.655406	-0.733134	-0.163539
4	6	0	-0.108350	-0.756597	-1.364560
5	7	0	-1.197727	-1.216177	-0.553388
6	16	0	-2.147742	0.095884	0.018118
7	8	0	-3.435794	0.025561	-0.724440
8	8	0	-1.420186	1.399232	0.068198
9	6	0	3.218222	-1.672073	0.501089
10	6	0	2.139569	1.137104	1.446197
11	6	0	2.000201	1.771004	-1.008906

12	6	0	-2.442217	-0.451367	1.719162
13	1	0	2.833426	-0.725588	-1.455166
14	1	0	0.212881	-1.533403	-2.084235
15	1	0	-0.196508	0.235727	-1.847999
16	1	0	2.842492	-2.645214	0.142003
17	1	0	2.916759	-1.557704	1.553769
18	1	0	4.325293	-1.713801	0.464790
19	1	0	2.853770	1.949704	1.683895
20	1	0	2.294677	0.320283	2.166756
21	1	0	1.121887	1.545125	1.587746
22	1	0	0.953427	2.113537	-0.897858
23	1	0	2.157005	1.420498	-2.042896
24	1	0	2.646751	2.654808	-0.842425
25	1	0	-3.140794	0.267888	2.173975
26	1	0	-1.482328	-0.461489	2.255302
27	1	0	-2.884518	-1.457671	1.687937

MPW1K/6-31+G* (gas phase)

E(RmPW+HF-PW91) = -954.007553840

Zero-point correction= 0.227924 (Hartree/Particle)
Thermal correction to Energy= 0.242726
Thermal correction to Enthalpy= 0.243671
Thermal correction to Gibbs Free Energy= 0.185515
Sum of electronic and zero-point Energies= -953.779630
Sum of electronic and thermal Energies= -953.764827
Sum of electronic and thermal Enthalpies= -953.763883
Sum of electronic and thermal Free Energies= -953.822039

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	152.313	52.188	122.399

C,0,0.5906921147,-2.1448182089,-1.5339747512
C,0,0.7640095217,-2.1974436158,-0.1725103094
O,0,-0.0348047674,-0.3601786402,-0.8817049459
C,0,0.8287839458,0.7266050476,-1.1121750246
N,0,-0.2774913177,1.523722274,-0.8112221727
S,0,-0.4105104415,1.8878588673,0.800683094
O,0,-0.2075774599,3.3156647503,0.9492672007
O,0,0.3811959436,0.9920864707,1.6359099239
C,0,-0.5789597491,-2.6208377944,-2.3183351023
C,0,-0.2968641589,-2.6099038511,0.783807364
C,0,2.0722794224,-1.85266055,0.4490449979
C,0,-2.120693234,1.549643616,1.0843086045
H,0,1.464423721,-1.8798485898,-2.1181198882
H,0,1.1306184584,0.8143110102,-2.1531056839
H,0,1.6751456395,0.7388102972,-0.4278791419
H,0,-0.7650306265,-1.9510342731,-3.1552549125
H,0,-1.4874421386,-2.677191725,-1.7275209513
H,0,-0.3772163254,-3.6119409322,-2.7299304707
H,0,-0.0090711102,-3.5414997454,1.2752239663
H,0,-1.2652449522,-2.755274978,0.3177683934
H,0,-0.3897739482,-1.849345314,1.5591584505
H,0,1.9406992935,-1.0290941372,1.1528600788
H,0,2.8260051272,-1.5806791772,-0.2863817079
H,0,2.445438919,-2.7051618614,1.0196739379
H,0,-2.3378498978,1.8343653251,2.109877069
H,0,-2.3002420295,0.4914359501,0.9298100274
H,0,-2.7058507475,2.146261849,0.3926744356

MPW1K/6-31+G* (Onsager)

```
E(RmPW+HF-PW91) =  -954.014252869

 Zero-point correction=                           0.227679 (Hartree/Particle)
 Thermal correction to Energy=                    0.242643
 Thermal correction to Enthalpy=                  0.243587
 Thermal correction to Gibbs Free Energy=         0.184617
 Sum of electronic and zero-point Energies=           -953.786574
 Sum of electronic and thermal Energies=              -953.771610
 Sum of electronic and thermal Enthalpies=            -953.770666
 Sum of electronic and thermal Free Energies=         -953.829636

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 152.261             52.340            124.113

 C,0,0.5558146894,-2.1941560092,-1.481077995
 C,0,0.7426912325,-2.280288347,-0.1283936199
 O,0,-0.0004957228,-0.3080378328,-0.8142972241
 C,0,0.9356330582,0.7002634086,-1.043784911
 N,0,-0.1714198206,1.5415264784,-0.844815682
 S,0,-0.4236575088,1.9772895307,0.7359023793
 O,0,-0.5597961561,3.4243579233,0.754941037
 O,0,0.5349042321,1.365738853,1.6454247745
 C,0,-0.6405857169,-2.6046213011,-2.2595182826
 C,0,-0.3176284753,-2.7012922751,0.8259177193
 C,0,2.0752850214,-2.0071384509,0.4790286684
 C,0,-2.0175875594,1.2855169454,1.060570557
 H,0,1.4304971985,-1.9478639616,-2.0722159896
 H,0,1.2987985375,0.7329090024,-2.0678970581
 H,0,1.7318304568,0.7244138039,-0.3031584817
 H,0,-0.8138734545,-1.9103778723,-3.0791849054
 H,0,-1.5435502369,-2.652394579,-1.6594364026
 H,0,-0.4757994848,-3.5903943514,-2.6987032829
 H,0,-0.10252491,-3.7080412392,1.1907109072
 H,0,-1.3100446385,-2.7118524173,0.3881937311
 H,0,-0.320040953,-2.041883512,1.6935766893
 H,0,1.9990028551,-1.2103265269,1.2207168756
 H,0,2.8227227392,-1.7352902336,-0.2628419227
 H,0,2.4301520684,-2.8962157053,1.0037109806
 H,0,-2.3096067471,1.6054688169,2.0568935661
 H,0,-1.945467983,0.2054454237,1.0060468311
 H,0,-2.7122688871,1.6629101402,0.3178586521
```

B3PW91/6-31G* (gas phase)

```
Filename: b3pw91

E(RB+HF-PW91) = -953.927497137

Zero-point correction=                           0.221702 (Hartree/Particle)
 Thermal correction to Energy=                    0.236925
 Thermal correction to Enthalpy=                  0.237870
 Thermal correction to Gibbs Free Energy=         0.178453
 Sum of electronic and zero-point Energies=           -953.705795
 Sum of electronic and thermal Energies=              -953.690572
 Sum of electronic and thermal Enthalpies=            -953.689628
 Sum of electronic and thermal Free Energies=         -953.749044

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

```
 Total                  148.673             53.488            125.052

C,0,0.6080337562,-2.2276342751,-1.5225311458
 C,0,0.8049938964,-2.3185691635,-0.1550286643
 O,0,-0.0383129584,-0.4569338809,-0.8603672334
 C,0,0.8150315603,0.6529505471,-1.0758819184
 N,0,-0.3036664402,1.4638534477,-0.7856417159
 S,0,-0.4148109413,1.8506754027,0.8485986814
 O,0,-0.1197877982,3.2826010756,0.9736986394
 O,0,0.3128497443,0.9091573573,1.718188089
 C,0,-0.5593939476,-2.7243781072,-2.310607948
 C,0,-0.2422262408,-2.7722667788,0.8088438563
 C,0,2.1212452668,-1.9576498015,0.4575399464
 C,0,-2.1676372032,1.6205734841,1.1168599898
 H,0,1.4763773055,-1.9369533029,-2.1141488593
 H,0,1.1333196084,0.7555955467,-2.1199350635
 H,0,1.6672978555,0.6749051479,-0.3861022291
 H,0,-0.7705622984,-2.041427153,-3.1390651101
 H,0,-1.4671197985,-2.8168603096,-1.7108802402
 H,0,-0.3335331936,-3.7086567351,-2.7438232854
 H,0,0.0920437101,-3.6806922552,1.3280318884
 H,0,-1.2047193129,-2.9798584938,0.3389144187
 H,0,-0.3827792393,-1.9956210304,1.5703456525
 H,0,1.9829966357,-1.1407176117,1.177700314
 H,0,2.8640573654,-1.6570319639,-0.2871615871
 H,0,2.5232515112,-2.8135333705,1.0165503213
 H,0,-2.3819674522,1.9362582794,2.1405779421
 H,0,-2.4107100007,0.5664560335,0.9764101167
 H,0,-2.7112913905,2.2414229113,0.4030861446
```

BB1K/6-31G* (gas phase)

```
Filename: bb95

E(RB+HF-B95) = -953.922255508

Zero-point correction=                           0.228031 (Hartree/Particle)
 Thermal correction to Energy=                    0.242355
 Thermal correction to Enthalpy=                  0.243299
 Thermal correction to Gibbs Free Energy=         0.187477
 Sum of electronic and zero-point Energies=           -953.694224
 Sum of electronic and thermal Energies=              -953.679901
 Sum of electronic and thermal Enthalpies=            -953.678957
 Sum of electronic and thermal Free Energies=         -953.734778

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 152.080             51.933            117.487

 C,0,0.5781044987,-2.2098083677,-1.5014813195
 C,0,0.7498153909,-2.2050487681,-0.1376892292
 O,0,-0.0000234185,-0.4122375123,-0.8959065392
 C,0,0.8943213686,0.6585531678,-1.0947727115
 N,0,-0.1913563357,1.4861678769,-0.7995770221
 S,0,-0.3702542135,1.7335620198,0.8264702393
 O,0,-0.2267720556,3.1498311302,1.088823207
 O,0,0.4334271641,0.8008784441,1.609624528
 C,0,-0.6071004651,-2.6765910202,-2.2636003647
 C,0,-0.3209033931,-2.5251932951,0.839636103
 C,0,2.068134564,-1.8723590655,0.4642810748
 C,0,-2.0689351341,1.3046770842,1.0478972624
 H,0,1.4593558089,-1.9927400054,-2.093377058
 H,0,1.2162451743,0.7535414197,-2.129082287
```

H,0,1.7297267548,0.6347128971,-0.3972966992
H,0,-0.784565184,-2.0212041361,-3.1129774748
H,0,-1.5091413093,-2.6964036976,-1.6612043734
H,0,-0.4342378731,-3.6810954908,-2.6534752908
H,0,-0.0480969431,-3.4095863381,1.4171200334
H,0,-1.2872792112,-2.6995470515,0.3796094615
H,0,-0.4020831183,-1.6897336503,1.5362294104
H,0,1.9504672921,-1.0346020943,1.1536978599
H,0,2.8160725548,-1.6248858068,-0.285267151
H,0,2.4330550425,-2.7214667035,1.044563947
H,0,-2.3236857045,1.5036373074,2.0845366065
H,0,-2.1930751575,0.2532753087,0.8120551729
H,0,-2.6682360969,1.9193313473,0.3853336143

BPW91/6-31G* (gas phase)

Filename: bpw91

E(RB-PW91) = -954.134645397

Zero-point correction= 0.215021 (Hartree/Particle)
Thermal correction to Energy= 0.230765
Thermal correction to Enthalpy= 0.231709
Thermal correction to Gibbs Free Energy= 0.170869
Sum of electronic and zero-point Energies= -953.919625
Sum of electronic and thermal Energies= -953.903880
Sum of electronic and thermal Enthalpies= -953.902936
Sum of electronic and thermal Free Energies= -953.963777

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	144.807	55.102	128.049

C,0,0.6056865935,-2.2408780201,-1.5308218534
C,0,0.8455933805,-2.3851992829,-0.1644129064
O,0,-0.0379012038,-0.4515036727,-0.8451553194
C,0,0.8215908888,0.6690396971,-1.0287126071
N,0,-0.3253207621,1.4894686142,-0.7861915991
S,0,-0.4619397827,1.9166109481,0.8686634781
O,0,-0.118144865,3.3620607297,0.9462878565
O,0,0.2125029485,0.9686879277,1.8009550782
C,0,-0.5835049979,-2.7279123932,-2.3060164657
C,0,-0.1776361931,-2.8803423863,0.8163112541
C,0,2.1854623957,-2.034284682,0.4207674926
C,0,-2.2514163893,1.7506011665,1.0883791528
H,0,1.4628996989,-1.9308866229,-2.1411835484
H,0,1.1858216744,0.7837352393,-2.0653903631
H,0,1.6524132506,0.7051065743,-0.3011276487
H,0,-0.8078611837,-2.0345158702,-3.1307526667
H,0,-1.486676177,-2.8220696742,-1.6875436416
H,0,-0.3702425216,-3.7166030897,-2.7536170497
H,0,0.1868636127,-3.794554373,1.3198032537
H,0,-1.1500180964,-3.1047438282,0.3588253205
H,0,-0.3271336158,-2.118315673,1.6003751424
H,0,2.0716662294,-1.2430130227,1.1825695322
H,0,2.9037502081,-1.6944529211,-0.3405416204
H,0,2.6194145581,-2.9109796983,0.9359698268
H,0,-2.4857064611,2.1067492262,2.1011967106
H,0,-2.52398157,0.6941133777,0.9717027215
H,0,-2.7532016196,2.36974671,0.3338314695

MPW3LYP/6-31G* (gas phase)

Filename: mpw3lyp

E(RmPW+HF-LYP) = -954.186869532

Zero-point correction= 0.221411 (Hartree/Particle)
 Thermal correction to Energy= 0.236516
 Thermal correction to Enthalpy= 0.237460
 Thermal correction to Gibbs Free Energy= 0.178832
 Sum of electronic and zero-point Energies= -953.965458
 Sum of electronic and thermal Energies= -953.950354
 Sum of electronic and thermal Enthalpies= -953.949409
 Sum of electronic and thermal Free Energies= -954.008037

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.416	53.532	123.392

C,0,0.6143517827,-2.2462677703,-1.5270742026
 C,0,0.789381446,-2.2944881753,-0.1528701058
 O,0,-0.0342056588,-0.4477149144,-0.9028933161
 C,0,0.8201153334,0.6741659241,-1.113272364
 N,0,-0.2803702575,1.501643719,-0.7909624479
 S,0,-0.390137932,1.8278725137,0.8651940246
 O,0,-0.1173899493,3.2615401399,1.0477150462
 O,0,0.35643773,0.8614505738,1.7004011847
 C,0,-0.552177561,-2.7499369453,-2.3186106307
 C,0,-0.2795582641,-2.7029677573,0.8132443514
 C,0,2.1037830889,-1.9318686572,0.4711992437
 C,0,-2.1466435152,1.5551373021,1.1343975824
 H,0,1.4926156487,-1.9810513332,-2.114310126
 H,0,1.1192560336,0.7894012425,-2.161067569
 H,0,1.6862646011,0.6737958452,-0.4422283883
 H,0,-0.7524719394,-2.0775187607,-3.1582887748
 H,0,-1.4642107944,-2.8286708863,-1.7239728595
 H,0,-0.3288151091,-3.7414232549,-2.7363867826
 H,0,0.0328064867,-3.6010302063,1.3629786107
 H,0,-1.2398955452,-2.9069427209,0.3377986779
 H,0,-0.4122309293,-1.8998789888,1.548561564
 H,0,1.9617656714,-1.0940295367,1.1660272932
 H,0,2.8604788308,-1.6602089583,-0.2704402564
 H,0,2.4860517626,-2.777465618,1.0587287008
 H,0,-2.3596017382,1.8239623122,2.1713613096
 H,0,-2.368681122,0.5032906263,0.9500269004
 H,0,-2.7039381003,2.1948692854,0.4489143342

MPWB1K/6-31G* (gas phase)

Filename: mpwb1k

E(RmPW+HF-B95) = -953.919326994

Zero-point correction= 0.228640 (Hartree/Particle)
 Thermal correction to Energy= 0.242928
 Thermal correction to Enthalpy= 0.243872
 Thermal correction to Gibbs Free Energy= 0.188136
 Sum of electronic and zero-point Energies= -953.690687
 Sum of electronic and thermal Energies= -953.676399
 Sum of electronic and thermal Enthalpies= -953.675455
 Sum of electronic and thermal Free Energies= -953.731191

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	152.440	51.800	117.307

```
C,0,0.5762501598,-2.2075678352,-1.4997257347
 C,0,0.7489208444,-2.2003025628,-0.1376465374
 O,0,0.0007987904,-0.4092468491,-0.8978319324
 C,0,0.8974361985,0.6574373469,-1.0958081184
 N,0,-0.1866422642,1.4840452843,-0.7983759346
 S,0,-0.3682196084,1.7217057311,0.8261455356
 O,0,-0.2280810713,3.1345057643,1.0983397695
 O,0,0.4358384082,0.7863432809,1.6027834298
 C,0,-0.6121520818,-2.6693178246,-2.2576887756
 C,0,-0.3214111896,-2.5134743094,0.8403601849
 C,0,2.0665989649,-1.8676111833,0.4627081196
 C,0,-2.0637904071,1.28844704,1.0426465572
 H,0,1.4565787689,-1.9935531181,-2.0929342156
 H,0,1.2183887657,0.7527898463,-2.1295306353
 H,0,1.732224421,0.6313035134,-0.398804456
 H,0,-0.7893873652,-2.0132071232,-3.1056648342
 H,0,-1.5115144957,-2.684435451,-1.6522898684
 H,0,-0.4456574509,-3.6739356669,-2.6477367615
 H,0,-0.0484482265,-3.3923606648,1.424668725
 H,0,-1.286822182,-2.6917853268,0.3812835701
 H,0,-0.4026379485,-1.6726959061,1.5296319752
 H,0,1.9492376457,-1.0293339522,1.1507829314
 H,0,2.8134695054,-1.621606392,-0.2874625781
 H,0,2.4310640846,-2.7156750404,1.0434120606
 H,0,-2.319641701,1.4783988383,2.0799876962
 H,0,-2.1864094232,0.2394968017,0.7978894237
 H,0,-2.6630111422,1.9073007588,0.3850314035
```

MPW1B95/6-31G* (gas phase)

```
Filename: mpwb95

E(RmPW+HF-B95) = -953.954312502

Zero-point correction=                           0.224836 (Hartree/Particle)
 Thermal correction to Energy=                    0.239323
 Thermal correction to Enthalpy=                  0.240267
 Thermal correction to Gibbs Free Energy=         0.184198
 Sum of electronic and zero-point Energies=           -953.729477
 Sum of electronic and thermal Energies=              -953.714990
 Sum of electronic and thermal Enthalpies=            -953.714046
 Sum of electronic and thermal Free Energies=         -953.770115

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                150.177             52.610           118.008

C,0,0.5765828929,-2.2164203646,-1.5073950707
 C,0,0.7480894467,-2.2094748257,-0.1386292821
 O,0,-0.0032273501,-0.4088627915,-0.9036676698
 C,0,0.8942933024,0.6645719751,-1.1015952582
 N,0,-0.1911780931,1.5037166485,-0.8041669942
 S,0,-0.3625269648,1.7439934525,0.8361662583
 O,0,-0.2210921687,3.1685090074,1.0970973293
 O,0,0.4480240124,0.8067340597,1.6209608999
 C,0,-0.6091253505,-2.6872953929,-2.2704029317
 C,0,-0.3258640657,-2.5304600437,0.8388394788
 C,0,2.0674872576,-1.8728897623,0.4646689165
 C,0,-2.0676514609,1.3069540763,1.0595754905
 H,0,1.4607164934,-1.9983282644,-2.1004881072
 H,0,1.2170813263,0.7646129223,-2.1392125382
 H,0,1.7348442962,0.6387439884,-0.4042463827
 H,0,-0.7873797422,-2.0328965467,-3.1243377594
```

H,0,-1.5142798285,-2.7072673405,-1.6669124397
H,0,-0.4348411585,-3.6955449165,-2.6592080675
H,0,-0.05669219,-3.4206887487,1.4152104307
H,0,-1.2958141962,-2.6994280319,0.3766931689
H,0,-0.4045377293,-1.695642727,1.5414065664
H,0,1.947699714,-1.0263759202,1.1484926031
H,0,2.8196162871,-1.6305376469,-0.2868813271
H,0,2.4323823383,-2.7184390901,1.0560542041
H,0,-2.3217525241,1.5011761937,2.1004113907
H,0,-2.1870630475,0.2530871536,0.8178518897
H,0,-2.6708114972,1.9241179361,0.3978862019

MPWLYP1M/6-31G* (gas phase)

Filename: mpwlyp

E(RmPW+HF-LYP) = -953.954553874

Zero-point correction= 0.215963 (Hartree/Particle)
Thermal correction to Energy= 0.231465
Thermal correction to Enthalpy= 0.232409
Thermal correction to Gibbs Free Energy= 0.172795
Sum of electronic and zero-point Energies= -953.738591
Sum of electronic and thermal Energies= -953.723089
Sum of electronic and thermal Enthalpies= -953.722145
Sum of electronic and thermal Free Energies= -953.781759

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	145.246	54.840	125.469

C,0,0.6265022616,-2.2689768125,-1.5434700706
C,0,0.8038276067,-2.3175248096,-0.1593865356
O,0,-0.0403625209,-0.4586962853,-0.9172245399
C,0,0.8053535564,0.6853532802,-1.1159871313
N,0,-0.3064862428,1.522616616,-0.7927630384
S,0,-0.3985877864,1.8512876749,0.8918543824
O,0,-0.0782738268,3.29367544,1.0656514032
O,0,0.3196812404,0.854671228,1.7445457897
C,0,-0.5394579288,-2.7887265719,-2.3381725072
C,0,-0.2670838713,-2.739047274,0.810491267
C,0,2.1242419624,-1.9477471201,0.4654721624
C,0,-2.184938409,1.6309987924,1.1574012925
H,0,1.5075152456,-1.9968940453,-2.1336693772
H,0,1.1088922468,0.8168406643,-2.1675684008
H,0,1.6777872364,0.6895650106,-0.4422208771
H,0,-0.7415018232,-2.1231435313,-3.1899164198
H,0,-1.4578895089,-2.8687359923,-1.743323055
H,0,-0.308150534,-3.7882617531,-2.7484372061
H,0,0.0517396058,-3.6420871131,1.3601815416
H,0,-1.2311243894,-2.9485994186,0.3322226605
H,0,-0.4072932317,-1.9369217343,1.5536458419
H,0,1.9805954858,-1.1093230378,1.1679331732
H,0,2.8811834579,-1.6668914959,-0.2805445974
H,0,2.516481672,-2.7966397712,1.0526352619
H,0,-2.3928364438,1.9102122977,2.1981517911
H,0,-2.4362450001,0.5800925477,0.9734507792
H,0,-2.7205900608,2.2885682146,0.4632174098

PBE1KCIS/6-31G* (gas phase)

Filename: pbe1kcis

```
E(RPBE+HF-KCIS) = -953.412515317

 Zero-point correction=                           0.221768 (Hartree/Particle)
 Thermal correction to Energy=                    0.236757
 Thermal correction to Enthalpy=                  0.237701
 Thermal correction to Gibbs Free Energy=         0.179457
 Sum of electronic and zero-point Energies=           -953.190748
 Sum of electronic and thermal Energies=              -953.175758
 Sum of electronic and thermal Enthalpies=            -953.174814
 Sum of electronic and thermal Free Energies=         -953.233059

C,0,0.6021494834,-2.2235872581,-1.5202425972
 C,0,0.7913759503,-2.2966831915,-0.1495726014
 O,0,-0.0320845449,-0.4462425808,-0.8841682596
 C,0,0.8251313108,0.6602270936,-1.0951937947
 N,0,-0.2814522849,1.4788387953,-0.7914395935
 S,0,-0.3986800079,1.8265329489,0.8497871331
 O,0,-0.134174756,3.2606648373,1.0085172066
 O,0,0.3479656451,0.8802650709,1.6997370932
 C,0,-0.5625167068,-2.7207018229,-2.3070839632
 C,0,-0.2662641787,-2.7161897657,0.8144434306
 C,0,2.1053405896,-1.9422655279,0.4647019008
 C,0,-2.1410982712,1.5511254349,1.1154056085
 H,0,1.4783725275,-1.951407031,-2.1099748584
 H,0,1.1374616773,0.7700743339,-2.1415556322
 H,0,1.685853287,0.6689551604,-0.4140826636
 H,0,-0.7693704112,-2.0431212261,-3.1414187832
 H,0,-1.4735410009,-2.8060858989,-1.7107241591
 H,0,-0.3405167871,-3.7086439429,-2.7339673532
 H,0,0.0551031344,-3.6114308407,1.3636808367
 H,0,-1.2276484538,-2.9285177535,0.3438063709
 H,0,-0.4047297049,-1.9162868196,1.5533078065
 H,0,1.970606068,-1.111836553,1.1710496149
 H,0,2.8582144085,-1.6623544894,-0.278122536
 H,0,2.4929052045,-2.7925828924,1.0422022323
 H,0,-2.3619104887,1.8377517257,2.146670104
 H,0,-2.3606375472,0.4946848974,0.9509794211
 H,0,-2.7028741419,2.1744822961,0.4174290363
```

PBE1W/6-31G* (gas phase)

```
Filename: pbepbe

E(RPBE+HF-PBE) = -1028.17773542

Zero-point correction=                           0.333271 (Hartree/Particle)
 Thermal correction to Energy=                    0.344838
 Thermal correction to Enthalpy=                  0.345782
 Thermal correction to Gibbs Free Energy=         0.295402
 Sum of electronic and zero-point Energies=          -1027.844464
 Sum of electronic and thermal Energies=             -1027.832898
 Sum of electronic and thermal Enthalpies=           -1027.831954
 Sum of electronic and thermal Free Energies=        -1027.882333

C,0,-0.5495717198,-2.2810503943,-1.944573432
 C,0,0.4827945884,-1.8961950584,-1.2818085014
 C,0,0.631117475,-1.9026364142,-0.1092310317
 C,0,1.7603333384,-1.5892442175,0.4241420107
 C,0,-0.2928858059,-2.2084912098,0.7313323773
 O,0,-0.0484154548,-0.3237818637,-0.7054581402
 C,0,0.7305409413,0.544534958,-0.9550470196
 N,0,-0.2180942745,1.2097410158,-0.6438483017
 S,0,-0.3980637822,1.5079763982,0.7001455925
```

C,0,-1.821712688,1.0688136348,0.960140672
O,0,-0.3413009743,2.7483811932,0.8761792532
O,0,0.3673183582,0.7915728905,1.4047072492
H,0,1.2208837981,-1.6859890225,-1.7860316994
H,0,0.9611083301,0.5929068723,-1.8463572069
H,0,1.4648239862,0.5576725102,-0.397441278
H,0,-0.7455714937,-1.6735250429,-2.6070181366
H,0,-1.2921925387,-2.3741741143,-1.4142088899
H,0,-0.3817446379,-3.0906659174,-2.3507867409
H,0,-0.0477283795,-2.9579472906,1.2072778056
H,0,-1.1045565378,-2.3673087832,0.3345484765
H,0,-0.3814187472,-1.5152835445,1.3316817533
H,0,1.6375299514,-0.8720592545,0.9916237643
H,0,2.4015591761,-1.3799672002,-0.1998931796
H,0,2.0701778921,-2.2924599297,0.932223857
H,0,-2.0073687981,1.262392996,1.8392442013
H,0,-1.8932743758,0.1674286586,0.804038103
H,0,-2.3794676275,1.5425831299,0.4053414421

PBELYP1W/6-31G* (gas phase)

Filename: pbev5lyp

E(RPBE+HF-V5LYP) = -1007.70225710

Zero-point correction= 0.308074 (Hartree/Particle)
Thermal correction to Energy= 0.320118
Thermal correction to Enthalpy= 0.321062
Thermal correction to Gibbs Free Energy= 0.269660
Sum of electronic and zero-point Energies= -1007.394183
Sum of electronic and thermal Energies= -1007.382139
Sum of electronic and thermal Enthalpies= -1007.381195
Sum of electronic and thermal Free Energies= -1007.432597

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.877	42.577	108.185

C,0,-0.5658292946,-2.3511176753,-2.0176643383
C,0,0.5035883165,-1.9544957241,-1.3247668005
C,0,0.6470527924,-1.9532079148,-0.1104101761
C,0,1.8158719348,-1.6300952056,0.4503898246
C,0,-0.3197584743,-2.2551042583,0.7580646052
O,0,-0.0531013983,-0.3029140587,-0.7469153337
C,0,0.7574677674,0.609155671,-0.9865701775
N,0,-0.2115786199,1.3167095489,-0.6616752049
S,0,-0.396810137,1.5910881,0.7429001301
C,0,-1.8767773715,1.1330704011,1.000696635
O,0,-0.3366862244,2.8674858618,0.9520554558
O,0,0.3902439651,0.8307955788,1.4535073715
H,0,1.2743966278,-1.7441750833,-1.8440270139
H,0,0.9971424886,0.6683186025,-1.9099865141
H,0,1.5175705082,0.5978963715,-0.40689781
H,0,-0.7575085837,-1.7233153174,-2.7129061916
H,0,-1.3426996605,-2.4335891492,-1.471346289
H,0,-0.3975060878,-3.1985927339,-2.4306565399
H,0,-0.070703085,-3.027149494,1.2667339533
H,0,-1.1598376053,-2.4244366594,0.3406700788
H,0,-0.4148321891,-1.5242673792,1.3697785203
H,0,1.6886704356,-0.8812620106,1.0354554182
H,0,2.4857566866,-1.4190493637,-0.1970910136
H,0,2.1315901122,-2.3610330105,0.9825895318
H,0,-2.0747318245,1.3193065431,1.9161594309
H,0,-1.9519988061,0.1992715641,0.8230646908

H,0,-2.4541722733,1.6339317953,0.4297707567

RHF/6-31G* (gas phase)

Filename: rhf

E(RHF) = -950.075192665

Zero-point correction=	0.237829 (Hartree/Particle)
Thermal correction to Energy=	0.252037
Thermal correction to Enthalpy=	0.252981
Thermal correction to Gibbs Free Energy=	0.196231
Sum of electronic and zero-point Energies=	-949.837363
Sum of electronic and thermal Energies=	-949.823156
Sum of electronic and thermal Enthalpies=	-949.822212
Sum of electronic and thermal Free Energies=	-949.878962

C,0,0.6327820007,-2.2421735355,-1.5086662073
C,0,0.7924151815,-2.3000878997,-0.1537803862
O,0,-0.0277609315,-0.4678318814,-0.831717522
C,0,0.7933075631,0.6804756706,-1.1003591928
N,0,-0.3088394818,1.4312306544,-0.7610153897
S,0,-0.4167769801,1.8546945071,0.8165579997
O,0,-0.1701985261,3.2633828985,0.9493215597
O,0,0.3516462604,0.9663884909,1.6596037345
C,0,-0.535703774,-2.7123852903,-2.3244287802
C,0,-0.2740092531,-2.7316893466,0.8097686392
C,0,2.1110159509,-1.9627164507,0.4846677343
C,0,-2.1322982924,1.5796148649,1.1391571074
H,0,1.5056040398,-1.9772435186,-2.0816233645
H,0,1.0438615376,0.7360003085,-2.1481557408
H,0,1.6605871856,0.6935259945,-0.4601866603
H,0,-0.7075756856,-2.0277338629,-3.1465358991
H,0,-1.4484457569,-2.7792776278,-1.7511882711
H,0,-0.3238756119,-3.6907630924,-2.7483234979
H,0,0.030992181,-3.6548284217,1.2958267296
H,0,-1.2330512313,-2.8930268081,0.3418901602
H,0,-0.382040683,-1.9733422102,1.5770284705
H,0,1.978686929,-1.1634799911,1.2054059696
H,0,2.8573525909,-1.6686463778,-0.2429111247
H,0,2.4843493876,-2.8314602713,1.0203922243
H,0,-2.3232700287,1.8968138431,2.155482978
H,0,-2.3523994804,0.5291800272,1.0208306123
H,0,-2.7133750915,2.1710443262,0.4471291177

TPSS1KCIS/6-31G* (gas phase)

Filename: tpsskcis

E(RTPSS+HF-KCIS) = -954.215717575

Zero-point correction=	0.221923 (Hartree/Particle)
Thermal correction to Energy=	0.237091
Thermal correction to Enthalpy=	0.238035
Thermal correction to Gibbs Free Energy=	0.179432
Sum of electronic and zero-point Energies=	-953.993794
Sum of electronic and thermal Energies=	-953.978626
Sum of electronic and thermal Enthalpies=	-953.977682
Sum of electronic and thermal Free Energies=	-954.036286

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.777	53.669	123.342

C,0,0.603844396,-2.2332901752,-1.5246925275
C,0,0.7920951482,-2.2989093322,-0.1505608931
O,0,-0.0189519369,-0.4537099282,-0.8732364736
C,0,0.8380015759,0.669853831,-1.0853789112
N,0,-0.280106417,1.4883324907,-0.7969037868
S,0,-0.4027365569,1.8492093989,0.8497877674
O,0,-0.1574753091,3.294660416,0.9949671048
O,0,0.3569777186,0.9149971243,1.7115460029
C,0,-0.5706746943,-2.726220985,-2.3103117533
C,0,-0.2680778779,-2.7236492887,0.8182903469
C,0,2.1158029251,-1.9498821969,0.4618535033
C,0,-2.1537259729,1.5540612581,1.1137909557
H,0,1.4758018014,-1.9616664758,-2.1161531875
H,0,1.1539403515,0.7692933583,-2.127464696
H,0,1.6859060235,0.6844606745,-0.3944246435
H,0,-0.7740539135,-2.0481001622,-3.1425415519
H,0,-1.4762589345,-2.8066105346,-1.7085790245
H,0,-0.3521940835,-3.7143762103,-2.7348033928
H,0,0.0423689897,-3.6407771063,1.3340889561
H,0,-1.2344093449,-2.9040141552,0.3482720904
H,0,-0.3847415476,-1.9443704883,1.5784645537
H,0,1.9877046183,-1.1285994811,1.1759279351
H,0,2.8593807614,-1.664094383,-0.2856768183
H,0,2.5052690068,-2.8083676403,1.0228747995
H,0,-2.3791026303,1.8483648156,2.1395827012
H,0,-2.3563084905,0.4951996901,0.9583148502
H,0,-2.7152956066,2.1638704859,0.4071370926

TPSSLYP1W/6-31G* (gas phase)

Filename: tpssv5lyp

E(RTPSS+HF-V5LYP) = -1029.05458335

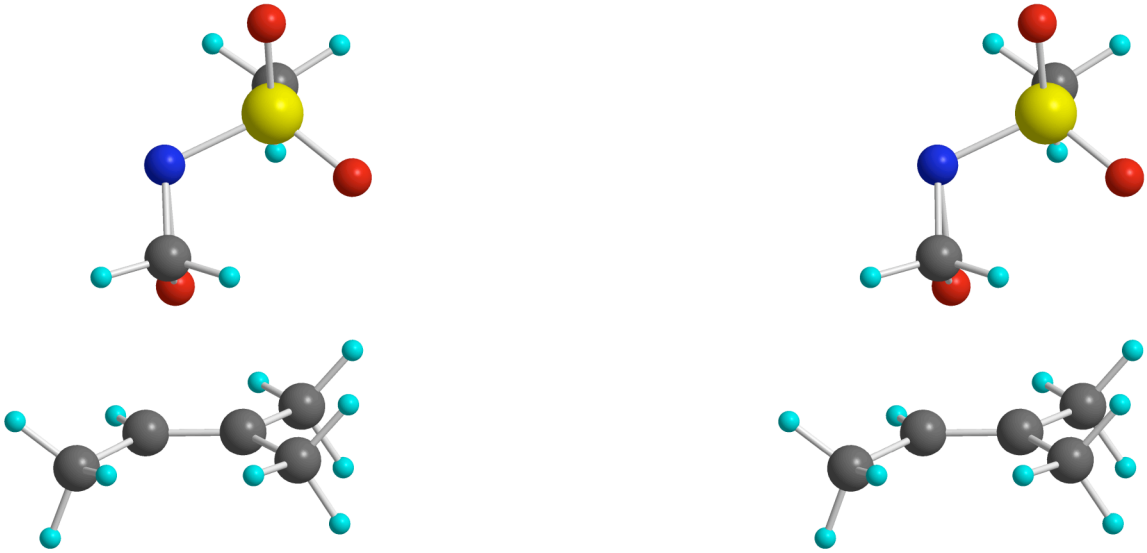
Zero-point correction=	0.336944 (Hartree/Particle)
Thermal correction to Energy=	0.348457
Thermal correction to Enthalpy=	0.349401
Thermal correction to Gibbs Free Energy=	0.299269
Sum of electronic and zero-point Energies=	-1028.717639
Sum of electronic and thermal Energies=	-1028.706127
Sum of electronic and thermal Enthalpies=	-1028.705183
Sum of electronic and thermal Free Energies=	-1028.755314

C,0,-0.5235887021,-2.4372222037,-1.9664691664
C,0,0.5236793454,-2.0460871262,-1.3196137505
C,0,0.6747607063,-2.0141786346,-0.1490654144
C,0,-0.2496703078,-2.291957573,0.7093522815
C,0,1.8112633355,-1.6838788625,0.3724849954
O,0,-0.0103218738,-0.4357763866,-0.762480797
C,0,0.7674706804,0.4407600056,-1.030167866
N,0,-0.1717852172,1.1150114851,-0.7012053631
S,0,-0.3449191072,1.3980651782,0.6478221243
O,0,0.4463450475,0.6918347191,1.3349394541
C,0,-1.7603920908,0.9204505209,0.9250389971
O,0,-0.3170437951,2.6376782872,0.8362553363
H,0,1.2537346267,-1.8481760393,-1.8339702367
H,0,0.9777461466,0.4804419099,-1.9230994097
H,0,1.5078635957,0.4472343159,-0.4873211982
H,0,-0.7277185999,-1.8337517149,-2.6275620932
H,0,-1.2538757332,-2.5249734201,-1.421583516
H,0,-0.3617480972,-3.2482487993,-2.3680110267
H,0,-0.0017189778,-3.0234513136,1.207628636
H,0,-1.0593595419,-2.4638234607,0.3184175405

```
H,0,-0.3360896105,-1.578506838,1.2822919273
H,0,1.6896284479,-0.9565035461,0.9228444523
H,0,2.4412925963,-1.4850745469,-0.2636035821
H,0,2.1271703684,-2.3760807593,0.8884162348
H,0,-1.9385319794,1.1037921995,1.8057576079
H,0,-1.8107977204,0.0204788671,0.7643760571
H,0,-2.3351135424,1.3823887363,0.3810877752
```

Epoxidation TS Isomer 9

B3LYP/6-31+G** (PCM)



```
E(RB+HF-LYP) = -954.242694686

Zero-point correction=                           0.218830 (Hartree/Particle)
 Thermal correction to Energy=                    0.234271
 Thermal correction to Enthalpy=                  0.235215
 Thermal correction to Gibbs Free Energy=         0.175540
 Sum of electronic and zero-point Energies=           -954.023864
 Sum of electronic and thermal Energies=              -954.008423
 Sum of electronic and thermal Enthalpies=            -954.007479
 Sum of electronic and thermal Free Energies=         -954.067155

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 147.007             54.328            125.598

 C,0,-1.5589331789,-2.0563971534,-0.8822884575
 C,0,-0.1979927504,-2.2519195265,-0.7709919799
 O,0,-0.8528997265,-0.1047137925,-0.2782401148
 C,0,-0.9363605548,0.2115714512,1.0974916206
 N,0,-0.7723883295,1.5556032697,0.6422487042
 S,0,0.847054168,2.0618081717,0.538706454
 O,0,1.8215350156,0.9790674801,0.8023127472
 O,0,0.9288376742,3.2777312846,1.3789736645
 C,0,-2.628746475,-2.4721643075,0.0795140322
 C,0,0.4753174715,-2.8440878898,0.4324320351
 C,0,0.7089055972,-1.9340698065,-1.9243568997
 C,0,0.9884783904,2.5602697654,-1.1808814677
 H,0,-1.9200333515,-1.6864609263,-1.8412920527
```

H,0,-0.1309198289,-0.223452391,1.6973008265
H,0,-1.9264755555,0.0529861023,1.5347840248
H,0,-3.3941056178,-1.6927039357,0.1603007813
H,0,-2.2572926721,-2.7025150235,1.0803474782
H,0,-3.1349964855,-3.3690114435,-0.3031429971
H,0,0.9361162635,-3.8023546598,0.1569100629
H,0,-0.1986867562,-3.023875071,1.2712611079
H,0,1.2906099627,-2.1916451949,0.7677310858
H,0,1.5258078174,-1.280057346,-1.5977144072
H,0,0.1744591048,-1.4527998609,-2.7468160356
H,0,1.1703003209,-2.8567096144,-2.3020465432
H,0,1.9801824966,3.0025897927,-1.2995329133
H,0,0.2077273784,3.2934659365,-1.3874392591
H,0,0.8731676216,1.6737106891,-1.8037724973

B3lYP/6-31+G** (gas phase)

Filename: b3BBgasPCMts9

E(RB+HF-LYP) = -954.227312703

Zero-point correction=	0.219494 (Hartree/Particle)
Thermal correction to Energy=	0.234767
Thermal correction to Enthalpy=	0.235711
Thermal correction to Gibbs Free Energy=	0.176494
Sum of electronic and zero-point Energies=	-954.007819
Sum of electronic and thermal Energies=	-953.992546
Sum of electronic and thermal Enthalpies=	-953.991602
Sum of electronic and thermal Free Energies=	-954.050819

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.318	54.092	124.633

C,0,-1.5766489109,-2.0953406491,-0.856735935
C,0,-0.2009316264,-2.2472366302,-0.7410191243
O,0,-0.9092292872,-0.2397544033,-0.3762407485
C,0,-1.0077486955,0.2165284307,0.9775240766
N,0,-0.7499549869,1.5264410129,0.5100773123
S,0,0.8999897769,1.9142994725,0.4744586445
O,0,1.7792496038,0.721772051,0.4716736734
O,0,1.1223466798,2.9378593053,1.5121725696
C,0,-2.6309704421,-2.5156659485,0.121585435
C,0,0.4939404673,-2.7448855874,0.4907431683
C,0,0.6947536422,-1.9561264521,-1.9081891081
C,0,1.0259604254,2.7182008062,-1.1299476286
H,0,-1.9480390014,-1.8062179535,-1.8363584228
H,0,-0.2613312058,-0.2532649702,1.6278154389
H,0,-2.0211257121,0.1272692749,1.3812631517
H,0,-3.4367432554,-1.7753817023,0.154022275
H,0,-2.2526744901,-2.661959855,1.1352571619
H,0,-3.0825025584,-3.4615833179,-0.206637906
H,0,1.0133853669,-3.6845920196,0.2610271609
H,0,-0.1762005982,-2.9264478492,1.332032474
H,0,1.2616699034,-2.0232958399,0.7946062888
H,0,1.4606375117,-1.2309808025,-1.6099134749
H,0,0.1419385977,-1.5583223381,-2.7621657112
H,0,1.2133489125,-2.8719460832,-2.2220872452
H,0,2.0461032391,3.0980323221,-1.2118158036
H,0,0.304024755,3.534689986,-1.1559628192
H,0,0.8154198887,1.9817757403,-1.9053859036

B3LYP/6-31+G** (Onsager)

Filename: b3BBonsts9

E(RB+HF-LYP) = -954.233576663

Zero-point correction=	0.219230 (Hartree/Particle)
Thermal correction to Energy=	0.234675
Thermal correction to Enthalpy=	0.235619
Thermal correction to Gibbs Free Energy=	0.175829
Sum of electronic and zero-point Energies=	-954.014347
Sum of electronic and thermal Energies=	-953.998902
Sum of electronic and thermal Enthalpies=	-953.997957
Sum of electronic and thermal Free Energies=	-954.057747

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.261	54.265	125.839

C,0,-1.5437445116,-2.0092887596,-0.8866719405
C,0,-0.1871812855,-2.2367288782,-0.7705884583
O,0,-0.8351256877,-0.0976506749,-0.2403383883
C,0,-0.8927531869,0.2085949155,1.1383981971
N,0,-0.7697293756,1.5641244071,0.7111671547
S,0,0.8373300924,2.1002580649,0.5587323493
O,0,1.8371582996,1.054829926,0.8645844998
O,0,0.9049082869,3.3752764287,1.3016780474
C,0,-2.6323657605,-2.441005086,0.0458198987
C,0,0.4605143334,-2.878231839,0.4213904878
C,0,0.7358648006,-1.9097403401,-1.9079339856
C,0,0.9368599656,2.4849395235,-1.1980895921
H,0,-1.8868829349,-1.6104081053,-1.8379598964
H,0,-0.0643501216,-0.218545103,1.7132201021
H,0,-1.8696429437,0.0186239104,1.5936055434
H,0,-3.3930950129,-1.6583381289,0.1334152226
H,0,-2.2782410772,-2.7012083348,1.0454647092
H,0,-3.1374207566,-3.3242590301,-0.367238124
H,0,0.8801037593,-3.8499141586,0.1285461736
H,0,-0.2230173891,-3.0485809363,1.2542620553
H,0,1.3008314641,-2.2661433692,0.7701788345
H,0,1.5648951309,-1.2838301073,-1.5573754369
H,0,0.2192496828,-1.3958895164,-2.7217256152
H,0,1.1766427304,-2.8320655742,-2.3092337825
H,0,1.9165857052,2.9362441601,-1.3670930813
H,0,0.1361308724,3.1854137657,-1.4361264828
H,0,0.8251439202,1.5573868401,-1.7582914917

MPW1K/6-31+G** (PCM)

E(RmPW+HF-PW91) = -954.050074826

Zero-point correction=	0.226408 (Hartree/Particle)
Thermal correction to Energy=	0.241210
Thermal correction to Enthalpy=	0.242154
Thermal correction to Gibbs Free Energy=	0.184017
Sum of electronic and zero-point Energies=	-953.823667
Sum of electronic and thermal Energies=	-953.808865
Sum of electronic and thermal Enthalpies=	-953.807921
Sum of electronic and thermal Free Energies=	-953.866057

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	151.362	52.483	122.359

```
C,0,-1.5392775757,-1.995454727,-0.8808751616
 C,0,-0.1869133936,-2.1706441878,-0.7598015666
 O,0,-0.8431869134,-0.1274709835,-0.2713709056
 C,0,-0.9418877839,0.1604429507,1.0929476957
 N,0,-0.7673128188,1.4831638098,0.6442660527
 S,0,0.8137323993,1.9601298756,0.5199930833
 O,0,1.7504014487,0.8764539589,0.7946569051
 O,0,0.9412921693,3.1728724514,1.3172090233
 C,0,-2.5976681175,-2.4234268568,0.070179371
 C,0,0.4814281194,-2.7547841618,0.4346266338
 C,0,0.7186707232,-1.8287762684,-1.8909664079
 C,0,0.9529263671,2.4101184695,-1.1786417619
 H,0,-1.8963790059,-1.6317794081,-1.8372359446
 H,0,-0.145823674,-0.2822762831,1.686716449
 H,0,-1.9316955654,-0.0030671609,1.5095264994
 H,0,-3.3668387978,-1.6572827191,0.1518909123
 H,0,-2.2261779903,-2.6512224393,1.0646101092
 H,0,-3.0885386104,-3.3191599511,-0.3138980757
 H,0,0.9564883789,-3.6963641444,0.1542657814
 H,0,-0.1917080413,-2.9527808115,1.2617736506
 H,0,1.2771678654,-2.0922242233,0.775294771
 H,0,1.5147390808,-1.1702808674,-1.5448429877
 H,0,0.1873201623,-1.3484482414,-2.7075390516
 H,0,1.19423662,-2.7340744482,-2.2717894502
 H,0,1.9475678148,2.8233478958,-1.3190646975
 H,0,0.1953533831,3.1549109289,-1.3974560605
 H,0,0.8107517558,1.5219435428,-1.7826758664
```

MPW1K/6-31+G** (gas phase)

```
Filename: mpBBgasPCMts9
E(RmPW+HF-PW91) = -954.033982853

Zero-point correction=                           0.227071 (Hartree/Particle)
 Thermal correction to Energy=                    0.241709
 Thermal correction to Enthalpy=                  0.242653
 Thermal correction to Gibbs Free Energy=         0.185285
 Sum of electronic and zero-point Energies=           -953.806911
 Sum of electronic and thermal Energies=              -953.792274
 Sum of electronic and thermal Enthalpies=            -953.791329
 Sum of electronic and thermal Free Energies=         -953.848698

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 151.675             52.276            120.743

C,0,-1.5616537571,-2.045743861,-0.8579341486
 C,0,-0.1968756309,-2.160567029,-0.7422673349
 O,0,-0.8997399791,-0.2148049268,-0.3534834103
 C,0,-1.0288139544,0.1813467636,0.9929133364
 N,0,-0.7555310921,1.4706141359,0.5296177648
 S,0,0.8621002654,1.8252384753,0.4817544504
 O,0,1.6920126439,0.62716925,0.5600333873
 O,0,1.1096061145,2.8876620703,1.4367926383
 C,0,-2.5937444152,-2.4791493485,0.1204308951
 C,0,0.5100737811,-2.645852083,0.472824216
 C,0,0.6860450703,-1.8280253721,-1.8929989031
 C,0,1.0191730457,2.5064457065,-1.1394267968
 H,0,-1.9384990174,-1.7518327636,-1.8277447701
 H,0,-0.2952724452,-0.298263672,1.6386760093
 H,0,-2.0442147452,0.0875728947,1.3687661783
 H,0,-3.3988539553,-1.748710024,0.1700524328
```

H,0,-2.2033984918,-2.6315813337,1.1217112348
H,0,-3.0399467468,-3.4185299179,-0.2092536973
H,0,1.0776902507,-3.5432752927,0.2239705853
H,0,-0.1503667954,-2.8838098073,1.2995596162
H,0,1.2294295918,-1.8905697693,0.7916069237
H,0,1.4333165595,-1.1030495987,-1.5718086394
H,0,0.1283776067,-1.4196357358,-2.7305807391
H,0,1.2153860732,-2.7210699819,-2.2279033736
H,0,2.0435344239,2.8504322996,-1.2422608049
H,0,0.32738742,3.336629054,-1.2253296928
H,0,0.7914461791,1.7352258675,-1.8659183576

MPW1K/6-31+G** (Onsager)

Filename: mpBBonsts9

E(RmPW+HF-PW91) = -954.040714342

Zero-point correction=	0.226889 (Hartree/Particle)
Thermal correction to Energy=	0.241667
Thermal correction to Enthalpy=	0.242611
Thermal correction to Gibbs Free Energy=	0.184551
Sum of electronic and zero-point Energies=	-953.813826
Sum of electronic and thermal Energies=	-953.799047
Sum of electronic and thermal Enthalpies=	-953.798103
Sum of electronic and thermal Free Energies=	-953.856163

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	151.648	52.407	122.198

C,0,-1.5327870325,-1.9697212687,-0.882608067
C,0,-0.1815963825,-2.154998365,-0.7606402545
O,0,-0.8352709925,-0.1170158954,-0.2517700567
C,0,-0.9240650665,0.1644048343,1.1131903587
N,0,-0.7669462472,1.4942255526,0.6854935388
S,0,0.8109605268,1.9799398101,0.540112807
O,0,1.7554261626,0.9140787877,0.8464741083
O,0,0.9339080403,3.233367901,1.2663584305
C,0,-2.5993166452,-2.4115264439,0.0521142231
C,0,0.4793537704,-2.7586618519,0.4282767797
C,0,0.7282432555,-1.8101712213,-1.8872022407
C,0,0.9308386347,2.3497522606,-1.1839151685
H,0,-1.882473708,-1.5936041442,-1.8342685763
H,0,-0.1182538686,-0.2780983972,1.6947827554
H,0,-1.9092912439,-0.0160516335,1.5343305814
H,0,-3.3696878741,-1.6475476503,0.1379786336
H,0,-2.2354544179,-2.6559602029,1.0451816176
H,0,-3.0857770492,-3.3015542759,-0.3491639704
H,0,0.9438968574,-3.7025560928,0.1395939206
H,0,-0.1991672264,-2.9611185616,1.2497315613
H,0,1.2795845076,-2.1062048581,0.7779405732
H,0,1.5366401748,-1.1720451883,-1.5314705326
H,0,0.2038988347,-1.3089483591,-2.6954173949
H,0,1.1840939796,-2.7172577072,-2.2865015525
H,0,1.9193949542,2.7649850162,-1.3535500402
H,0,0.1616125719,3.073039803,-1.4292909617
H,0,0.7909034841,1.4331131516,-1.7439630731

B3LYP/6-31G* (gas phase)

E(RB+HF-LYP) = -954.183501704

```
 Zero-point correction=                           0.221508 (Hartree/Particle)
 Thermal correction to Energy=                    0.236517
 Thermal correction to Enthalpy=                  0.237461
 Thermal correction to Gibbs Free Energy=         0.179352
 Sum of electronic and zero-point Energies=           -953.961993
 Sum of electronic and thermal Energies=              -953.946984
 Sum of electronic and thermal Enthalpies=            -953.946040
 Sum of electronic and thermal Free Energies=         -954.004150

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                148.417             53.526            122.303

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0   C     2.649638   -0.281205   -0.707056
    2          6             0   C     2.205013    0.793393    0.052621
    3          8             0   O     0.652612   -0.480693   -0.639731
    4          6             0   C     0.066817   -1.409399    0.278986
    5          7             0   N    -1.153095   -1.279145   -0.421638
    6         16             0   S    -2.117622   -0.021213    0.163400
    7          8             0   O    -1.361144    0.980908    0.947885
    8          8             0   O    -3.306439   -0.631019    0.780523
    9          6             0   C     3.299333   -1.541086   -0.222396
   10          6             0   C     2.166692    0.815360    1.551162
   11          6             0   C     1.762379    2.062052   -0.614833
   12          6             0   C    -2.628284    0.750135   -1.379935
   13          1             0   H     2.703094   -0.122129   -1.780995
   14          1             0   H     0.112481   -1.054022    1.314411
   15          1             0   H     0.481360   -2.418324    0.179168
   16          1             0   H     2.941117   -2.399818   -0.800452
   17          1             0   H     3.125106   -1.740854    0.837414
   18          1             0   H     4.385657   -1.483045   -0.378420
   19          1             0   H     2.818168    1.617757    1.923361
   20          1             0   H     2.484737   -0.120534    2.014584
   21          1             0   H     1.147209    1.049704    1.881886
   22          1             0   H     0.745499    2.307354   -0.286030
   23          1             0   H     1.773586    1.980036   -1.704912
   24          1             0   H     2.415925    2.894649   -0.319953
   25          1             0   H    -3.342051    1.537192   -1.126093
   26          1             0   H    -3.099972   -0.009107   -2.005312
   27          1             0   H    -1.748059    1.165496   -1.872298
```

B3LYP/6-31G* (Onsager)

```
E(RB+HF-LYP) =  -954.188616462

 Zero-point correction=                           0.221341 (Hartree/Particle)
 Thermal correction to Energy=                    0.236465
 Thermal correction to Enthalpy=                  0.237409
 Thermal correction to Gibbs Free Energy=         0.178657
 Sum of electronic and zero-point Energies=           -953.967275
 Sum of electronic and thermal Energies=              -953.952151
 Sum of electronic and thermal Enthalpies=            -953.951207
 Sum of electronic and thermal Free Energies=         -954.009959

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                148.384             53.627            123.655
```

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	2.642419	-0.288703	-0.734387
2	6	0	C	2.250502	0.777801	0.053892
3	8	0	O	0.567458	-0.494108	-0.593830
4	6	0	C	0.043519	-1.397009	0.363437
5	7	0	N	-1.180836	-1.303430	-0.354160
6	16	0	S	-2.158077	-0.018000	0.152572
7	8	0	O	-1.500126	0.877136	1.127515
8	8	0	O	-3.463959	-0.601522	0.508875
9	6	0	C	3.287752	-1.567646	-0.300401
10	6	0	C	2.290693	0.783587	1.553270
11	6	0	C	1.799307	2.061879	-0.578626
12	6	0	C	-2.368707	0.892245	-1.387294
13	1	0	H	2.631339	-0.123888	-1.808999
14	1	0	H	0.069419	-1.004586	1.385373
15	1	0	H	0.470957	-2.403156	0.295434
16	1	0	H	2.872916	-2.412762	-0.860902
17	1	0	H	3.183601	-1.771623	0.767890
18	1	0	H	4.361608	-1.533968	-0.530410
19	1	0	H	2.993713	1.553530	1.899094
20	1	0	H	2.596500	-0.169502	1.988859
21	1	0	H	1.302616	1.054130	1.946331
22	1	0	H	0.813996	2.341938	-0.186710
23	1	0	H	1.742331	1.986697	-1.667717
24	1	0	H	2.494607	2.873675	-0.324813
25	1	0	H	-3.080460	1.698033	-1.192556
26	1	0	H	-2.757427	0.207231	-2.142130
27	1	0	H	-1.400535	1.291280	-1.690587

BP86/6-31* (gas phase)

E(RB-P86) = -954.232178847

Zero-point correction= 0.214385 (Hartree/Particle)
Thermal correction to Energy= 0.229856
Thermal correction to Enthalpy= 0.230800
Thermal correction to Gibbs Free Energy= 0.171565
Sum of electronic and zero-point Energies= -954.017793
Sum of electronic and thermal Energies= -954.002323
Sum of electronic and thermal Enthalpies= -954.001379
Sum of electronic and thermal Free Energies= -954.060614

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	144.237	55.106	124.672

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.690467	-0.283055	-0.710824
2	6	0	2.230034	0.792168	0.053580
3	8	0	0.641235	-0.477260	-0.647694
4	6	0	0.071778	-1.394539	0.287036
5	7	0	-1.152308	-1.278809	-0.447011
6	16	0	-2.135364	-0.014595	0.165375
7	8	0	-1.388592	1.016016	0.949201

8	8	0	-3.311412	-0.673313	0.796683
9	6	0	3.326856	-1.550976	-0.222846
10	6	0	2.178704	0.804671	1.555668
11	6	0	1.796139	2.068893	-0.613991
12	6	0	-2.678700	0.745391	-1.386231
13	1	0	2.742225	-0.121237	-1.794551
14	1	0	0.093851	-1.021232	1.329080
15	1	0	0.486973	-2.417182	0.212082
16	1	0	2.956303	-2.416621	-0.800089
17	1	0	3.152787	-1.745555	0.847556
18	1	0	4.422791	-1.509239	-0.382442
19	1	0	2.831942	1.609044	1.946803
20	1	0	2.492192	-0.143108	2.020157
21	1	0	1.148549	1.041065	1.883103
22	1	0	0.771841	2.324625	-0.285930
23	1	0	1.809612	1.989191	-1.713198
24	1	0	2.458098	2.905414	-0.314727
25	1	0	-3.414343	1.522340	-1.126386
26	1	0	-3.139276	-0.033641	-2.010911
27	1	0	-1.803074	1.182462	-1.887336

MPW1K/6-31+G* (gas phase)

E(RmPW+HF-PW91) = -954.006948184

Zero-point correction= 0.228239 (Hartree/Particle)
Thermal correction to Energy= 0.242838
Thermal correction to Enthalpy= 0.243782
Thermal correction to Gibbs Free Energy= 0.186493
Sum of electronic and zero-point Energies= -953.778710
Sum of electronic and thermal Energies= -953.764110
Sum of electronic and thermal Enthalpies= -953.763166
Sum of electronic and thermal Free Energies= -953.820455

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	152.383	52.073	120.576

C,0,-1.5565380241,-2.0392896417,-0.8585108692
C,0,-0.1935253835,-2.1694254282,-0.7403048061
O,0,-0.8907101436,-0.2171452851,-0.3489626409
C,0,-1.0144874409,0.175920883,0.9981167255
N,0,-0.7535616843,1.4677946507,0.5362015361
S,0,0.8603724129,1.8374777047,0.4802998298
O,0,1.7027036837,0.6483890972,0.5522790063
O,0,1.1016885313,2.9019399458,1.4345192153
C,0,-2.5975093839,-2.4660783223,0.1141444615
C,0,0.5054459235,-2.6677323083,0.4745778363
C,0,0.6955090533,-1.840907099,-1.8878872768
C,0,1.0013741907,2.5224951518,-1.1418068408
H,0,-1.9288868305,-1.7392619235,-1.8284483789
H,0,-0.2749533443,-0.3004746119,1.6390548558
H,0,-2.0272006831,0.0737659661,1.3787808218
H,0,-3.3973910517,-1.7285989578,0.1611390301
H,0,-2.2146682742,-2.6235490847,1.1183345266
H,0,-3.0505452906,-3.4019893067,-0.2190272275
H,0,1.0501647884,-3.5811354888,0.2280617337
H,0,-0.1578807843,-2.8875390836,1.3050788096
H,0,1.2452929149,-1.9317465716,0.7925987979
H,0,1.4470438096,-1.1194424104,-1.5667469094
H,0,0.14332297,-1.4288191858,-2.7284438399
H,0,1.2219245418,-2.7367198136,-2.2231248183
H,0,2.0219546502,2.8779102458,-1.2520317822

H,0,0.3013226171,3.3469169617,-1.2254289086
H,0,0.7784029688,1.7511079589,-1.8706647677

MPW1K/6-31+G* (Onsager)

E(RmPW+HF-PW91) = -954.013157109

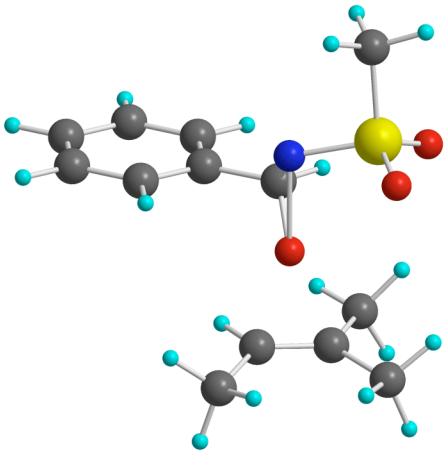
Zero-point correction=	0.228042 (Hartree/Particle)
Thermal correction to Energy=	0.242780
Thermal correction to Enthalpy=	0.243724
Thermal correction to Gibbs Free Energy=	0.185745
Sum of electronic and zero-point Energies=	-953.785115
Sum of electronic and thermal Energies=	-953.770377
Sum of electronic and thermal Enthalpies=	-953.769433
Sum of electronic and thermal Free Energies=	-953.827412

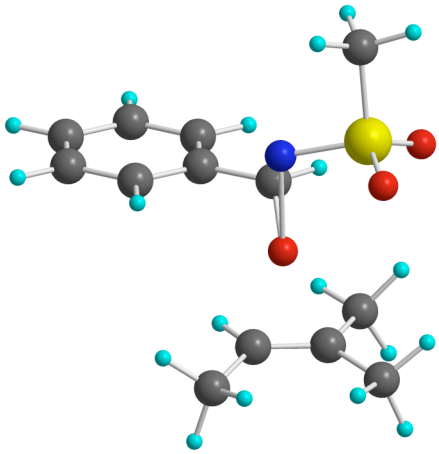
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	152.347	52.202	122.028

C,0,-1.5257065958,-2.0304677418,-0.907283481
C,0,-0.1744617074,-2.2164814048,-0.7844196324
O,0,-0.8303058121,-0.1839564797,-0.2830838698
C,0,-0.920440914,0.1033730772,1.0806107802
N,0,-0.7560609583,1.4313045994,0.6531712192
S,0,0.8241224557,1.9089023671,0.5086945561
O,0,1.7635236434,0.8314321608,0.7881317767
O,0,0.9603669403,3.147896129,1.2560810775
C,0,-2.5944120336,-2.4684706869,0.0277404658
C,0,0.4876170101,-2.8154163348,0.406544903
C,0,0.7366317306,-1.8716562307,-1.910329096
C,0,0.9338910584,2.3100515123,-1.2098655037
H,0,-1.8758551547,-1.6574852206,-1.8602806525
H,0,-0.1201367914,-0.3444317166,1.665388626
H,0,-1.9077260338,-0.0718228197,1.4989498789
H,0,-3.3649471678,-1.7031251149,0.1098909424
H,0,-2.2329623204,-2.7084791045,1.0235633002
H,0,-3.0816994985,-3.3607486824,-0.3699050158
H,0,0.9537857499,-3.7609080661,0.1222870111
H,0,-0.1898677036,-3.0156577576,1.2304781517
H,0,1.2877344151,-2.1609152193,0.7547790801
H,0,1.5403192022,-1.2257313207,-1.5558036545
H,0,0.2122718662,-1.3764276546,-2.7233790585
H,0,1.2005265852,-2.7776090155,-2.3053308417
H,0,1.9225700728,2.7270059876,-1.38011058
H,0,0.1655640297,3.0405950322,-1.4393124843
H,0,0.7895007038,1.4056029807,-1.7895486262

Epoxidation TS Isomer 3 + trans-Phenyl

B3LYP/6-31+G** (PCM)





Filename: b3BBPCMts3transfreq
E(RB+HF-LYP) = -1185.31458190

Zero-point correction=	0.298578 (Hartree/Particle)
Thermal correction to Energy=	0.318880
Thermal correction to Enthalpy=	0.319824
Thermal correction to Gibbs Free Energy=	0.247747
Sum of electronic and zero-point Energies=	-1185.016004
Sum of electronic and thermal Energies=	-1184.995702
Sum of electronic and thermal Enthalpies=	-1184.994758
Sum of electronic and thermal Free Energies=	-1185.066834

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.100	73.603	151.698

1	6	0	-3.595238	-0.994777	-1.183554
2	6	0	-2.224346	-0.750931	-1.093517
3	6	0	-1.601323	-0.691484	0.162091
4	6	0	-2.364487	-0.881969	1.320269
5	6	0	-3.739146	-1.128744	1.230337
6	6	0	-4.355906	-1.184120	-0.021997
7	6	0	-0.123606	-0.434637	0.286843
8	8	0	0.403768	0.658032	-0.468227
9	7	0	0.696587	-1.205845	-0.597238
10	16	0	2.304334	-1.407234	-0.078730
11	8	0	2.515924	-0.950897	1.316483
12	8	0	3.220261	-0.896699	-1.117621
13	6	0	2.401105	-3.207050	-0.103595
14	6	0	-0.564129	2.549370	-0.379778
15	6	0	-0.595074	2.917497	-1.830428
16	6	0	0.481064	2.726242	0.504699
17	6	0	0.279228	2.513997	1.978028
18	6	0	1.841329	3.209999	0.100658
19	1	0	-1.523040	2.265094	0.050647
20	1	0	0.200953	-0.400916	1.332363
21	1	0	-1.217906	2.210860	-2.386390
22	1	0	0.395874	2.935605	-2.287748
23	1	0	-1.044630	3.912953	-1.951491
24	1	0	1.979714	4.242246	0.452297
25	1	0	2.002980	3.192705	-0.977301
26	1	0	2.616650	2.601821	0.578444
27	1	0	1.022540	1.813499	2.376397
28	1	0	-0.723127	2.147934	2.214228
29	1	0	0.429541	3.463685	2.509599
30	1	0	3.432900	-3.462437	0.150468
31	1	0	2.152388	-3.552264	-1.107893
32	1	0	1.708641	-3.609742	0.637064

33	1	0	-1.883818	-0.842253	2.297191
34	1	0	-4.323388	-1.277218	2.136203
35	1	0	-5.424646	-1.375470	-0.095966
36	1	0	-4.073112	-1.041535	-2.160174
37	1	0	-1.630434	-0.611765	-1.993002

B3LYP/6-31+G** (gas phase)

```
 Filename: b3BBts3trans

E(RB+HF-LYP) = -1185.29952993

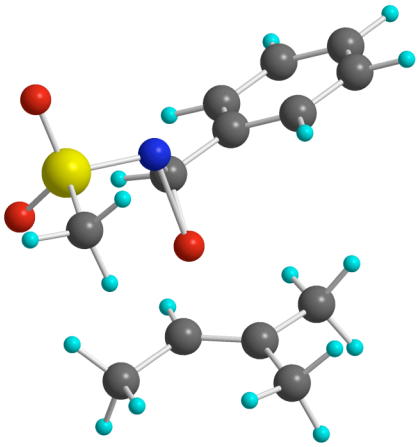
 Zero-point correction=                           0.299617 (Hartree/Particle)
 Thermal correction to Energy=                    0.319845
 Thermal correction to Enthalpy=                  0.320789
 Thermal correction to Gibbs Free Energy=         0.248596
 Sum of electronic and zero-point Energies=          -1184.999913
 Sum of electronic and thermal Energies=             -1184.979685
 Sum of electronic and thermal Enthalpies=           -1184.978741
 Sum of electronic and thermal Free Energies=        -1185.050934

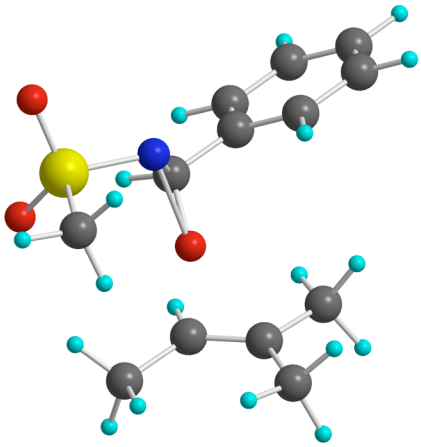
                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 200.706             73.345            151.944

 C,0,-2.7797565147,-2.3528621792,-0.5707525375
 C,0,-1.4308927052,-2.094236614,-1.1682770192
 C,0,-0.192946938,-2.3170687221,-0.5845783042
 C,0,1.0685816002,-2.2010642199,-1.3906947531
 C,0,-0.010388979,-2.7088771927,0.8505018037
 O,0,-0.9230261479,-0.2665073132,-0.3783244913
 C,0,-0.5860434878,0.8048232217,-1.2843414511
 N,0,-0.6600675831,1.6411354945,-0.1393081176
 S,0,0.7747380897,1.6512904219,0.7819640448
 C,0,0.9362551882,3.430427014,1.0309293798
 O,0,1.9349506052,1.1856118658,-0.0149738879
 O,0,0.5446021417,1.0411062704,2.1013800099
 H,0,-1.428805888,-1.8689949743,-2.2332402
 C,0,-1.6201029154,1.1017307181,-2.3390412816
 H,0,0.4116108577,0.659321543,-1.7141543971
 H,0,-3.4986627034,-1.6182227085,-0.9442624639
 H,0,-2.7768132015,-2.3029080636,0.5191018893
 H,0,-3.141242346,-3.3462915119,-0.8705056128
 H,0,0.5474749239,-3.6524995482,0.9081172646
 H,0,-0.9498049272,-2.8274340606,1.3897346023
 H,0,0.5847524843,-1.9456113412,1.3647919611
 H,0,1.7490936889,-1.4737388737,-0.9320298335
 H,0,0.8750087601,-1.9034901475,-2.4243894267
 H,0,1.589586012,-3.1674344142,-1.4033179137
 H,0,1.8044223917,3.5710914636,1.6782211606
 H,0,0.0288125181,3.7916208793,1.5152757191
 H,0,1.0891631783,3.9127271157,0.0650306193
 C,0,-1.2547210784,1.1087720278,-3.6896618164
 C,0,-2.2044590107,1.3782164615,-4.6811207986
 C,0,-3.527814318,1.6422074197,-4.3232259616
 C,0,-3.8977650505,1.6395688162,-2.9723852259
 C,0,-2.9501921893,1.3714951964,-1.984950602
 H,0,-0.2223791702,0.9100896752,-3.9685379947
 H,0,-1.9093742224,1.3839111973,-5.7264808675
 H,0,-4.2679553371,1.8527372524,-5.0899604767
 H,0,-4.9254213783,1.8523165395,-2.69127967
 H,0,-3.223881348,1.3786142907,-0.9347273497
```

Epoxidation TS Isomer 5 + trans-Phenyl

B3LYP/6-31+G** (PCM)





Filename: b3BBPCMts5transfreq

E(RB+HF-LYP) = -1185.31642864

Zero-point correction=	0.298694 (Hartree/Particle)
Thermal correction to Energy=	0.318848
Thermal correction to Enthalpy=	0.319792
Thermal correction to Gibbs Free Energy=	0.248619
Sum of electronic and zero-point Energies=	-1185.017734
Sum of electronic and thermal Energies=	-1184.997581
Sum of electronic and thermal Enthalpies=	-1184.996637
Sum of electronic and thermal Free Energies=	-1185.067810

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.080	73.480	149.796

1	6	0	-3.317368	-1.400349	1.271835
2	6	0	-1.983259	-1.027247	1.104741
3	6	0	-1.429636	-0.949185	-0.181817
4	6	0	-2.224086	-1.251841	-1.293398
5	6	0	-3.562452	-1.625469	-1.126809
6	6	0	-4.110662	-1.698838	0.156143
7	6	0	0.007878	-0.549670	-0.385257
8	8	0	0.419176	0.684653	0.216483
9	7	0	0.917486	-1.133589	0.549944
10	16	0	2.514348	-1.277882	0.012379
11	8	0	2.776093	-0.602141	-1.279904
12	8	0	2.840667	-2.719666	0.103327
13	6	0	3.424931	-0.423540	1.304531
14	6	0	0.140499	2.377985	-0.958965
15	6	0	1.567835	2.774100	-1.175257
16	6	0	-0.689854	2.740426	0.086242
17	6	0	-2.166730	2.491744	0.014916
18	6	0	-0.207137	3.443243	1.319177
19	1	0	-0.346001	1.930665	-1.826628
20	1	0	0.298996	-0.594971	-1.441824
21	1	0	2.137054	1.919389	-1.554402

22	1	0	2.054094	3.139467	-0.268745
23	1	0	1.617155	3.569677	-1.930985
24	1	0	-0.560072	4.484361	1.311726
25	1	0	0.878866	3.454036	1.414418
26	1	0	-0.632454	2.973347	2.213141
27	1	0	-2.501439	1.881810	0.861989
28	1	0	-2.463192	1.993499	-0.910397
29	1	0	-2.701651	3.449131	0.082833
30	1	0	4.486266	-0.562898	1.086586
31	1	0	3.161248	-0.876194	2.261158
32	1	0	3.151485	0.630856	1.277004
33	1	0	-1.794651	-1.201566	-2.293342
34	1	0	-4.171466	-1.861987	-1.996947
35	1	0	-5.150205	-1.991831	0.289626
36	1	0	-3.740150	-1.463553	2.272678
37	1	0	-1.363101	-0.802927	1.968706

B3LYP/6-31+G** (gas phase)

E(RB+HF-LYP) = -1185.29948564

Zero-point correction= 0.299676 (Hartree/Particle)
Thermal correction to Energy= 0.319764
Thermal correction to Enthalpy= 0.320708
Thermal correction to Gibbs Free Energy= 0.249297
Sum of electronic and zero-point Energies= -1184.999810
Sum of electronic and thermal Energies= -1184.979721
Sum of electronic and thermal Enthalpies= -1184.978777
Sum of electronic and thermal Free Energies= -1185.050189

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.655	73.265	150.299

C,0,-0.940579635,-2.0665434589,1.209565621
C,0,0.1492063586,-2.220986704,0.1925054803
C,0,1.4992887574,-2.4493024317,0.4298862871
C,0,2.4100251079,-2.9007015497,-0.670957931
C,0,2.1305986912,-2.2888875891,1.7798413005
O,0,0.6946422847,-0.3553072803,-0.05599276
C,0,0.5069756069,0.2233832527,-1.3708851767
N,0,0.4347822019,1.4765023111,-0.7138567976
S,0,-1.1333400408,1.9442057034,-0.2678739337
C,0,-0.8724987993,2.4425460519,1.441804332
O,0,-2.0994916801,0.8235521158,-0.2857549523
O,0,-1.4478686834,3.1524565294,-1.0494218081
H,0,-0.1998578679,-2.4522324582,-0.8128633219
H,0,-0.4231666682,-0.1492027557,-1.8167146724
C,0,1.6727039808,0.0822332439,-2.3150860333
H,0,-1.6657191175,-1.3255924177,0.8593386718
H,0,-0.5663683057,-1.752771774,2.186183132
H,0,-1.4635539863,-3.0235238843,1.3380469023
H,0,2.3330594801,-3.2777707689,2.2164623843
H,0,1.5072493597,-1.7312893603,2.4791933929
H,0,3.096220808,-1.7792556838,1.6908524422
H,0,3.2109343049,-2.1699943443,-0.8376157939
H,0,1.8839434713,-3.0519284514,-1.6154618513
H,0,2.8952580239,-3.8441340817,-0.3852767188
H,0,-1.8203475481,2.8528114519,1.7956093225
H,0,-0.0903484846,3.2018441949,1.4581777171
H,0,-0.5834460397,1.5638530624,2.0181899776
C,0,1.4895810762,-0.5308022489,-3.5588225686
C,0,2.5614222906,-0.670722895,-4.4468212061

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C,0,3.8252679339,-0.1952298633,-4.0922723118
C,0,4.0122732695,0.4256243337,-2.8508592904
C,0,2.9422872806,0.5654607987,-1.967231165
H,0,0.502724936,-0.8908702733,-3.8407827409
H,0,2.4063512098,-1.1432612307,-5.4124908751
H,0,4.6592820711,-0.2988545371,-4.780497368
H,0,4.9919031484,0.8080442123,-2.5779787151
H,0,3.0741092029,1.0602007802,-1.0102539714
```

B3LYP/6-31+G** (gas phase)

```
Filename: progSI b3BBts5trans
E(RB+HF-LYP) =  -1185.24166509

 Zero-point correction=                           0.301728 (Hartree/Particle)
 Thermal correction to Energy=                    0.321648
 Thermal correction to Enthalpy=                  0.322592
 Thermal correction to Gibbs Free Energy=         0.251148
 Sum of electronic and zero-point Energies=          -1184.939937
 Sum of electronic and thermal Energies=             -1184.920017
 Sum of electronic and thermal Enthalpies=           -1184.919073
 Sum of electronic and thermal Free Energies=        -1184.990517

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 201.837             72.692           150.367

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.249384    2.380085   -0.789652
    2          6             0       -0.921999    2.655016   -0.094975
    3          8             0        0.375553    0.778446    0.261992
    4          6             0        0.063467   -0.488969   -0.348128
    5          7             0        0.999515   -1.053825    0.557806
    6         16             0        2.574208   -1.148730   -0.057260
    7          8             0        2.834365   -0.188939   -1.149587
    8          8             0        2.852541   -2.573329   -0.297813
    9          6             0        1.609048    2.962221   -0.540234
   10          6             0       -0.949769    3.344586    1.235362
   11          6             0       -2.255845    2.279728   -0.667316
   12          6             0        3.517123   -0.629311    1.384610
   13          1             0        0.123400    1.950338   -1.782325
   14          1             0        0.341592   -0.485447   -1.409421
   15          6             0       -1.347257   -0.974143   -0.137515
   16          1             0        2.368458    2.226708   -0.821031
   17          1             0        1.761771    3.245343    0.504209
   18          1             0        1.749644    3.858568   -1.159497
   19          1             0       -1.388097    4.348460    1.131792
   20          1             0        0.038444    3.450132    1.685077
   21          1             0       -1.591221    2.793851    1.934163
   22          1             0       -2.809416    1.620351    0.012724
   23          1             0       -2.168714    1.778472   -1.634464
   24          1             0       -2.868308    3.183744   -0.800794
   25          1             0        4.574308   -0.735836    1.130762
   26          1             0        3.255222   -1.277814    2.221683
   27          1             0        3.273369    0.410638    1.606175
   28          6             0       -2.097199   -1.449654   -1.216123
   29          6             0       -3.401564   -1.912454   -1.022605
   30          6             0       -3.962945   -1.897568    0.253890
```

31	6	0	-3.215694	-1.422905	1.337523
32	6	0	-1.914479	-0.964703	1.143985
33	1	0	-1.657024	-1.466813	-2.210973
34	1	0	-3.974819	-2.284241	-1.867609
35	1	0	-4.976866	-2.257286	0.407952
36	1	0	-3.648372	-1.418065	2.334707
37	1	0	-1.320603	-0.605660	1.978721

B3LYP/6-31G* (Onsager)

E(RB+HF-LYP) = -1185.24497052

Zero-point correction= 0.301770 (Hartree/Particle)
Thermal correction to Energy= 0.321658
Thermal correction to Enthalpy= 0.322602
Thermal correction to Gibbs Free Energy= 0.251771
Sum of electronic and zero-point Energies= -1184.943201
Sum of electronic and thermal Energies= -1184.923313
Sum of electronic and thermal Enthalpies= -1184.922369
Sum of electronic and thermal Free Energies= -1184.993200

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	201.843	72.721	149.076

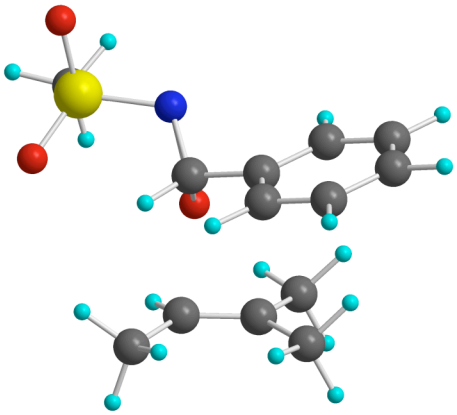
Standard orientation:

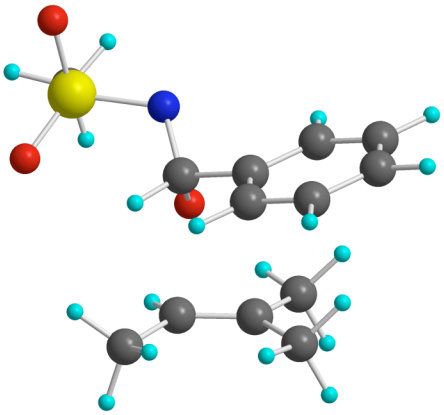
Center Number	Atomic Number	Atomic Type		X	Y	Z
1	6	0	C	0.253438	2.386613	-0.801897
2	6	0	C	-0.909253	2.642637	-0.091073
3	8	0	O	0.404122	0.728922	0.245529
4	6	0	C	0.058947	-0.520677	-0.366835
5	7	0	N	0.993553	-1.098025	0.540249
6	16	0	S	2.578937	-1.167486	-0.047505
7	8	0	O	2.800050	-0.344121	-1.253818
8	8	0	O	2.947526	-2.592613	-0.097949
9	6	0	C	1.617947	2.951897	-0.543566
10	6	0	C	-0.929106	3.311866	1.249339
11	6	0	C	-2.247292	2.287448	-0.666444
12	6	0	C	3.476648	-0.410926	1.318030
13	1	0	H	0.121095	1.968040	-1.798430
14	1	0	H	0.335662	-0.528137	-1.428075
15	6	0	C	-1.357224	-0.983486	-0.145336
16	1	0	H	2.373748	2.225535	-0.857068
17	1	0	H	1.779776	3.199338	0.508581
18	1	0	H	1.759924	3.868937	-1.131323
19	1	0	H	-1.350557	4.323617	1.156949
20	1	0	H	0.058855	3.396418	1.704015
21	1	0	H	-1.583632	2.763721	1.937433
22	1	0	H	-2.811688	1.633521	0.009304
23	1	0	H	-2.167003	1.794315	-1.638398
24	1	0	H	-2.845772	3.201471	-0.792869
25	1	0	H	4.541105	-0.480101	1.081677
26	1	0	H	3.247183	-0.962136	2.230977
27	1	0	H	3.163899	0.630167	1.404479
28	6	0	C	-2.126875	-1.435663	-1.220021
29	6	0	C	-3.439925	-1.869259	-1.017754
30	6	0	C	-3.989451	-1.849621	0.263914
31	6	0	C	-3.221943	-1.399405	1.343853

32	6	0	C	-1.912553	-0.969372	1.141303
33	1	0	H	-1.697774	-1.450834	-2.219844
34	1	0	H	-4.031652	-2.216490	-1.860492
35	1	0	H	-5.011879	-2.181114	0.424178
36	1	0	H	-3.647507	-1.386055	2.343860
37	1	0	H	-1.305385	-0.624073	1.972199

Epoxidation TS Isomer 7 + trans-Phenyl

B3LYP/6-31+G** (PCM)





Filename: b3BBPCMts7transfreq

[jen@das1 trans]$ progSIb b3BBPCMts7transfreq
b3BBPCMts7transfreq
E(RB+HF-LYP) = -1185.31476994

Zero-point correction=	0.298949 (Hartree/Particle)
Thermal correction to Energy=	0.318997
Thermal correction to Enthalpy=	0.319941
Thermal correction to Gibbs Free Energy=	0.249134
Sum of electronic and zero-point Energies=	-1185.015821
Sum of electronic and thermal Energies=	-1184.995773
Sum of electronic and thermal Enthalpies=	-1184.994829
Sum of electronic and thermal Free Energies=	-1185.065636

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.174	73.414	149.027

1	6	0	-1.728118	-1.233956	-1.142425
2	6	0	-1.159096	-1.061126	0.127735
3	6	0	-1.853999	-1.501384	1.260016
4	6	0	-3.109672	-2.105290	1.128844
5	6	0	-3.675297	-2.270815	-0.137973
6	6	0	-2.980613	-1.834729	-1.274223
7	6	0	0.195020	-0.424384	0.292865
8	7	0	1.198464	-0.943306	-0.586558
9	16	0	2.780490	-0.825517	0.006132
10	8	0	2.867306	-0.158043	1.326510
11	8	0	0.420952	0.809836	-0.404064
12	6	0	3.601165	0.214493	-1.209079
13	8	0	3.346874	-2.188968	-0.107230
14	6	0	-0.010216	2.610823	0.473967
15	6	0	-1.176645	2.549450	-0.270504
16	6	0	-2.504322	2.136693	0.285947

17	6	0	0.137784	2.431702	1.953706
18	6	0	-1.177456	2.982665	-1.706716
19	1	0	0.849440	3.064262	-0.016786
20	1	0	1.092944	1.946867	2.178668
21	1	0	-0.667511	1.849591	2.406952
22	1	0	0.153406	3.416796	2.439331
23	1	0	-3.181561	3.002786	0.269426
24	1	0	-2.456191	1.765224	1.309498
25	1	0	-2.963910	1.367173	-0.344321
26	1	0	-1.651058	2.225779	-2.342415
27	1	0	-0.169458	3.175326	-2.080268
28	1	0	-1.770966	3.901730	-1.815193
29	1	0	0.479266	-0.345103	1.346771
30	1	0	4.658996	0.238045	-0.937392
31	1	0	3.157341	1.208432	-1.163215
32	1	0	3.461932	-0.235886	-2.192801
33	1	0	-1.411665	-1.377771	2.247950
34	1	0	-3.641601	-2.446265	2.014737
35	1	0	-4.651270	-2.740621	-0.242704
36	1	0	-3.415510	-1.968719	-2.262773
37	1	0	-1.181986	-0.903693	-2.022376

B3LYP/6-31+G** (gas phase)

E(RB+HF-LYP) = -1185.29793461

Zero-point correction= 0.300102 (Hartree/Particle)
Thermal correction to Energy= 0.319957
Thermal correction to Enthalpy= 0.320902
Thermal correction to Gibbs Free Energy= 0.250685
Sum of electronic and zero-point Energies= -1184.997833
Sum of electronic and thermal Energies= -1184.977977
Sum of electronic and thermal Enthalpies= -1184.977033
Sum of electronic and thermal Free Energies= -1185.047250

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.776	73.125	147.783

C,0,0.7077469047,-2.5384220752,0.4042549761
C,0,-0.4824290387,-2.1037155049,-0.3969849776
C,0,-0.6580618184,-2.1932253981,-1.7758038777
C,0,-2.0124948834,-1.960876947,-2.3768485809
C,0,0.4335725077,-2.5442678722,-2.7378225022
O,0,-0.3455976888,-0.2022664579,-0.6882975328
C,0,0.9276633119,0.4914677467,-0.7468552028
N,0,0.2534780462,1.6325039421,-0.2420360059
S,0,0.2719495132,1.7553499734,1.4486871741
C,0,-1.4613498051,2.0966255616,1.7947376105
O,0,1.0441504295,2.966890668,1.7759417339
O,0,0.6403693203,0.4867240296,2.1169063874
H,0,-1.3912023947,-1.9897768354,0.1880893423
H,0,0.8416448218,-1.8633172791,1.2552026173
H,0,1.6340009031,-2.568852405,-0.173370222
H,0,0.5270845871,-3.5450724121,0.8032032063
H,0,0.1559145193,-3.45811536,-3.2814843117
H,0,1.3994668579,-2.7114224271,-2.2616876375
H,0,0.5523981926,-1.7549659706,-3.4897222692
H,0,-1.958604225,-1.2139346746,-3.1775271795
H,0,-2.7397910196,-1.6238896599,-1.6353902604
H,0,-2.3839901435,-2.8888758216,-2.8346750381
C,0,1.4940888246,0.681553736,-2.1307845191

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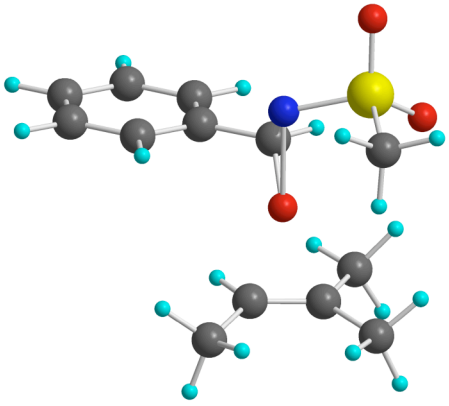
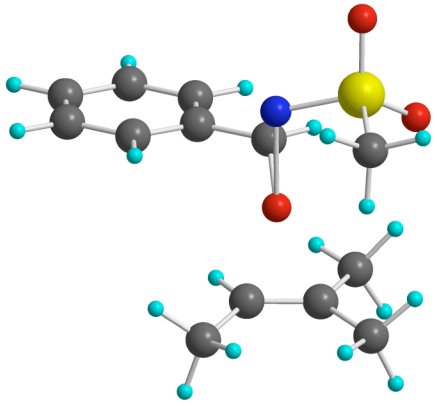
H,0,1.6517935158,0.0167093566,-0.0762385458
H,0,-1.5327753245,2.2915503007,2.8665840607
H,0,-2.0507802953,1.2246759244,1.5121142958
H,0,-1.7545537043,2.9753005499,1.2197969215
C,0,2.818732792,0.3202009309,-2.3965551941
C,0,3.361939966,0.4993105017,-3.6732131885
C,0,2.5782195742,1.0415473969,-4.6935127089
C,0,1.2524735833,1.4096677556,-4.4311201719
C,0,0.7136275851,1.2333669663,-3.1567947617
H,0,3.4333149527,-0.0944186377,-1.6008410098
H,0,4.3936579122,0.2198778378,-3.8664059829
H,0,2.9969529844,1.1839035072,-5.6856393477
H,0,0.6438938627,1.8429892069,-5.2199573375
H,0,-0.3071011271,1.5318798461,-2.9402299598
```

Epoxidation TS Isomer 8 + trans-Phenyl

B3LYP/6-31+G** (PCM)





Filename: b3BBPCMts8transfreq

```
[jen@das1 trans]$ progSIb b3BBPCMts8transfreq
b3BBPCMts8transfreq
E(RB+HF-LYP) = -1185.31652650

 Zero-point correction=                           0.298876 (Hartree/Particle)
 Thermal correction to Energy=                    0.319019
 Thermal correction to Enthalpy=                  0.319963
 Thermal correction to Gibbs Free Energy=         0.248505
 Sum of electronic and zero-point Energies=          -1185.017650
 Sum of electronic and thermal Energies=             -1184.997507
 Sum of electronic and thermal Enthalpies=           -1184.996563
 Sum of electronic and thermal Free Energies=        -1185.068021

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 200.188             73.470           150.396

    1          6             0       -2.257375   -0.697280   -1.102268
    2          6             0       -1.660922   -0.646916    0.166469
    3          6             0       -2.460209   -0.768864    1.309048
    4          6             0       -3.844574   -0.936566    1.190291
    5          6             0       -4.434743   -0.981814   -0.075151
    6          6             0       -3.637600   -0.862662   -1.221440
    7          6             0       -0.173045   -0.473251    0.318852
    8          7             0        0.615109   -1.314313   -0.533031
    9         16             0        2.173549   -1.641350    0.040953
   10          8             0        2.515556   -0.907112    1.281796
   11          8             0        0.421103    0.588044   -0.434536
```

12	6	0	0.615344	2.640415	0.512812
13	6	0	1.992691	3.055601	0.093264
14	6	0	-0.446816	2.505113	-0.361926
15	6	0	-0.480593	2.873581	-1.812162
16	6	0	0.424303	2.433283	1.987047
17	6	0	3.216267	-1.029197	-1.288588
18	8	0	2.290484	-3.117353	0.068534
19	1	0	-1.413093	2.269989	0.081032
20	1	0	0.128827	-0.439703	1.370713
21	1	0	-1.133241	2.187397	-2.359313
22	1	0	0.504890	2.860314	-2.281346
23	1	0	-0.898854	3.883030	-1.928504
24	1	0	2.207164	4.059501	0.485258
25	1	0	2.129064	3.078133	-0.988346
26	1	0	2.736469	2.380268	0.531423
27	1	0	1.127751	1.681254	2.365056
28	1	0	-0.595129	2.130111	2.237916
29	1	0	0.646002	3.366478	2.522198
30	1	0	4.243982	-1.295206	-1.031117
31	1	0	3.090109	0.051349	-1.350026
32	1	0	2.908000	-1.516684	-2.214369
33	1	0	-2.000777	-0.743064	2.296333
34	1	0	-4.456891	-1.034060	2.084425
35	1	0	-5.510781	-1.113008	-0.171120
36	1	0	-4.094184	-0.904774	-2.208387
37	1	0	-1.635345	-0.616808	-1.989692

B3LYP/6-31+G** (gas phase)

```
E(RB+HF-LYP) = -1185.29999809

 Zero-point correction=                           0.299644 (Hartree/Particle)
 Thermal correction to Energy=                    0.319817
 Thermal correction to Enthalpy=                  0.320761
 Thermal correction to Gibbs Free Energy=         0.248652
 Sum of electronic and zero-point Energies=          -1185.000354
 Sum of electronic and thermal Energies=             -1184.980181
 Sum of electronic and thermal Enthalpies=           -1184.979237
 Sum of electronic and thermal Free Energies=        -1185.051346

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 200.688             73.324            151.767
```

1	6	0	-0.618530	2.857834	-1.773873
2	6	0	-0.471420	2.462151	-0.336222
3	6	0	0.652059	2.618711	0.467189
4	6	0	0.573175	2.397418	1.948573
5	6	0	1.999015	3.018468	-0.049964
6	8	0	0.372993	0.661343	-0.458623
7	6	0	-0.162367	-0.446981	0.304044
8	7	0	0.618088	-1.295406	-0.522666
9	16	0	2.172903	-1.594824	0.074765
10	6	0	3.154224	-1.395873	-1.420871
11	8	0	2.223727	-3.015828	0.462975
12	8	0	2.621829	-0.586267	1.062677
13	1	0	-1.401199	2.225678	0.176758
14	6	0	-1.651945	-0.642993	0.174601
15	1	0	0.142503	-0.370244	1.353673
16	1	0	-1.318353	2.183332	-2.274525
17	1	0	0.326945	2.835131	-2.318339
18	1	0	-1.031402	3.873313	-1.844126

19	1	0	2.316353	3.956817	0.423851
20	1	0	2.026896	3.152023	-1.131381
21	1	0	2.730254	2.251253	0.232153
22	1	0	1.302244	1.637309	2.255159
23	1	0	-0.424756	2.092926	2.272940
24	1	0	0.837895	3.323944	2.475164
25	1	0	4.181290	-1.656765	-1.158529
26	1	0	3.081976	-0.358384	-1.747296
27	1	0	2.761719	-2.075951	-2.177185
28	6	0	-2.455191	-0.652109	1.319910
29	6	0	-3.839508	-0.826727	1.215887
30	6	0	-4.427116	-0.993647	-0.039209
31	6	0	-3.626532	-0.991660	-1.188411
32	6	0	-2.246895	-0.819040	-1.083029
33	1	0	-1.997109	-0.534601	2.299378
34	1	0	-4.452556	-0.837438	2.112481
35	1	0	-5.501177	-1.131971	-0.124030
36	1	0	-4.080180	-1.133791	-2.165303
37	1	0	-1.616612	-0.834856	-1.966389

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

Filename: b3BB1PCMtransts8freq
E(RB+HF-LYP) = -1185.50608450

Zero-point correction=	0.297706 (Hartree/Particle)
Thermal correction to Energy=	0.317886
Thermal correction to Enthalpy=	0.318830
Thermal correction to Gibbs Free Energy=	0.247179
Sum of electronic and zero-point Energies=	-1185.208378
Sum of electronic and thermal Energies=	-1185.188198
Sum of electronic and thermal Enthalpies=	-1185.187254
Sum of electronic and thermal Free Energies=	-1185.258905

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	199.477	73.568	150.802

1	6	0	-2.244747	-0.744036	-1.098399
2	6	0	-1.655692	-0.660741	0.168491
3	6	0	-2.459223	-0.748788	1.306979
4	6	0	-3.840066	-0.916658	1.186173
5	6	0	-4.422353	-0.994966	-0.077145
6	6	0	-3.621176	-0.909583	-1.219362
7	6	0	-0.170263	-0.478342	0.322375
8	7	0	0.624769	-1.316976	-0.521311
9	16	0	2.181460	-1.632037	0.052759
10	8	0	2.526181	-0.878733	1.273476
11	8	0	0.416526	0.583953	-0.432107
12	6	0	0.592544	2.650293	0.501387
13	6	0	1.973428	3.060645	0.097615
14	6	0	-0.454992	2.508777	-0.382842
15	6	0	-0.469754	2.864226	-1.833949
16	6	0	0.382311	2.455687	1.972346
17	6	0	3.212233	-1.042315	-1.293638
18	8	0	2.300285	-3.100180	0.107856
19	1	0	-1.425306	2.276711	0.048479
20	1	0	0.129672	-0.438706	1.372607
21	1	0	-1.101793	2.165821	-2.386466
22	1	0	0.521667	2.864810	-2.285946
23	1	0	-0.902522	3.864165	-1.963987
24	1	0	2.182500	4.066054	0.484249
25	1	0	2.124587	3.074623	-0.980265
26	1	0	2.709140	2.389858	0.551568
27	1	0	1.080503	1.708812	2.364988

28	1	0	-0.638739	2.155369	2.211529
29	1	0	0.597235	3.392071	2.501350
30	1	0	4.240716	-1.298044	-1.036572
31	1	0	3.079296	0.034187	-1.373902
32	1	0	2.899964	-1.549925	-2.204801
33	1	0	-2.005926	-0.697456	2.293971
34	1	0	-4.456389	-0.988361	2.077678
35	1	0	-5.496287	-1.126428	-0.174856
36	1	0	-4.072661	-0.978113	-2.205097
37	1	0	-1.619837	-0.689545	-1.983477

B3LYP/6-31G* (gas phase)

E(RB+HF-LYP) = -1185.24269945

Zero-point correction= 0.301882 (Hartree/Particle)
Thermal correction to Energy= 0.321773
Thermal correction to Enthalpy= 0.322717
Thermal correction to Gibbs Free Energy= 0.251654
Sum of electronic and zero-point Energies= -1184.940817
Sum of electronic and thermal Energies= -1184.920927
Sum of electronic and thermal Enthalpies= -1184.919982
Sum of electronic and thermal Free Energies= -1184.991046

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	201.916	72.695	149.565

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.566792	2.408315	-0.253580
2	6	0	0.626909	2.606430	0.428790
3	8	0	0.348366	0.660111	-0.450568
4	6	0	-0.143747	-0.458028	0.323611
5	7	0	0.648353	-1.289902	-0.506530
6	16	0	2.214723	-1.525705	0.075300
7	8	0	2.303844	-2.911128	0.564177
8	8	0	2.678539	-0.441718	0.969299
9	6	0	-0.887185	2.781476	-1.668001
10	6	0	1.899765	3.048322	-0.224742
11	6	0	0.713747	2.374965	1.908070
12	6	0	3.146714	-1.417223	-1.460709
13	1	0	-1.427584	2.136155	0.353755
14	6	0	-1.629188	-0.683404	0.198411
15	1	0	0.163089	-0.364869	1.371747
16	1	0	-1.567505	2.039261	-2.096581
17	1	0	-0.001655	2.842688	-2.303915
18	1	0	-1.398849	3.753717	-1.696687
19	1	0	2.233653	4.001064	0.208620
20	1	0	1.812518	3.173395	-1.305001
21	1	0	2.679066	2.305007	-0.015953
22	1	0	1.470195	1.607562	2.116694
23	1	0	-0.242157	2.064544	2.339339
24	1	0	1.037115	3.294949	2.414090
25	1	0	4.188552	-1.641428	-1.220656
26	1	0	3.047546	-0.406929	-1.859942
27	1	0	2.746971	-2.152520	-2.160428
28	6	0	-2.212229	-0.898968	-1.057994
29	6	0	-3.589292	-1.074477	-1.170309
30	6	0	-4.399357	-1.037444	-0.030169
31	6	0	-3.824224	-0.829916	1.222941

32	6	0	-2.442240	-0.653300	1.334727
33	1	0	-1.571531	-0.941557	-1.933250
34	1	0	-4.034492	-1.246078	-2.146944
35	1	0	-5.473563	-1.175222	-0.120788
36	1	0	-4.446391	-0.807876	2.113665
37	1	0	-1.992302	-0.499874	2.313601

B3LYP/6-31G* (Onsager)

E(RB+HF-LYP) = -1185.24706290

Zero-point correction= 0.301923 (Hartree/Particle)
Thermal correction to Energy= 0.321806
Thermal correction to Enthalpy= 0.322750
Thermal correction to Gibbs Free Energy= 0.252193
Sum of electronic and zero-point Energies= -1184.945140
Sum of electronic and thermal Energies= -1184.925257
Sum of electronic and thermal Enthalpies= -1184.924313
Sum of electronic and thermal Free Energies= -1184.994869

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	201.936	72.742	148.499

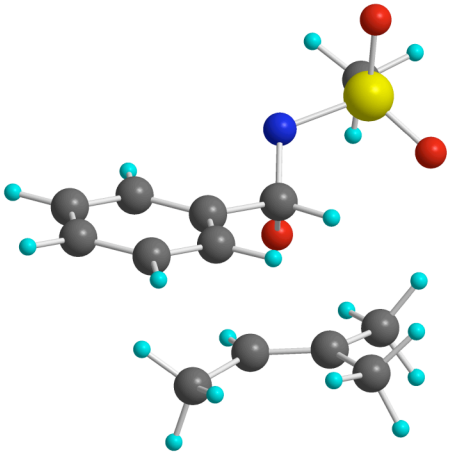
Standard orientation:

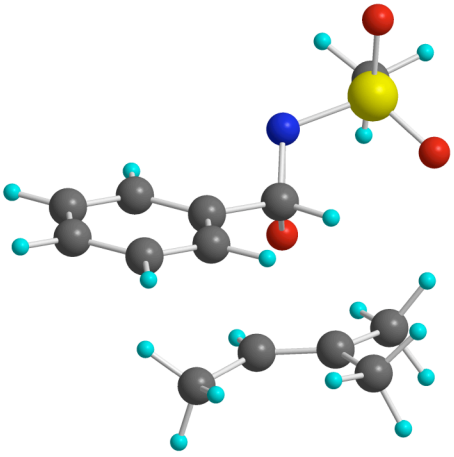
Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	-0.619784	2.394642	-0.231568
2	6	0	C	0.575122	2.609207	0.434714
3	8	0	O	0.371738	0.603020	-0.428661
4	6	0	C	-0.136429	-0.496124	0.342897
5	7	0	N	0.668087	-1.320702	-0.494703
6	16	0	S	2.249595	-1.528375	0.057363
7	8	0	O	2.457102	-2.977730	0.224558
8	8	0	O	2.607877	-0.637594	1.181754
9	6	0	C	-0.962515	2.751733	-1.643003
10	6	0	C	1.819002	3.112903	-0.231875
11	6	0	C	0.685315	2.378255	1.913040
12	6	0	C	3.189685	-1.005384	-1.387865
13	1	0	H	-1.464728	2.089869	0.382554
14	6	0	C	-1.619455	-0.724416	0.205337
15	1	0	H	0.170538	-0.417796	1.391552
16	1	0	H	-1.619241	1.986706	-2.068496
17	1	0	H	-0.086493	2.853334	-2.286770
18	1	0	H	-1.513290	3.702350	-1.664515
19	1	0	H	2.038244	4.132621	0.114338
20	1	0	H	1.747420	3.134144	-1.320311
21	1	0	H	2.670635	2.485326	0.056347
22	1	0	H	1.451799	1.618431	2.113916
23	1	0	H	-0.261833	2.057646	2.356092
24	1	0	H	1.003575	3.301699	2.415391
25	1	0	H	4.244977	-1.187754	-1.171345
26	1	0	H	3.003433	0.055317	-1.558592
27	1	0	H	2.863536	-1.597621	-2.244022
28	6	0	C	-2.195642	-0.921208	-1.057245
29	6	0	C	-3.573294	-1.085310	-1.180280
30	6	0	C	-4.390249	-1.054810	-0.044892
31	6	0	C	-3.821708	-0.867094	1.214489
32	6	0	C	-2.439160	-0.703170	1.337186
33	1	0	H	-1.551111	-0.948750	-1.930240
34	1	0	H	-4.014824	-1.233440	-2.162270

35	1	0	H	-5.465763	-1.173228	-0.145077
36	1	0	H	-4.450958	-0.841338	2.100040
37	1	0	H	-1.995117	-0.555504	2.319696

Epoxidation TS Isomer 9 + trans-Phenyl

B3LYP/6-31+G** (PCM)





Filename: b3BBPCMts9transfreq

[jen@das1 trans]$ progSIb b3BBPCMts9transfreq
b3BBPCMts9transfreq
E(RB+HF-LYP) = -1185.31505098

Zero-point correction=	0.298867 (Hartree/Particle)
Thermal correction to Energy=	0.318898
Thermal correction to Enthalpy=	0.319842
Thermal correction to Gibbs Free Energy=	0.248973
Sum of electronic and zero-point Energies=	-1185.016184
Sum of electronic and thermal Energies=	-1184.996153
Sum of electronic and thermal Enthalpies=	-1184.995209
Sum of electronic and thermal Free Energies=	-1185.066078

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.112	73.479	149.158

1	6	0	1.927226	2.533512	-0.730939
2	6	0	0.442711	2.539773	-0.897971
3	6	0	-0.520144	2.686345	0.087349
4	6	0	-1.953261	2.934906	-0.279216
5	6	0	-0.211884	2.732668	1.555136
6	8	0	-0.425772	0.600930	-0.635149
7	6	0	0.075420	-0.402433	0.266958
8	7	0	-0.785646	-1.294153	-0.443221
9	16	0	-2.360473	-1.394817	0.157467
10	6	0	-3.352248	-1.017624	-1.292975
11	8	0	-2.663287	-0.394263	1.208948
12	8	0	-2.580132	-2.820417	0.495330
13	1	0	0.092426	2.599680	-1.927829
14	1	0	-0.208221	-0.179248	1.300809
15	6	0	1.537924	-0.744222	0.151343
16	1	0	2.383353	1.769783	-1.367725
17	1	0	2.255984	2.368254	0.295954
18	1	0	2.322368	3.504292	-1.062375

19	1	0	-0.330816	3.764043	1.914945
20	1	0	0.799351	2.405828	1.800202
21	1	0	-0.930124	2.121236	2.112586
22	1	0	-2.599779	2.207914	0.225626
23	1	0	-2.117128	2.875046	-1.357752
24	1	0	-2.256502	3.933632	0.063434
25	1	0	-4.396606	-1.160163	-1.006286
26	1	0	-3.068932	-1.709656	-2.087067
27	1	0	-3.159319	0.015100	-1.582306
28	6	0	2.343858	-0.719778	1.295112
29	6	0	3.704391	-1.036851	1.209914
30	6	0	4.263855	-1.381912	-0.022790
31	6	0	3.458989	-1.412644	-1.169415
32	6	0	2.102878	-1.096216	-1.083346
33	1	0	1.908192	-0.461221	2.259433
34	1	0	4.322085	-1.017158	2.105504
35	1	0	5.320982	-1.630886	-0.091948
36	1	0	3.890408	-1.687896	-2.129871
37	1	0	1.474593	-1.125578	-1.970262

B3LYP/6-31+G** (gas phase)

Filename: b3BBts9trans

E(RB+HF-LYP) = -1185.29776352

Zero-point correction=	0.299981 (Hartree/Particle)
Thermal correction to Energy=	0.319847
Thermal correction to Enthalpy=	0.320791
Thermal correction to Gibbs Free Energy=	0.250576
Sum of electronic and zero-point Energies=	-1184.997782
Sum of electronic and thermal Energies=	-1184.977917
Sum of electronic and thermal Enthalpies=	-1184.976973
Sum of electronic and thermal Free Energies=	-1185.047187

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	200.707	73.284	147.779

C,0,1.9210150065,2.6437592614,-0.2851455636
C,0,0.5006545348,2.5996330607,-0.7443874588
C,0,-0.6523937105,2.6229508257,0.035102116
C,0,-1.9928269299,2.8614205939,-0.5980128928
C,0,-0.652578715,2.6070061265,1.5362689614
O,0,-0.3699849976,0.7026935594,-0.6401428629
C,0,0.0960339751,-0.3668723686,0.2347920045
N,0,-0.7453509861,-1.2481805827,-0.483131527
S,0,-2.2979034781,-1.405386852,0.1635215979
C,0,-3.2755877976,-1.4925451796,-1.3442310154
O,0,-2.735024723,-0.216954002,0.9344154624
O,0,-2.3710868209,-2.7196421561,0.8279781287
H,0,0.3551394995,2.7006720837,-1.8170144857
H,0,-0.1843544075,-0.1502900407,1.2718050423
C,0,1.5622334695,-0.697515344,0.1191396537
H,0,2.5295008939,1.9221742085,-0.8389014307
H,0,2.0439687122,2.4481455773,0.7806881067
H,0,2.3321784611,3.6407657424,-0.497596999
H,0,-0.9483419457,3.5974764396,1.9068867155
H,0,0.3164754254,2.3603315526,1.9722938448
H,0,-1.4010038865,1.8918364469,1.8938301242
H,0,-2.7106502697,2.1238402068,-0.2242408245

H,0,-1.9463305392,2.7998866339,-1.6877326366
H,0,-2.3602019874,3.8586803504,-0.3205331337
H,0,-4.3055705037,-1.6859805361,-1.0388069352
H,0,-2.8894967418,-2.3116853585,-1.9511868317
H,0,-3.1922958668,-0.5404173691,-1.8685952925
C,0,2.359448921,-0.7407955942,1.2671409976
C,0,3.7196680259,-1.055444992,1.1761173294
C,0,4.2894755539,-1.3270051776,-0.0690772704
C,0,3.4936260872,-1.289822908,-1.2211761167
C,0,2.1372548503,-0.979762321,-1.1279878367
H,0,1.9148417456,-0.5396068978,2.2391653321
H,0,4.3282688081,-1.0915892825,2.0751089792
H,0,5.3448547231,-1.5731271049,-0.1436608762
H,0,3.9317966339,-1.5109859934,-2.1904209925
H,0,1.5103870209,-0.9629335247,-2.0137407106

B3LYP/6-31G* (gas phase)

E(RB+HF-LYP) = -1185.24045395

Zero-point correction= 0.302262 (Hartree/Particle)
Thermal correction to Energy= 0.321828
Thermal correction to Enthalpy= 0.322772
Thermal correction to Gibbs Free Energy= 0.253633
Sum of electronic and zero-point Energies= -1184.938192
Sum of electronic and thermal Energies= -1184.918626
Sum of electronic and thermal Enthalpies= -1184.917682
Sum of electronic and thermal Free Energies= -1184.986821

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	201.950	72.657	145.516

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.501144	2.573305	-0.747719
2	6	0	-0.645385	2.577677	0.041462
3	8	0	-0.374163	0.692654	-0.628091
4	6	0	0.094068	-0.374339	0.250502
5	7	0	-0.744250	-1.259708	-0.462853
6	16	0	-2.297793	-1.396673	0.176003
7	8	0	-2.710192	-0.221374	0.977310
8	8	0	-2.411750	-2.726753	0.795226
9	6	0	1.926108	2.615853	-0.303180
10	6	0	-0.634416	2.555577	1.543029
11	6	0	-1.991302	2.827128	-0.578327
12	6	0	-3.270038	-1.403663	-1.338553
13	1	0	0.345675	2.688315	-1.817723
14	1	0	-0.182928	-0.153312	1.286941
15	6	0	1.560395	-0.696296	0.125460
16	1	0	2.532786	1.911884	-0.882084
17	1	0	2.061877	2.390553	0.755978
18	1	0	2.329725	3.621751	-0.491524
19	1	0	-0.926439	3.544523	1.922397
20	1	0	0.338695	2.305518	1.970429
21	1	0	-1.379356	1.836366	1.900484
22	1	0	-2.708458	2.090490	-0.201047
23	1	0	-1.954874	2.768702	-1.669534
24	1	0	-2.352381	3.826019	-0.296319
25	1	0	-4.310290	-1.575368	-1.052698

26	1	0	-2.908552	-2.210993	-1.976931
27	1	0	-3.156020	-0.437840	-1.832762
28	6	0	2.365743	-0.750355	1.265884
29	6	0	3.725807	-1.053758	1.159788
30	6	0	4.287413	-1.301676	-0.092218
31	6	0	3.484323	-1.252173	-1.237167
32	6	0	2.127889	-0.953846	-1.129606
33	1	0	1.926126	-0.564701	2.243792
34	1	0	4.341812	-1.097753	2.054003
35	1	0	5.344777	-1.537644	-0.178491
36	1	0	3.917942	-1.453712	-2.213307
37	1	0	1.492672	-0.924899	-2.009363

B3LYP/6-31G* (Onsager)

```
Zero-point correction=                           0.302147 (Hartree/Particle)
Thermal correction to Energy=                    0.321792
Thermal correction to Enthalpy=                  0.322736
Thermal correction to Gibbs Free Energy=         0.253173
Sum of electronic and zero-point Energies=          -1184.942755
Sum of electronic and thermal Energies=             -1184.923111
Sum of electronic and thermal Enthalpies=           -1184.922167
Sum of electronic and thermal Free Energies=        -1184.991730
```

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	201.928	72.714	146.408

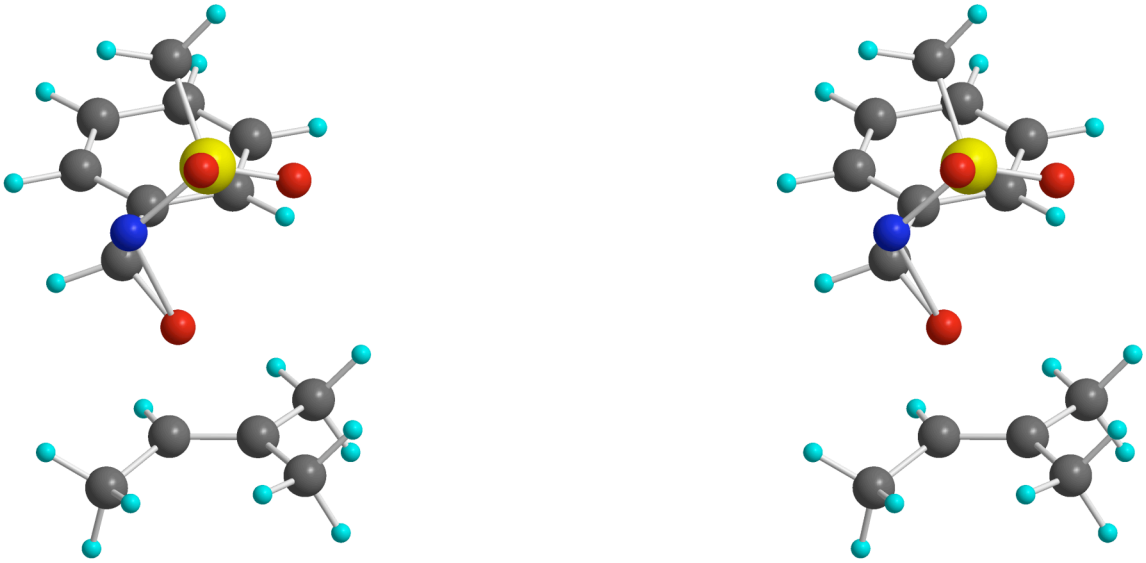
Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	0.492505	2.528534	-0.808689
2	6	0	C	-0.591403	2.600129	0.055371
3	8	0	O	-0.398484	0.621674	-0.615605
4	6	0	C	0.087786	-0.405808	0.276731
5	7	0	N	-0.759028	-1.304789	-0.425944
6	16	0	S	-2.331671	-1.389498	0.171097
7	8	0	O	-2.661707	-0.318033	1.137147
8	8	0	O	-2.568785	-2.785724	0.579709
9	6	0	C	1.945145	2.556786	-0.465456
10	6	0	C	-0.475237	2.613377	1.551725
11	6	0	C	-1.972799	2.847948	-0.478794
12	6	0	C	-3.282860	-1.094248	-1.330515
13	1	0	H	0.265299	2.613400	-1.868753
14	1	0	H	-0.189821	-0.179786	1.311747
15	6	0	C	1.552809	-0.731240	0.148698
16	1	0	H	2.505718	1.859822	-1.095940
17	1	0	H	2.154242	2.318135	0.578532
18	1	0	H	2.338555	3.563210	-0.670429
19	1	0	H	-0.730825	3.613894	1.927123
20	1	0	H	0.523741	2.364965	1.915282
21	1	0	H	-1.200374	1.912988	1.981897
22	1	0	H	-2.674931	2.132700	-0.035891
23	1	0	H	-2.010574	2.764137	-1.568242
24	1	0	H	-2.304814	3.857709	-0.200154
25	1	0	H	-4.338430	-1.213082	-1.074753
26	1	0	H	-2.981999	-1.829189	-2.078512
27	1	0	H	-3.078075	-0.082058	-1.680554
28	6	0	C	2.371529	-0.732308	1.280918
29	6	0	C	3.734954	-1.018419	1.169777

30	6	0	C	4.285687	-1.304622	-0.079011
31	6	0	C	3.468805	-1.310872	-1.215143
32	6	0	C	2.109549	-1.027672	-1.102579
33	1	0	H	1.941853	-0.508041	2.255283
34	1	0	H	4.364165	-1.010704	2.055773
35	1	0	H	5.347132	-1.518587	-0.170703
36	1	0	H	3.896055	-1.534537	-2.189128
37	1	0	H	1.465987	-1.032322	-1.976717

Epoxidation TS Isomer 3 + cis-Phenyl

B3LYP/6-31+G** (PCM)



Filename: b3BBPCMts3cisfreq
E(RB+HF-LYP) = -1185.30104674

Zero-point correction=	0.298591 (Hartree/Particle)
Thermal correction to Energy=	0.317900
Thermal correction to Enthalpy=	0.318844
Thermal correction to Gibbs Free Energy=	0.250056
Sum of electronic and zero-point Energies=	-1185.002455
Sum of electronic and thermal Energies=	-1184.983147
Sum of electronic and thermal Enthalpies=	-1184.982202
Sum of electronic and thermal Free Energies=	-1185.050991

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	199.485	71.533	144.778

1	6	0	0.892059	1.308474	-0.858763
2	6	0	0.849454	1.046974	0.518449
3	6	0	1.579204	1.870056	1.391244
4	6	0	2.354215	2.923553	0.899254
5	6	0	2.394973	3.175296	-0.475515
6	6	0	1.660374	2.367214	-1.349958
7	8	0	0.804386	-1.664764	-1.555429
8	16	0	1.215978	-2.160757	-0.225344
9	7	0	0.404260	-1.469286	1.093826
10	6	0	0.045662	-0.075288	1.138348
11	8	0	-1.135143	-0.523903	0.486325
12	6	0	2.940686	-1.688143	0.043087

13	8	0	1.121766	-3.615597	0.013089
14	6	0	-2.747786	0.779810	0.772349
15	6	0	-2.971913	0.553078	-0.573287
16	6	0	-3.717163	-0.636503	-1.093499
17	6	0	-3.402565	0.083135	1.927154
18	6	0	-2.510459	1.537553	-1.604362
19	1	0	-2.230438	1.707213	1.020943
20	1	0	-0.145476	0.168786	2.192663
21	1	0	-2.717381	0.025999	2.778484
22	1	0	-3.729728	-0.929159	1.685411
23	1	0	-4.278686	0.658823	2.255926
24	1	0	-4.670742	-0.311598	-1.533525
25	1	0	-3.928691	-1.383965	-0.329090
26	1	0	-3.145785	-1.113000	-1.898456
27	1	0	-1.945929	1.041040	-2.401885
28	1	0	-1.900918	2.336661	-1.178265
29	1	0	-3.389729	1.991767	-2.083576
30	1	0	3.520158	-2.211637	-0.721493
31	1	0	3.235947	-2.015875	1.040854
32	1	0	3.036670	-0.608231	-0.068560
33	1	0	1.539697	1.684311	2.464219
34	1	0	2.916730	3.549962	1.588587
35	1	0	2.992276	3.998218	-0.863156
36	1	0	1.686294	2.559152	-2.420880
37	1	0	0.341738	0.671504	-1.538372

B3LYP/6-31+G** (gas phase)

Filename: b3BBts3cis

E(RB+HF-LYP) = -1185.28779736

Zero-point correction=	0.299716 (Hartree/Particle)
Thermal correction to Energy=	0.319779
Thermal correction to Enthalpy=	0.320723
Thermal correction to Gibbs Free Energy=	0.249408
Sum of electronic and zero-point Energies=	-1184.988082
Sum of electronic and thermal Energies=	-1184.968018
Sum of electronic and thermal Enthalpies=	-1184.967074
Sum of electronic and thermal Free Energies=	-1185.038389

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	200.664	73.270	150.095

C,0,-2.8451099191,-1.5606190823,-0.088629411
C,0,-1.5904438971,-1.7289935415,-0.89838086
C,0,-0.4516242972,-2.4268657556,-0.517538106
C,0,0.5785367204,-2.8243332805,-1.5287993706
C,0,-0.1580940379,-2.8011309557,0.9024380701
O,0,-0.6497618735,-0.0965024733,-0.3716992333
C,0,-0.431750905,0.9228057581,-1.3655594745
N,0,-0.408039621,1.8365270529,-0.2763477196
S,0,1.0208339676,2.2433401398,0.5285535171
C,0,0.2770498476,3.0917584626,1.9312382568
O,0,1.7502996862,3.2432823976,-0.2761638784
O,0,1.7766105694,1.0894733401,1.0599037403
H,0,-1.7042054565,-1.559470306,-1.9685441304
H,0,-1.356880234,1.1046937404,-1.9291303012
C,0,0.6965228536,0.7145132364,-2.3542468897
H,0,-3.3798096723,-0.6617471844,-0.4064690898

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H,0,-2.6407656625,-1.4662002242,0.9789699819
H,0,-3.5135517721,-2.4185603414,-0.2413479586
H,0,0.263879725,-3.8116274532,0.9552499414
H,0,-1.029903373,-2.7496747158,1.555633585
H,0,0.6021608013,-2.1137631474,1.2992472397
H,0,1.5853909082,-2.5406798798,-1.2025150474
H,0,0.3957348859,-2.3863003712,-2.5117399161
H,0,0.5781058025,-3.9194645304,-1.6302487927
H,0,1.1068558833,3.4570236727,2.5389363814
H,0,-0.3290440385,2.3764137863,2.4873109008
H,0,-0.3282935688,3.9177103347,1.5585053165
C,0,0.4307941846,0.9946850977,-3.7020070363
C,0,1.4175381797,0.832650639,-4.6777894586
C,0,2.687410006,0.382425735,-4.3115879919
C,0,2.9595299108,0.0971389398,-2.9696056725
C,0,1.9737577729,0.2580473368,-1.9953785475
H,0,-0.5555989873,1.3505841396,-3.9908618394
H,0,1.1945928604,1.0600042875,-5.7162712787
H,0,3.4610361555,0.2581995378,-5.0640000335
H,0,3.9483779346,-0.2448123221,-2.6772748446
H,0,2.1974806604,0.05006893,-0.9554220486
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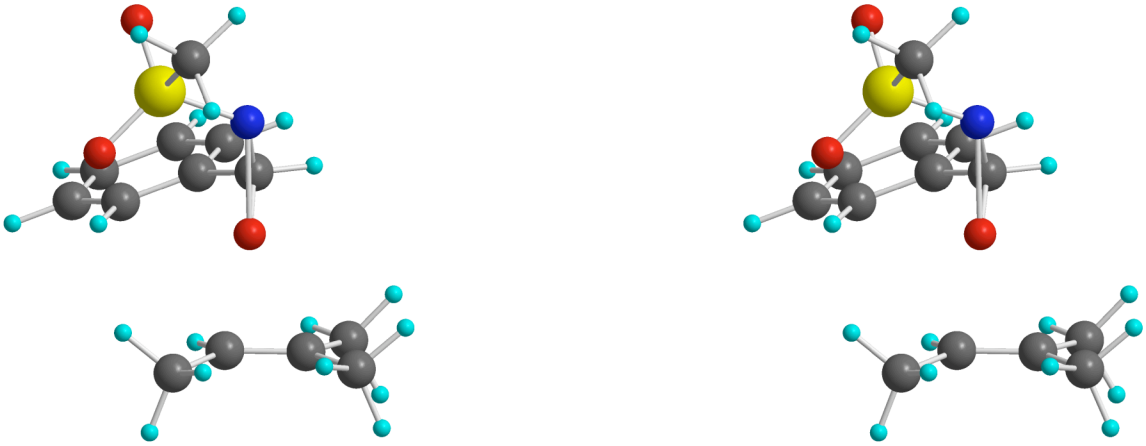
Epoxidation TS Isomer 5 + cis-Phenyl

B3LYP/6-31+G** (PCM)



Filename: b3BBPCMts5cisfreq

E(RB+HF-LYP) = -1185.30484579

Zero-point correction=	0.298717 (Hartree/Particle)
Thermal correction to Energy=	0.318978
Thermal correction to Enthalpy=	0.319922
Thermal correction to Gibbs Free Energy=	0.248231
Sum of electronic and zero-point Energies=	-1185.006128
Sum of electronic and thermal Energies=	-1184.985868
Sum of electronic and thermal Enthalpies=	-1184.984924
Sum of electronic and thermal Free Energies=	-1185.056614

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.162	73.591	150.885

1	6	0	0.738181	1.427559	0.979299
2	6	0	0.494602	1.275646	-0.393976

3	6	0	0.753794	2.353001	-1.253730
4	6	0	1.260420	3.557766	-0.758470
5	6	0	1.501155	3.701300	0.610651
6	6	0	1.236417	2.633857	1.476044
7	6	0	-0.056960	0.010700	-1.017226
8	7	0	0.670108	-1.219274	-1.145585
9	16	0	1.855437	-1.676708	-0.039377
10	8	0	3.130617	-1.031562	-0.438605
11	8	0	-0.972515	-0.782888	-0.260564
12	6	0	1.957955	-3.419546	-0.467883
13	8	0	1.476530	-1.588229	1.388586
14	6	0	-2.423554	0.051936	0.996355
15	6	0	-3.149942	-0.082206	-0.172595
16	6	0	-3.906167	-1.321380	-0.546103
17	6	0	-2.357102	-0.909834	2.140138
18	6	0	-3.287895	1.078294	-1.115727
19	1	0	-1.990764	1.031408	1.185899
20	1	0	-0.464006	0.251651	-2.007811
21	1	0	-1.336887	-0.956317	2.532343
22	1	0	-2.663965	-1.921336	1.869066
23	1	0	-3.008817	-0.560652	2.952634
24	1	0	-4.984324	-1.139797	-0.430641
25	1	0	-3.639932	-2.187214	0.060302
26	1	0	-3.737903	-1.567951	-1.600103
27	1	0	-3.016763	0.789218	-2.138526
28	1	0	-2.681528	1.935459	-0.814060
29	1	0	-4.338945	1.396686	-1.153838
30	1	0	2.753526	-3.840906	0.150250
31	1	0	2.198680	-3.506745	-1.527678
32	1	0	0.999102	-3.887089	-0.241166
33	1	0	0.559329	2.248500	-2.320580
34	1	0	1.460834	4.381715	-1.440302
35	1	0	1.891842	4.638449	1.002219
36	1	0	1.423548	2.737718	2.543029
37	1	0	0.556750	0.598317	1.652093

B3LYP/6-31+G** (gas phase)

E(RB+HF-LYP) = -1185.28906824

Zero-point correction=	0.299722 (Hartree/Particle)
Thermal correction to Energy=	0.319880
Thermal correction to Enthalpy=	0.320824
Thermal correction to Gibbs Free Energy=	0.249687
Sum of electronic and zero-point Energies=	-1184.989347
Sum of electronic and thermal Energies=	-1184.969189
Sum of electronic and thermal Enthalpies=	-1184.968244
Sum of electronic and thermal Free Energies=	-1185.039381

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	200.728	73.370	149.719

C,0,-0.6407985986,-2.3469754229,1.8232384346
C,0,0.0529832511,-2.4058195876,0.498285537
C,0,1.4214591107,-2.4356438435,0.261460833
C,0,1.9477118361,-2.754504654,-1.1087235338
C,0,2.453818459,-2.2328469277,1.3294768186
O,0,0.4014343505,-0.4826033736,0.1623900952
C,0,0.1715262771,0.1714522342,-1.1086439508
N,0,0.0961197617,1.38578624,-0.3759780847
S,0,-1.3659565968,1.940957281,0.2555648206

```
C,0,-0.7000308011,3.1972671957,1.359459225
O,0,-2.0943598628,0.9595867907,1.0905701537
O,0,-2.1170512702,2.6258101402,-0.81561606
H,0,-0.5857181157,-2.6515362809,-0.3462444007
C,0,-0.9262633916,-0.3785995562,-1.9994394034
H,0,1.103310668,0.1943231683,-1.6873218753
H,0,-1.4730130803,-1.6386506629,1.7726926479
H,0,0.0158562133,-2.0368179165,2.6374706651
H,0,-1.0495050423,-3.3361395507,2.0686072145
H,0,2.9363457135,-3.1924615665,1.5646130264
H,0,2.0403484225,-1.8234135727,2.2508443612
H,0,3.2408404079,-1.5588798391,0.9748413812
H,0,2.665131847,-1.9944361761,-1.4410153236
H,0,1.1519983713,-2.8397322478,-1.8521840558
H,0,2.4959893373,-3.7065059242,-1.0807372026
H,0,-1.5614631448,3.6873126887,1.8167063585
H,0,-0.1154424755,3.9035479301,0.7702975202
H,0,-0.0839637351,2.7062596328,2.1129528117
C,0,-0.6481727294,-0.4740304758,-3.3703036423
C,0,-1.6016649963,-0.9649694274,-4.2658041633
C,0,-2.8489602422,-1.3780874255,-3.7943437544
C,0,-3.134020219,-1.2907192273,-2.4279560618
C,0,-2.183933128,-0.7939647376,-1.5345790692
H,0,0.3216031466,-0.152742528,-3.7433614188
H,0,-1.3692314487,-1.0232496149,-5.3252547475
H,0,-3.5952583764,-1.7604575851,-4.4848157855
H,0,-4.1063170883,-1.5996424981,-2.0549398927
H,0,-2.4272258305,-0.7012826793,-0.4826094784
```

B3LYP/6-31G* (gas phase)

```
E(RB+HF-LYP) =  -1185.23169719

 Zero-point correction=                           0.301996 (Hartree/Particle)
 Thermal correction to Energy=                    0.321851
 Thermal correction to Enthalpy=                  0.322795
 Thermal correction to Gibbs Free Energy=         0.252972
 Sum of electronic and zero-point Energies=          -1184.929701
 Sum of electronic and thermal Energies=             -1184.909846
 Sum of electronic and thermal Enthalpies=           -1184.908902
 Sum of electronic and thermal Free Energies=        -1184.978725

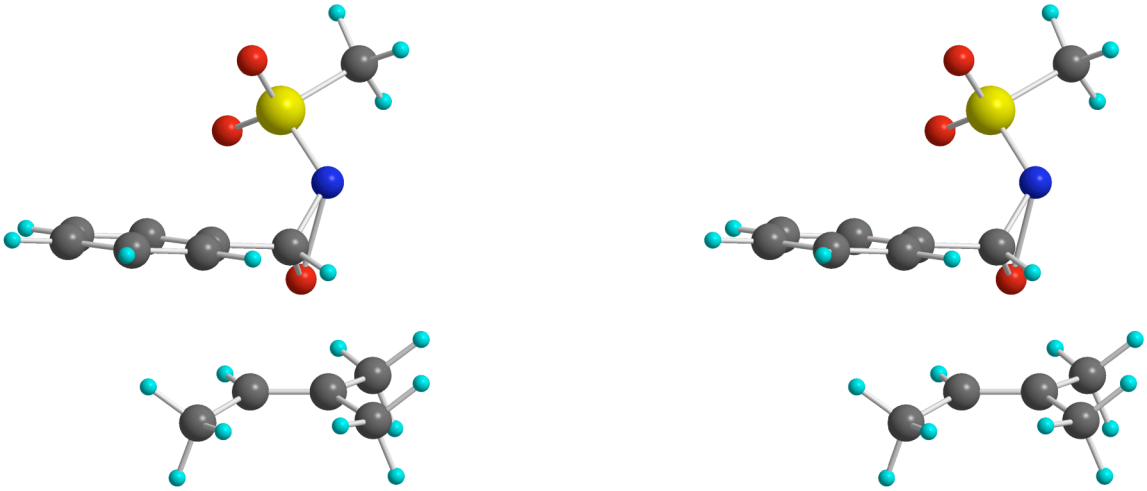
                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 201.965             72.762           146.955

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -2.134497   -0.631210    1.024966
    2          6             0       -2.938122   -0.865929   -0.082989
    3          8             0       -0.766462   -1.014466   -0.326803
    4          6             0       -0.042625    0.002406   -1.059052
    5          7             0        0.984611   -0.962623   -1.221604
    6         16             0        2.195940   -1.145685   -0.069634
    7          8             0        1.715491   -1.318107    1.318878
    8          8             0        3.248294   -0.144418   -0.316598
    9          6             0       -1.752007   -1.601611    2.099158
   10          6             0       -3.421519   -2.227115   -0.485735
   11          6             0       -3.430408    0.281421   -0.918418
   12          6             0        2.806135   -2.749510   -0.614104
   13          1             0       -1.919768    0.409983    1.251800
```

14	1	0	-0.510494	0.149317	-2.040986
15	6	0	0.121294	1.364860	-0.411882
16	1	0	-0.675274	-1.531360	2.285250
17	1	0	-1.985427	-2.637385	1.844103
18	1	0	-2.280232	-1.350750	3.028872
19	1	0	-4.497096	-2.321033	-0.274685
20	1	0	-2.900714	-3.034592	0.029915
21	1	0	-3.295976	-2.371665	-1.564781
22	1	0	-3.226977	0.109876	-1.983010
23	1	0	-2.981562	1.233696	-0.624599
24	1	0	-4.522374	0.370586	-0.822081
25	1	0	3.656104	-2.994299	0.026726
26	1	0	3.117398	-2.674675	-1.656595
27	1	0	2.010069	-3.486196	-0.497924
28	6	0	0.495917	1.564690	0.926142
29	6	0	0.605521	2.856989	1.437865
30	6	0	0.348400	3.967127	0.629687
31	6	0	-0.021619	3.778748	-0.701404
32	6	0	-0.138349	2.485291	-1.212654
33	1	0	0.724320	0.711783	1.554816
34	1	0	0.902410	2.996542	2.473929
35	1	0	0.439865	4.971305	1.035126
36	1	0	-0.221180	4.633683	-1.341940
37	1	0	-0.427724	2.343483	-2.251867

Epoxidation TS Isomer 7 + cis-Phenyl

B3LYP/6-31+G** (PCM)



Filename: b3BBPCMts7cisfreq
E(RB+HF-LYP) = -1185.30159596

Zero-point correction=	0.298892 (Hartree/Particle)
Thermal correction to Energy=	0.318871
Thermal correction to Enthalpy=	0.319815
Thermal correction to Gibbs Free Energy=	0.249614
Sum of electronic and zero-point Energies=	-1185.002704
Sum of electronic and thermal Energies=	-1184.982725
Sum of electronic and thermal Enthalpies=	-1184.981781
Sum of electronic and thermal Free Energies=	-1185.051982

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.095	73.550	147.751

1	6	0	-2.706801	1.742756	-0.813359
2	6	0	-2.687440	0.259469	-0.978482
3	6	0	-3.086217	-0.693497	-0.054098
4	6	0	-3.316092	-2.112114	-0.494483
5	6	0	-3.546554	-0.364829	1.337219
6	8	0	-0.996897	-0.834746	0.000861
7	6	0	-0.126538	-0.121101	0.889767
8	7	0	0.632826	-1.333233	0.936368
9	16	0	1.921336	-1.633877	-0.099296
10	6	0	2.112184	-3.392289	0.225948
11	8	0	3.125615	-0.942177	0.425049
12	8	0	1.636031	-1.478096	-1.543889
13	1	0	-2.456209	-0.101864	-1.979951
14	1	0	-1.824784	2.199797	-1.269627
15	1	0	-2.772285	2.071927	0.225177
16	1	0	-3.582603	2.140460	-1.347849
17	1	0	-4.641291	-0.443280	1.383370
18	1	0	-3.268938	0.637678	1.666110
19	1	0	-3.145868	-1.093324	2.049804
20	1	0	-2.925820	-2.816638	0.246085
21	1	0	-2.848827	-2.318407	-1.459903
22	1	0	-4.396026	-2.292412	-0.585329
23	1	0	-0.593636	0.017090	1.873649
24	6	0	0.443137	1.200446	0.420198
25	1	0	2.972847	-3.719902	-0.361013
26	1	0	1.204374	-3.903478	-0.096069
27	1	0	2.288860	-3.536369	1.292084
28	6	0	0.663868	2.189797	1.388179
29	6	0	1.196914	3.431981	1.031692
30	6	0	1.506079	3.698545	-0.304837
31	6	0	1.279134	2.717914	-1.277414
32	6	0	0.750705	1.475754	-0.920164
33	1	0	0.418988	1.986892	2.430269
34	1	0	1.365976	4.188281	1.795553
35	1	0	1.919085	4.664534	-0.588657
36	1	0	1.517059	2.919790	-2.320022
37	1	0	0.585665	0.717035	-1.676688

B3LYP/6-31+G** (gas phase)

Filename: b3BBts7cis

E(RB+HF-LYP) = -1185.28417982

Zero-point correction=	0.299732 (Hartree/Particle)
Thermal correction to Energy=	0.319700
Thermal correction to Enthalpy=	0.320644
Thermal correction to Gibbs Free Energy=	0.250122
Sum of electronic and zero-point Energies=	-1184.984448
Sum of electronic and thermal Energies=	-1184.964480
Sum of electronic and thermal Enthalpies=	-1184.963536
Sum of electronic and thermal Free Energies=	-1185.034058

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	200.615	73.482	148.426

C,0,2.8712322419,0.7156534443,1.3629748653
C,0,2.468936517,-0.7139183001,1.230400222
C,0,2.6574290196,-1.5542939222,0.1363286679
C,0,2.5196073568,-3.0436099781,0.3120430329
C,0,3.3209724623,-1.1119140311,-1.1398275874
O,0,0.7303921063,-1.1328936211,0.0127238155

```
C,0,0.1406465878,-0.1746198746,-0.9151648784
N,0,-0.9475872642,-1.0683256003,-1.0542101429
S,0,-2.3245437983,-0.9643440574,-0.0878304504
C,0,-3.0923417646,-2.5133941385,-0.5913916403
O,0,-3.1734753009,0.1421882983,-0.5752256702
O,0,-2.0638755614,-1.0521880663,1.3643829423
H,0,2.0698746613,-1.1788878276,2.1284595447
H,0,2.0925839483,1.2965022286,1.8650244071
H,0,3.1000137103,1.1991154015,0.4121357689
H,0,3.7692262232,0.7709412319,1.9965034934
H,0,4.3753060162,-1.4185053587,-1.1257031363
H,0,3.2884448688,-0.0324802624,-1.2949582333
H,0,2.8561389442,-1.6041458072,-1.9996392261
H,0,2.054982059,-3.4960113712,-0.5684343307
H,0,1.9161349462,-3.2895366461,1.1882606551
H,0,3.5144531,-3.4926195187,0.4362313149
H,0,0.7043414929,-0.1805502684,-1.8560297413
C,0,0.0185643586,1.2562499084,-0.4329477263
H,0,-4.0438385737,-2.5660571892,-0.0592688133
H,0,-2.4374265766,-3.3352742808,-0.3016623999
H,0,-3.2480980156,-2.4925501153,-1.6697641876
C,0,0.362587196,2.2728248516,-1.3339047085
C,0,0.2667588899,3.6186196896,-0.9694863462
C,0,-0.1739078167,3.9608615837,0.3101653573
C,0,-0.5157904102,2.951533455,1.2165203694
C,0,-0.419894232,1.6078537748,0.8528770878
H,0,0.699024048,2.0110130883,-2.3347306565
H,0,0.5317421542,4.3930739281,-1.6835937546
H,0,-0.2548990184,5.004866966,0.599198343
H,0,-0.8687581129,3.2112427352,2.2105710038
H,0,-0.7041554715,0.8328911669,1.5560278027
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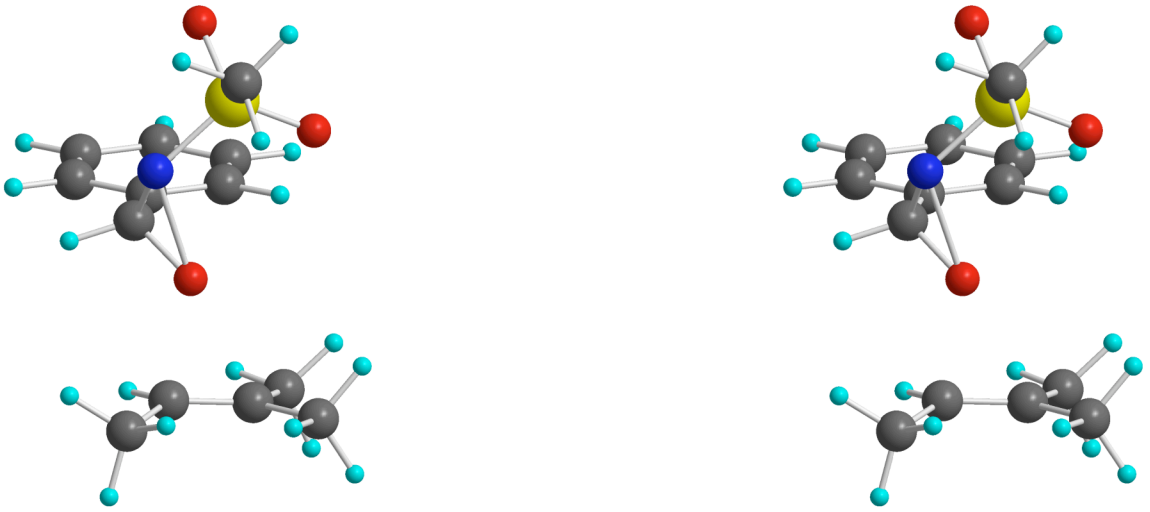
Epoxidation TS Isomer 8 + cis-Phenyl

B3LYP/6-31+G** (PCM)



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Filename: b3BBPCMts8cisfreq
E(RB+HF-LYP) = -1185.30329038

 Zero-point correction=                           0.298644 (Hartree/Particle)
 Thermal correction to Energy=                    0.318887
 Thermal correction to Enthalpy=                  0.319832
 Thermal correction to Gibbs Free Energy=         0.247857
 Sum of electronic and zero-point Energies=          -1185.004646
```

```
 Sum of electronic and thermal Energies=             -1184.984403
 Sum of electronic and thermal Enthalpies=           -1184.983459
 Sum of electronic and thermal Free Energies=        -1185.055434

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 200.105             73.529           151.484

    1          6             0       -2.796428    0.491827    0.797648
    2          6             0       -2.938628    0.436171   -0.577603
    3          8             0       -1.071631   -0.596186    0.473789
    4          6             0        0.076723   -0.064572    1.137469
    5          7             0        0.561759   -1.409604    1.052182
    6          6             0        0.768313    1.140416    0.538930
    7          6             0        0.885255    1.363149   -0.840443
    8          6             0        1.537743    2.502779   -1.314799
    9          6             0        2.081145    3.432374   -0.420937
   10          6             0        1.964388    3.219327    0.955476
   11          6             0        1.305949    2.081409    1.429571
   12         16             0        1.512794   -1.948400   -0.231379
   13          8             0        2.914088   -1.535714    0.026929
   14          6             0       -3.446755   -0.403662    1.810633
   15          6             0       -3.544207   -0.728456   -1.297776
   16          6             0       -2.506835    1.582517   -1.440447
   17          8             0        0.972105   -1.691284   -1.584625
   18          6             0        1.388923   -3.715138    0.075584
   19          1             0       -2.379079    1.416456    1.197419
   20          1             0       -0.138868    0.140435    2.195288
   21          1             0       -2.819223   -0.486402    2.702851
   22          1             0       -3.631905   -1.409811    1.431458
   23          1             0       -4.406753    0.027599    2.126014
   24          1             0       -2.824555   -1.123861   -2.025601
   25          1             0       -4.421149   -0.398043   -1.871002
   26          1             0       -3.848257   -1.539861   -0.636862
   27          1             0       -1.877916    1.238807   -2.269470
   28          1             0       -1.968255    2.349138   -0.880556
   29          1             0       -3.395726    2.044507   -1.893891
   30          1             0        2.013070   -4.200465   -0.677778
   31          1             0        0.345304   -4.012383   -0.033160
   32          1             0        1.755833   -3.923898    1.080806
   33          1             0        1.211617    1.920247    2.502880
   34          1             0        2.380882    3.937046    1.659348
   35          1             0        2.591150    4.317515   -0.796043
   36          1             0        1.625645    2.663319   -2.387571
   37          1             0        0.481157    0.637901   -1.535935
```

B3LYP/6-31+G** (gas phase)

```
Filename: b3BBts8cis

E(RB+HF-LYP) = -1185.28779729

 Zero-point correction=                           0.299718 (Hartree/Particle)
 Thermal correction to Energy=                    0.319780
 Thermal correction to Enthalpy=                  0.320724
 Thermal correction to Gibbs Free Energy=         0.249412
 Sum of electronic and zero-point Energies=          -1184.988080
 Sum of electronic and thermal Energies=             -1184.968017
 Sum of electronic and thermal Enthalpies=           -1184.967073
 Sum of electronic and thermal Free Energies=        -1185.038386

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 200.665             73.269           150.090
```

```
C,0,-0.450326748,-2.3387607701,-2.3790126649
 C,0,0.6831246099,-2.1624371287,-1.4082220262
 C,0,0.7996369138,-2.7608299747,-0.1602977862
 C,0,2.1151495656,-2.7956538116,0.5539020834
 C,0,-0.3580401346,-3.3764172925,0.5631510709
 O,0,0.0575093357,-0.5606241749,-0.4754925698
 C,0,0.8021578579,0.66206284,-0.633042944
 N,0,-0.4248667295,1.3254874949,-0.3571536857
 S,0,-0.8880331425,1.7492709524,1.2115876141
 C,0,-2.5988412994,2.1791819556,0.8526021149
 O,0,-0.1778130324,2.9843792512,1.5984559987
 O,0,-0.9067337109,0.6253582588,2.1714879478
 H,0,1.6112461011,-1.7927470129,-1.8427924963
 H,0,1.0360296901,0.8277692745,-1.6934218592
 C,0,2.0781452674,0.8193551468,0.1675780424
 H,0,-0.5106703152,-1.4757111716,-3.0471440329
 H,0,-1.414282956,-2.4397149056,-1.8779761513
 H,0,-0.2842354996,-3.2301160552,-2.9987693297
 H,0,-0.6864666539,-2.68836451,1.3547553523
 H,0,-0.0541811579,-4.3085820828,1.0537665427
 H,0,-1.2148192309,-3.5807274158,-0.0799228774
 H,0,2.0143512617,-2.4505305753,1.5889882691
 H,0,2.8794721224,-2.1930683054,0.0597720296
 H,0,2.4696246547,-3.835644778,0.6026992424
 H,0,-3.0293114232,2.5213722081,1.795414584
 H,0,-3.1113306002,1.2880791801,0.4898706561
 H,0,-2.6098879768,2.9732272702,0.106320266
 C,0,3.198109416,1.3329891442,-0.5013228922
 C,0,4.4129639061,1.5130981877,0.1648267694
 C,0,4.5198305191,1.1753861343,1.5153487846
 C,0,3.4081959373,0.6588640246,2.1890142874
 C,0,2.1953195906,0.4781154512,1.5234171653
 H,0,3.1177372615,1.6022140863,-1.5520992488
 H,0,5.2683021949,1.9174875843,-0.3687500092
 H,0,5.4598522435,1.3167101072,2.0411243945
 H,0,3.4826773575,0.4027683057,3.2421411919
 H,0,1.3342098041,0.0922661072,2.0567341661
```

B3LYP/6-31G* (gas phase)

```
E(RB+HF-LYP) =  -1185.23044279

 Zero-point correction=                           0.301915 (Hartree/Particle)
 Thermal correction to Energy=                    0.321729
 Thermal correction to Enthalpy=                  0.322673
 Thermal correction to Gibbs Free Energy=         0.252442
 Sum of electronic and zero-point Energies=          -1184.928528
 Sum of electronic and thermal Energies=             -1184.908714
 Sum of electronic and thermal Enthalpies=           -1184.907770
 Sum of electronic and thermal Free Energies=        -1184.978001

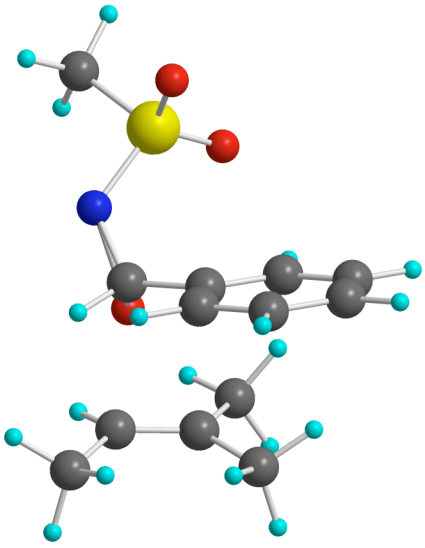
                     E (Thermal)             CV                S
                      KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  201.888             72.694            147.813

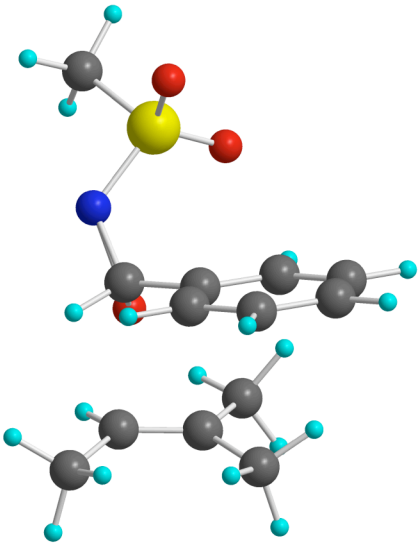
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.903232    2.671054   -0.777584
    2          6             0        0.573598    2.740378    0.569523
```

3	8	0	0.980069	0.754493	-0.548909
4	6	0	0.033361	-0.115245	-1.194086
5	7	0	1.050777	-1.105212	-1.123265
6	16	0	1.238847	-2.089317	0.231425
7	8	0	0.274450	-3.200761	0.158648
8	8	0	1.367575	-1.358158	1.509226
9	6	0	2.268212	2.884549	-1.368953
10	6	0	1.596245	2.646520	1.661595
11	6	0	-0.854029	2.865731	1.002262
12	6	0	2.871330	-2.733650	-0.170151
13	1	0	0.075169	2.780895	-1.477130
14	6	0	-1.349381	-0.235372	-0.587031
15	1	0	-0.078725	0.164980	-2.250529
16	1	0	2.346077	2.364923	-2.327899
17	1	0	3.061598	2.509024	-0.719764
18	1	0	2.443287	3.954039	-1.550637
19	1	0	1.279199	3.208591	2.546933
20	1	0	2.584862	2.998883	1.357736
21	1	0	1.694001	1.590785	1.955490
22	1	0	-1.113383	2.102805	1.745419
23	1	0	-1.556442	2.784602	0.169191
24	1	0	-0.999886	3.842303	1.488074
25	1	0	3.127655	-3.444886	0.618245
26	1	0	3.581487	-1.905876	-0.188585
27	1	0	2.828226	-3.231141	-1.139637
28	6	0	-2.442725	-0.117312	-1.454920
29	6	0	-3.751894	-0.217514	-0.981120
30	6	0	-3.982415	-0.434461	0.376836
31	6	0	-2.898724	-0.548676	1.251411
32	6	0	-1.590958	-0.447012	0.779175
33	1	0	-2.267432	0.046168	-2.516373
34	1	0	-4.585940	-0.128113	-1.672090
35	1	0	-4.998909	-0.517468	0.752451
36	1	0	-3.071529	-0.724798	2.309889
37	1	0	-0.758168	-0.548705	1.465819

Epoxidation TS Isomer 9 + cis-Phenyl

B3LYP/6-31+G** (PCM)





Filename: b3BBPCMts9cisfreq
E(RB+HF-LYP) = -1185.30311091

```
 Zero-point correction=                           0.298994 (Hartree/Particle)
 Thermal correction to Energy=                    0.319040
 Thermal correction to Enthalpy=                  0.319984
 Thermal correction to Gibbs Free Energy=         0.249121
 Sum of electronic and zero-point Energies=          -1185.004117
 Sum of electronic and thermal Energies=             -1184.984071
 Sum of electronic and thermal Enthalpies=           -1184.983127
 Sum of electronic and thermal Free Energies=        -1185.053990

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 200.201             73.409            149.144

 C,0,-0.5346187483,2.2265457833,-1.3480076792
 C,0,-0.2257237514,1.1687963941,-0.4806734182
 C,0,-0.2488846677,1.3928021326,0.9033290173
 C,0,-0.5646584816,2.6569303081,1.4048691986
 C,0,-0.8628839802,3.7108184139,0.5338191681
 C,0,-0.8477080997,3.4932577192,-0.8465720303
 C,0,0.1141381771,-0.1671056301,-1.1043067948
 N,0,1.4228082189,-0.75280491,-1.0824909448
 S,0,2.5343025399,-0.4529824043,0.1474184109
 O,0,3.2099444864,0.8351095875,-0.145915089
 O,0,-0.2772698904,-1.3588837561,-0.4201107452
 C,0,3.6903450221,-1.7802811795,-0.2192356416
 O,0,2.0421370782,-0.6554868123,1.5278009798
 C,0,-2.1691908847,-2.1131242084,-0.6180557786
 C,0,-2.4382389606,-1.5661830977,0.6254809938
 C,0,-3.2275923706,-0.3083968621,0.8228682503
 C,0,-2.7053527306,-1.6413827625,-1.9370828636
 C,0,-2.0048145807,-2.2751143617,1.8725966114
 H,0,-1.7493082664,-3.1170154343,-0.6262940864
 H,0,-0.2294024385,-0.1740997979,-2.1463654863
 H,0,-2.0035984285,-1.8811231046,-2.741784486
 H,0,-2.9164160901,-0.5698393773,-1.9638775605
 H,0,-3.6413415957,-2.1704049475,-2.1624606721
 H,0,-4.2451303759,-0.5794655715,1.1424567196
 H,0,-3.3116376919,0.3012633874,-0.07735313
 H,0,-2.7989538518,0.3053856979,1.6206293791
 H,0,-1.3413666077,-1.6346798545,2.4661608213
 H,0,-1.4814051985,-3.209205255,1.6575901693
 H,0,-2.8778863186,-2.4951509218,2.5026210866
 H,0,4.5155603946,-1.6708805181,0.4876303289
 H,0,4.0380449184,-1.6691761333,-1.2465478908
 H,0,3.1789542521,-2.7329550767,-0.0763268453
 H,0,-0.0047161169,0.5835617438,1.5811302318
 H,0,-0.5742030323,2.8203687387,2.4807966142
 H,0,-1.106288487,4.6948020987,0.9297686458
 H,0,-1.0804934066,4.3049899566,-1.532779835
 H,0,-0.526298881,2.0596891588,-2.4246273292
```

B3LYP/6-31+G** (gas phase)

```
E(RB+HF-LYP) = -1185.28651191

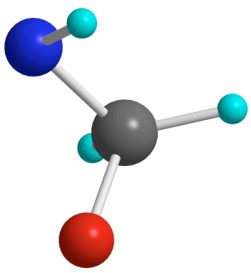
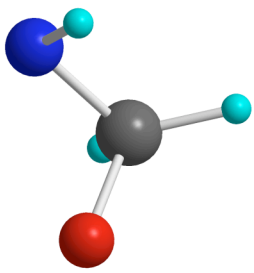
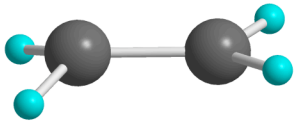
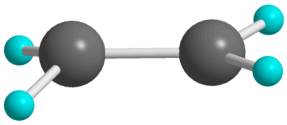
 Zero-point correction=                           0.299825 (Hartree/Particle)
 Thermal correction to Energy=                    0.319818
 Thermal correction to Enthalpy=                  0.320762
 Thermal correction to Gibbs Free Energy=         0.249943
 Sum of electronic and zero-point Energies=          -1184.986687
 Sum of electronic and thermal Energies=             -1184.966694
 Sum of electronic and thermal Enthalpies=           -1184.965750
```

Sum of electronic and thermal Free Energies= -1185.036569

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.689	73.308	149.052

C,0,-2.4642703525,-2.4549310935,0.250554391
C,0,-1.5073576981,-2.079218178,-0.844500683
C,0,-0.2106740144,-2.5588988344,-1.0032348406
C,0,0.5564757393,-2.2490758019,-2.2516313927
C,0,0.4835315961,-3.4153642132,0.0092856326
O,0,-0.6247130326,-0.3986561802,-0.3926804438
C,0,-0.6929168242,0.1796839423,0.934229966
N,0,-0.4669828745,1.4368901471,0.3170507913
S,0,1.0860046171,2.0349220145,0.0435807221
C,0,0.643548471,3.3669283984,-1.0836014877
O,0,1.9864529568,1.1171038719,-0.688731691
O,0,1.5880238708,2.6428407407,1.2924233662
H,0,-1.9695675178,-1.6458177856,-1.7267521625
C,0,0.1838981613,-0.4256273617,2.0125339827
H,0,-1.7303497972,0.1731669451,1.2900769646
H,0,-3.200966851,-1.6605103845,0.4015673899
H,0,-1.9695770109,-2.6552978602,1.2033270672
H,0,-3.0204510374,-3.3572189337,-0.0363767509
H,0,0.4421135389,-4.4622920775,-0.3276388322
H,0,0.0394752472,-3.3646078011,1.0035788788
H,0,1.5417902967,-3.1497837183,0.0885640853
H,0,1.3937252247,-1.5804262285,-2.0128395955
H,0,-0.0616830503,-1.7573637302,-3.0058288585
H,0,0.9822679574,-3.1663110796,-2.6793971012
H,0,1.5736548348,3.8884144036,-1.3165432699
H,0,-0.0607079482,4.0290215761,-0.5803472885
H,0,0.2042070691,2.9315193696,-1.9812075393
C,0,1.536359822,-0.7527837739,1.8319797057
C,0,2.2730132018,-1.2973414384,2.8845291676
C,0,1.6756290057,-1.5270803815,4.1281291025
C,0,0.3296581905,-1.2071761098,4.3159695497
C,0,-0.4075894895,-0.6614971235,3.2619181209
H,0,2.0137968411,-0.5606362132,0.8779930996
H,0,3.3226603647,-1.5341666447,2.7348391666
H,0,2.2567933963,-1.9469811535,4.9442000536
H,0,-0.1451366678,-1.376342565,5.2781948196
H,0,-1.4538152367,-0.4067237435,3.4155349138

CCSDT Parent

Bond Distances: C-O = 1.82 Å C-O = 2.52 Å N-O = 1.99 Å

SCF Done: E(RHF) = -246.751356758   A.U. after   9 cycles

1	1	0	-1.630272	-1.553035	-0.232507
2	6	0	-1.450640	-0.619297	0.286415
3	6	0	-1.994737	0.555707	-0.225604
4	1	0	-2.005497	1.469908	0.356772
5	1	0	-2.297570	0.618561	-1.263556
6	8	0	0.283399	-0.520815	-0.263311
7	6	0	1.007821	0.563366	0.290861
8	7	0	2.222367	-0.121572	-0.046401
9	1	0	2.348657	0.019501	-1.057310
10	1	0	-1.297877	-0.707497	1.357271
11	1	0	0.875901	0.653081	1.373572
12	1	0	0.808244	1.518353	-0.212975

B3LYP Parent

Bond Distances: C-O = 1.69 Å C-O = 2.24 Å N-O = 2.01 Å
E(RB+HF-LYP) = -248.343323795

Zero-point correction=	0.097363 (Hartree/Particle)
Thermal correction to Energy=	0.103481
Thermal correction to Enthalpy=	0.104425
Thermal correction to Gibbs Free Energy=	0.068115
Sum of electronic and zero-point Energies=	-248.245961
Sum of electronic and thermal Energies=	-248.239843
Sum of electronic and thermal Enthalpies=	-248.238898
Sum of electronic and thermal Free Energies=	-248.275209

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	64.935	20.578	76.421

H,0,-1.5323233145,-1.5785160178,-0.0797768357
C,0,-1.3975259659,-0.5720606364,0.3042798963
C,0,-2.0645989262,0.4867212715,-0.3151659724
H,0,-2.1028516267,1.4690173105,0.1435182463
H,0,-2.4542393236,0.3852359044,-1.3214515304
O,0,0.0815835395,-0.1578235365,-0.4111383814
C,0,1.1007393537,0.5491703857,0.3720134821
N,0,2.076155941,-0.2829849212,-0.1706035374
H,0,2.3299333044,0.0924388928,-1.090697857
H,0,-1.193902828,-0.5231736867,1.3721647931
H,0,0.9383816968,0.3905780606,1.4449200008
H,0,1.0884441494,1.6176579732,0.1151646957

mPW1K Parent

Bond Distances: C-O = 1.66 Å C-O = 2.17 Å N-O = 1.97 Å

E(RmPW+HF-PW91) = -248.231240077

Zero-point correction=	0.100793 (Hartree/Particle)
Thermal correction to Energy=	0.106737
Thermal correction to Enthalpy=	0.107682
Thermal correction to Gibbs Free Energy=	0.071749
Sum of electronic and zero-point Energies=	-248.130447
Sum of electronic and thermal Energies=	-248.124503
Sum of electronic and thermal Enthalpies=	-248.123559
Sum of electronic and thermal Free Energies=	-248.159491

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	66.979	19.846	75.625

H,0,-1.5175308832,-1.5731082011,-0.0896436
C,0,-1.3729005167,-0.5776597628,0.3017962764
C,0,-2.0058386778,0.4893050354,-0.313256214
H,0,-2.0340433939,1.4615359577,0.1529870744
H,0,-2.3904042353,0.398435874,-1.3157770184
O,0,0.0667453925,-0.1593494206,-0.3996621045
C,0,1.063350681,0.5535022249,0.3683408654
N,0,2.0155620467,-0.2791112763,-0.1638939738
H,0,2.276845166,0.0815049945,-1.0757817611
H,0,-1.1747496749,-0.5394782956,1.3648898268
H,0,0.8956969194,0.409450488,1.4357785543
H,0,1.0470631762,1.6112333818,0.0974490746

Table of B3LYP/6-31+G** Energies

Table of Energies for Reactions of 2-methyl-2-butene with 2-(methylsulfonyl)oxaziridine from B3LYP/6-31+G**

Isomer	Fig in Paper	Gas Phase Energy	PCM Energy	Gas Phase Free Energy	PCM Free Energy
ts 1 **	Not shown	-954.00759	-954.021744	-954.051787	-954.065809
ts 2	Not shown	-954.005568	-954.021264	-954.048877	-954.065078
ts 3	Not shown	-954.00759	-954.021744	-954.051791	-954.065795
ts 4	Not shown	-954.006634	-954.021471	-954.049977	-954.064988
ts 5	4	-954.008573	-954.024275	-954.051931	-954.067828
ts 6	Not shown	-954.007131	-954.021958	-954.050913	-954.065875
ts 7	6	-954.007067	-954.023098	-954.049925	-954.066459
ts 8	3	-954.009354	-954.024651	-954.052959	-954.068434
ts 9	5	-954.007819	-954.023864	-954.050819	-954.067155

**ts 1 optimizes to ts 3 when the larger basis sets is used in the calculations.

Table of Energies for Reactions of 2-methyl-2-butene with *trans*-3-phenyl-2-methanesulfonyloxaziridine from B3LYP/6-31+G**

Isomer	Fig in Paper	Gas Phase Energy	PCM Energy	Gas Phase Free Energy	PCM Free Energy
ts 3	Not shown	-1184.999913	-1185.016004	-1185.050934	-1185.066834
ts 5	8	-1184.99981	-1185.017734	-1185.050189	-1185.06781
ts 7	10	-1184.997833	-1185.015821	-1185.04725	-1185.065636
ts 8	7	-1185.000354	-1185.01765	-1185.051346	-1185.068021
ts 9	9	-1184.997782	-1185.016184	-1185.047187	-1185.066078

Table of Energies for Reactions of 2-methyl-2-butene with *cis*-3-phenyl-2-methanesulfonyloxaziridine from B3LYP/6-31+G**

Isomer	Fig in Paper	Gas Phase Energy	PCM Energy	Gas Phase Free Energy	PCM Free Energy	GP Barrier	PCM Barrier
ts 3	Not shown	-1184.988082	-1185.002455	-1185.038389	-1185.050991		

ts 5	12	-1184.989347	-1185.006128	-1185.039381	-1185.056614		
ts 7	Not shown	-1184.984448	-1185.002704	-1185.034058	-1185.051982		
ts 8	11	-1184.98808	-1185.004646	-1185.038386	-1185.055434		
ts 9	Not shown	-1184.986687	-1185.004117	-1185.036569	-1185.05399		

Table of Free Energy Barriers

Free Energy Barriers*

	enthalpic barrier (kcal/mol)	free energy barrier (kcal/mol)	experimental free energy barrier (kcal/mol)**
B3LYP/6-31+G** (gas phase)	17.6	29.1	24.7
B3LYP/6-31+G** (PCM)	15.3	26.6	22.2
MPW1K/6-31+G** (gas phase)	23.4	35.4	31.0
MPW1K/6-31+G** (PCM)	24.0	35.4	31.0
bpw91/6-31G* (gas phase)	12.8	24.1	19.7
mpwb95/6-31G* (gas phase)	20.5	33.5	29.1
mpwb1k/6-31G* (gas phase)	25.1	38.0	33.6
b3pw91/6-31G* (gas phase)	19.4	31.0	26.6
rhf/6-31G* (gas phase)	48.0	60.0	55.6
mpw3lyp/6-31G* (gas phase)	15.2	27.0	22.6
tpsskcis/6-31G* (gas phase)	16.3	28.2	23.8
pbepbe/6-31G* (gas phase)	62.8	75.4	71
pbev5lyp/6-31G* (gas phase)	52.7	65.4	61.0
tpssv5lyp/6-31G* (gas phase)	57.6	70.3	65.9
bb95/6-31G* (gas phase)	26.3	39.1	34.7
bp86/6-31G* (gas phase)	17.6	29.1	24.7
pbe1kcis/6-31G* (gas phase)	18.3	30.2	25.8
mpwlp1m/6-31G* (gas phase)	9.3	21.1	16.7

*All energies based upon structure 3.

**Free Energies calculated using the experimental conditions as standard state.

	Energy based upon structure (from paper)	enthalpic barrier (kcal/mol)	free energy barrier (kcal/mol)	experimental free energy barrier (kcal/mol)**
B3LYP/6-31+G** *trans*-phenyl (gas phase)	7	20.4	32.2	27.8
B3LYP/6-31+G** *trans*-phenyl (PCM)	7	19.1	31.2	26.8
B3LYP/6-31+G** *cis*-phenyl (gas phase)	12	21.1	21.1	27.3
B3LYP/6-31+G** *cis*-phenyl (PCM)	12	19.9	19.9	28.9

**Free Energies calculated using the experimental conditions as standard state.

Table of KIEs and C-O Bond Distances

(All C-O Bond Distances are reported in angstroms)

Table of KIEs for the Gas Phase Reactions of 2-methyl-2-butene with 2-(methylsulfonyl)oxaziridine from B3LYP/6-31+G**

		monosubstituted olefin		disubstituted olefin	
Isomer	fig #	C-O	KIE	C-O	KIE

ts 2	Not shown	2.029	1.006	2.237	0.999
ts 3	Not shown	2.078	1.015	2.206	1.009
ts 4	Not shown	2.106	1.014	2.160	1.011
ts 5	4	1.995	1.019	2.244	1.008
ts 6	Not shown	2.053	1.015	2.243	1.007
ts 7	6	1.978	1.018	2.238	1.008
ts 8	3	2.031	1.016	2.194	1.008
ts 9	5	2.030	1.015	2.160	1.009

*All KIEs normalized to set the 4th carbon of 2-methyl-2-butene as the standard, similar to experiment

Table of KIEs for Reactions of 2-methyl-2-butene with 2-(methylsulfonyl)oxaziridine from B3LYP/6-31+G with PCM solvent model**

		monosubstituted olefin		disubstituted olefin	
Isomer	fig #	C-O	KIE	C-O	KIE
ts 2	Not shown	2.159	1.011	2.340	1.007
ts 3	Not shown	2.165	1.011	2.340	1.006
ts 4	Not shown	2.182	1.011	2.319	1.008
ts 5	4	2.150	1.012	2.316	1.007
ts 6	Not shown	2.174	1.011	2.333	1.007
ts 7	6	2.144	1.012	2.309	1.008
ts 8	3	2.150	1.012	2.316	1.007
ts 9	5	2.162	1.012	2.298	1.008

*All KIEs normalized to set the 4th carbon of 2-methyl-2-butene as the standard, similar to experiment

Table of KIEs for the Reactions of 2-methyl-2-butene with 2-(methylsulfonyl)oxaziridine from B3LYP/6-31+G with Onsager solvent model**

		monosubstituted olefin		disubstituted olefin	
Isomer	fig #	C-O	KIE	C-O	KIE
ts 2	Not shown	2.100	1.013	2.300	1.008
ts 3	Not shown	2.128	1.013	2.251	1.008
ts 4	Not shown	2.136	1.012	2.240	1.009
ts 5	4	2.132	1.013	2.336	1.006
ts 6	Not shown	2.112	1.013	2.303	1.007
ts 7	6	2.126	1.013	2.329	1.007
ts 8	3	2.130	1.013	2.302	1.007
ts 9	5	2.139	1.012	2.297	1.007

*All KIEs normalized to set the 4th carbon of 2-methyl-2-butene as the standard, similar to experiment

Table of KIEs for Gas Phase Reactions of 2-methyl-2-butene with trans-3-phenyl-2-methanesulfonyloxaziridine from B3LYP/6-31+G**

	11.008	monosubstituted olefin		disubstituted olefin	
Isomer	fig #	C-O	KIE	C-O	KIE
ts 3	Not shown	2.055	1.016	2.186	1.009
ts 5	8	1.960	1.022	2.295	1.007
ts 7	10	1.928	1.021	2.290	1.008
ts 8	7	1.993	1.018	2.183	1.009
ts 9	9	2.090	1.014	2.055	1.016

*All KIEs normalized to set the 4th carbon of 2-methyl-2-butene as the standard, similar to experiment

Table of KIEs for Gas Phase Reactions of 2-methyl-2-butene with cis-3-phenyl-2-methanesulfonyloxaziridine from B3LYP/6-31+G**

		monosubstituted olefin		disubstituted olefin	
Isomer	fig #	C-O	KIE	C-O	KIE
ts 3	Not shown	1.956	1.024	2.343	1.006
ts 5	8	1.983	1.018	2.206	1.009
ts 7	10	2.164	1.012	1.976	1.021
ts 8	7	1.956	1.024	2.343	1.006
ts 9	9	1.951	1.022	2.283	1.008

*All KIEs normalized to set the 4th carbon of 2-methyl-2-butene as the standard, similar to experiment

Table of KIEs for Reactions of 2-methyl-2-butene with trans-3-phenyl-2-methanesulfonyloxaziridine from B3LYP/6-31+G with PCM solvent model]**

		monosubstituted olefin		disubstituted olefin	
Isomer	fig #	C-O	KIE	C-O	KIE
ts 3	Not shown	2.126	1.013	2.287	1.007
ts 5	8	2.080	1.016	2.339	1.007
ts 7	10	2.049	1.016	2.366	1.007
ts 8	7	2.106	1.014	2.269	1.008
ts 9	9	2.141	1.013	2.209	1.011

*All KIEs normalized to set the 4th carbon of 2-methyl-2-butene as the standard, similar to experiment

Table of KIEs for Reactions of 2-methyl-2-butene with cis-3-phenyl-2-methanesulfonyloxaziridine from B3LYP/6-31+G with PCM solvent model**

		monosubstituted olefin		disubstituted olefin	
Isomer	fig #	C-O	KIE	C-O	KIE
ts 3	Not shown	2.093	1.017	2.378	1.005
ts 5	8	2.093	1.014	2.289	1.007
ts 7	10	2.239	1.011	2.095	1.015
ts 8	7	2.065	1.019	2.378	1.006
ts 9	9	2.046	1.017	2.410	1.006

*All KIEs normalized to set the 4th carbon of 2-methyl-2-butene as the standard, similar to experiment

GAS	C3		C2	
b3lyp/6-31+G**	C-O	KIE	C-O	KIE
ts 1	2.078	1.0145	2.206	1.0081
ts 2	2.029	1.0152	2.237	1.0082
ts 3	2.078	1.0145	2.206	1.0081
ts 4	2.106	1.0124	2.160	1.0099
ts 5	1.995	1.0184	2.244	1.0075
ts 6	2.053	1.0152	2.243	1.0072
ts 7	1.978	1.0180	2.238	1.0083
ts 8	2.031	1.0163	2.194	1.0081
ts 9	2.030	1.0151	2.160	1.0095

PCM	C3		C2	
b3lyp/6-31+G**	C-O	KIE	C-O	KIE
ts 1	2.165	1.01091	2.338	1.00570
ts 2	2.159	1.01053	2.340	1.00636
ts 3	2.165	1.01111	2.340	1.00571
ts 4	2.182	1.00997	2.319	1.00663
ts 5	2.150	1.01158	2.316	1.00605
ts 6	2.174	1.01044	2.333	1.00616
ts 7	2.144	1.01111	2.309	1.00710
ts 8	2.150	1.01169	2.316	1.00606
ts 9	2.162	1.01067	2.298	1.00669

ONSAGER	C3		C2	
b3lyp/6-31+G**	C-O	KIE	C-O	KIE
ts 1	2.123	1.013	2.247	1.008
ts 2	2.100	1.012	2.300	1.007
ts 3	2.128	1.012	2.251	1.007
ts 4	2.136	1.011	2.240	1.008
ts 5	2.132	1.013	2.336	1.006
ts 6	2.112	1.013	2.303	1.006
ts 7	2.126	1.012	2.329	1.007
ts 8	2.130	1.012	2.302	1.006
ts 9	2.139	1.011	2.297	1.007

GAS	C3		C2	
mpw1k/6-31+G**	C-O	KIE	C-O	KIE
ts 1	2.036	1.014	2.132	1.009
ts 2	1.990	1.014	2.160	1.009
ts 3	2.036	1.014	2.132	1.009
ts 4	2.058	1.012	2.106	1.010
ts 5	1.969	1.016	2.150	1.008
ts 6	2.008	1.014	2.152	1.008
ts 7	1.958	1.016	2.160	1.009
ts 8	2.004	1.015	2.121	1.009
ts 9	2.011	1.014	2.105	1.010

PCM	C3		C2	

mpw1k/6-31+G**	C-O	KIE	C-O	KIE
ts 1	2.088	1.012	2.211	1.007
ts 2	2.076	1.011	2.228	1.007
ts 3	2.087	1.012	2.212	1.007
ts 4	2.096	1.011	2.210	1.008
ts 5	2.071	1.012	2.213	1.007
ts 6	2.082	1.012	2.222	1.007
ts 7	2.054	1.012	2.237	1.007
ts 8	2.077	1.012	2.206	1.007
ts 9	2.085	1.011	2.201	1.008

ONSAGER	C3		C2	
mpw1k/6-31+G**	C-O	KIE	C-O	KIE
ts 1	2.061	1.013	2.157	1.009
ts 2	2.026	1.013	2.205	1.008
ts 3	2.063	1.013	2.159	1.009
ts 4	2.073	1.012	2.155	1.009
ts 5	2.036	1.014	2.213	1.007
ts 6	2.038	1.013	2.201	1.008
ts 7	2.031	1.014	2.234	1.008
ts 8	2.063	1.013	2.196	1.007
ts 9	2.078	1.013	2.200	1.007

Gas	C3		C2	
mpw1k/6-31G*	C-O	KIE	C-O	KIE
ts 1	2.032	1.014	2.135	1.009
ts 2	1.957	1.016	2.160	1.009
ts 3	2.032	1.014	2.135	1.009
ts 4	2.051	1.013	2.112	1.010
ts 5	1.967	1.016	2.154	1.008
ts 6	2.006	1.014	2.156	1.008
ts 7	1.957	1.016	2.160	1.009
ts 8	2.000	1.015	2.125	1.009
ts 9	2.006	1.014	2.110	1.010

GAS PHASE TRANS	C3		C2	
b3lyp/6-31+G**	C-O	KIE	C-O	KIE

ts 3	2.055	1.0154	2.186	1.0086
ts 5	1.960	1.0216	2.295	1.0068
ts 7	1.928	1.0211	2.290	1.0078
ts 8	1.993	1.0176	2.183	1.0085
ts 9	2.090	1.0120	2.055	1.0143

GAS PHASE CIS	C3		C2	
b3lyp/6-31+G**	C-O	KIE	C-O	KIE
ts 3	1.956	1.0233	2.343	1.0059
ts 5	1.983	1.0178	2.206	1.0088
ts 7	2.164	1.0094	1.976	1.0192
ts 8	1.956	1.0233	2.343	1.0059
ts 9	1.951	1.0214	2.283	1.0073

PCM TRANS	C3		C2	
b3lyp/6-31+G**	C-O	KIE	C-O	KIE
ts 3	2.126	1.0123	2.287	1.0068
ts 5	2.080	1.0158	2.339	1.0060
ts 7	2.049	1.0159	2.366	1.0066
ts 8	2.106	1.0131	2.269	1.0070
ts 9	2.141	1.0115	2.209	1.0093

PCM CIS	C3		C2	
b3lyp/6-31+G**	C-O	KIE	C-O	KIE
ts 3	2.093	1.01648	2.378	1.0049
ts 5	2.093	1.01340	2.289	1.0071
ts 7	2.239	1.00884	2.095	1.0136
ts 8	2.065	1.01817	2.378	1.0051
ts 9	2.046	1.01666	2.410	1.0060

PCM Trans	C3		C2	
b3lyp/6-311+G**	C-O	KIE	C-O	KIE
TS 8	2.114	1.013	2.274	1.007

gas phase		C3		C2
b3lyp/6-31G*	KIE	C-O	KIE	C-O
ts 1	1.016	2.053	1.009	2.176
ts 2	1.019	1.964	1.009	2.236
ts 3	1.018	2.029	1.008	2.190

ts 4	1.014	2.065	1.012	2.112
ts 5	1.020	1.971	1.008	2.304
ts 6	1.019	1.981	1.008	2.292
ts 7	1.021	1.936	1.009	2.231
ts 8	1.018	2.006	1.010	2.162
ts 9	1.016	2.008	1.011	2.124

Onsager		C3		C2
b3lyp/6-31G*	KIE	C-O	KIE	C-O
ts 1	1.014	2.115	1.009	2.184
ts 5	1.016	2.059	1.008	2.272
ts 7	1.016	2.045	1.008	2.305
ts 8	1.014	2.102	1.008	2.235
ts 9	1.014	2.090	1.009	2.207

TRANS-phenyl gas phase		C3		C2
b3lyp/6-31G*	KIE	C-O	KIE	C-O
ts 1	1.017	2.029	1.010	2.167
ts 5	1.024	1.920	1.008	2.309
ts 8	1.018	1.967	1.010	2.154
ts 9	1.013	2.078	1.016	2.019

TRANS-phenyl Onsager		C3		C2
b3lyp/6-31G*	KIE	C-O	KIE	C-O
ts 1	1.015	2.061	1.010	2.164
ts 5	1.022	1.967	1.007	2.345
ts 8	1.015	2.057	1.009	2.193
ts 9	1.012	2.114	1.014	2.098

CIS-phenyl gas phase		C3		C2
b3lyp/6-31G*	KIE	C-O	KIE	C-O
ts 5	1.019	1.961	1.010	2.190
ts 8	1.025	1.932	1.007	2.315

gas phase		C3		C2
b3lyp/6-311+G**	KIE	C-O	KIE	C-O
ts 8	1.016	2.043	1.008	2.189

gas phase		C3		C2
rhf/6-31G*	KIE	C-O	KIE	C-O
is 5	1.016	1.990	1.011	2.128

gas phase		C3		C2
BP86/6-31G*	KIE	C-O	KIE	C-O
ts 5	1.020	2.024	1.007	2.325
ts 7	1.020	1.992	1.008	2.282
ts 8	1.016	2.073	1.009	2.193
ts 9	1.015	2.059	1.011	2.151

Onsager		C3		C2
MPW1K/6-31G*	KIE	C-O	KIE	C-O
ts 2	1.013	2.042	1.008	2.236
ts 3	1.013	2.056	1.009	2.16
ts 4	1.012	2.064	1.009	2.154
ts 5	1.014	2.043	1.007	2.222
ts 6	1.014	2.037	1.008	2.205
ts 7	1.013	2.047	1.008	2.24
ts 8	1.012	2.076	1.007	2.216
ts 9	1.012	2.069	1.008	2.194

gas phase		C3		C2
ts 8 6-31G*	KIE	C-O	KIE	C-O
bpw91/6-31G* (gas phase)	1.019	2.021	1.008	2.232
mpwb95/6-31G* (gas phase)	1.016	1.992	1.011	2.096
mpwb1k/6-31G* (gas phase)	1.018	1.982	1.013	2.085
b3pw91/6-31G* (gas phase)	1.017	1.998	1.009	2.162
rhf/6-31G* (gas phase)	1.018	2.011	1.011	2.119
mpw3lyp/6-31G* (gas phase)	1.017	2.011	1.010	2.157
tpsskcis/6-31G* (gas phase)	1.017	1.995	1.010	2.141
pbepbe/6-31G* (gas phase) †	1.016	1.757	1.013	1.819
pbev5lyp/6-31G* (gas phase) †	1.015	1.836	1.012	1.902
tpssv5lyp/6-31G* (gas phase) †	1.015	1.788	1.013	1.827
bb95/6-31G* (gas phase)	1.017	1.983	1.012	2.086
pbe1kcis/6-31G* (gas phase)	1.018	1.991	1.009	2.154

mpwlp1m/6-31G* (gas phase)	1.019	2.028	1.010	2.178

† Wigner tunneling correction used in these cases.

Plot of C-O Bond Distance versus KIEs for the Shi Epoxidation

Energies and geometries of all fully optimized transition structures can be found in the supporting information of Singleton, D. A.; Wang, Z. J. Am. Chem. Soc. 2005, 127, 6679-6685.

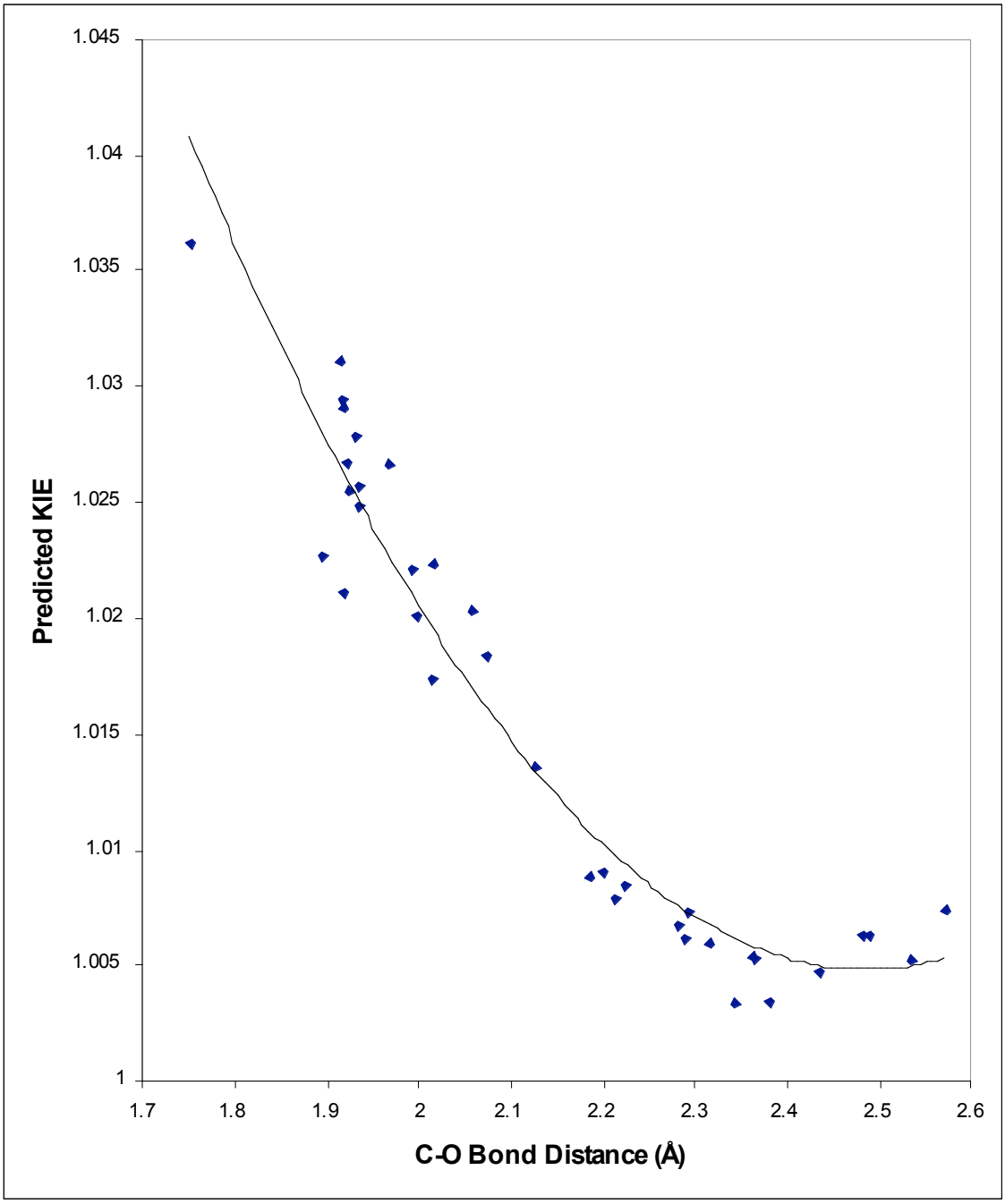


Fig 1. Plot of KIEs versus C-O Bond Distances for the epoxidation of □-methyl styrene with the Shi catalyst.

Table of KIEs and C-O Bond Distances for the Shi Epoxidation

	Bond Distances		KIEs	
	beta	alpha	beta	alpha
ts a	1.991	2.315	1.022	1.006
ts b	1.996	2.184	1.020	1.009
ts c	2.125	2.013	1.014	1.017
ts d	1.915	2.488	1.029	1.006
ts e	1.914	2.380	1.031	1.004
ts g	1.750	2.433	1.036	1.005
ts h	1.929	2.342	1.028	1.003
ts aa	1.934	2.291	1.025	1.007
ts ab	1.917	2.198	1.021	1.009
ts ad	1.934	2.288	1.026	1.006
ts bd	1.916	2.481	1.029	1.006
ts ca	1.923	2.571	1.026	1.007
ts cb	1.894	2.222	1.023	1.009
ts cd	1.920	2.281	1.027	1.007
ts da	2.056	2.361	1.020	1.005
ts dd	1.965	2.534	1.027	1.005
ts ea	2.015	2.364	1.022	1.005
ts eb	2.072	2.211	1.018	1.008

Energies and Geometries of Non-Stationary Point Structures

All geometries are based upon structure **3** in the paper (ts 8). Structures were optimized using B3LYP/6-31G* in the gas-phase with the olefinic C-O bond distances fixed at the bond lengths listed below.

Grid Structure C3 fixed at 1.9 / C2 fixed at 1.9

```
E(RB+HF-LYP) = -954.190519874

 Zero-point correction=                           0.220903 (Hartree/Particle)
 Thermal correction to Energy=                    0.235133
 Thermal correction to Enthalpy=                  0.236077
 Thermal correction to Gibbs Free Energy=         0.180063
 Sum of electronic and zero-point Energies=           -953.969617
 Sum of electronic and thermal Energies=              -953.955387
 Sum of electronic and thermal Enthalpies=            -953.954443
 Sum of electronic and thermal Free Energies=         -954.010457

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 147.548             51.832            117.891

 C,0,2.7771875976,-0.4878137195,-0.3681855454
 C,0,2.0813711073,0.7309296921,-0.0702642247
 O,0,0.9381958166,-0.7847727775,0.0058768613
 C,0,-0.0926246561,-1.0904508337,-1.079518262
 N,0,-1.2060442794,-1.3141978694,-0.2975611283
 S,0,-2.1157981568,0.042081858,-0.0124260565
 O,0,-3.2421566847,0.1283987291,-0.9620336969
 O,0,-1.2972062025,1.2760129043,0.1538942624
 C,0,3.5808853358,-1.3175938529,0.5754695129
```

C,0,1.971383726,1.3008384943,1.3104143302
C,0,1.6475991486,1.6385005553,-1.1814497283
C,0,-2.7979170367,-0.3692971169,1.6012682975
H,0,2.8915761856,-0.7175308572,-1.4257123922
H,0,0.2543411464,-2.0073551053,-1.5660124749
H,0,-0.0858073856,-0.2483381656,-1.7816520615
H,0,3.4713630373,-2.3785005868,0.3308821689
H,0,3.292272089,-1.1688594925,1.6170172107
H,0,4.6466579698,-1.0653898666,0.47245934
H,0,2.6554838834,2.1545315515,1.4116983549
H,0,2.199086071,0.5749923983,2.0917803226
H,0,0.9474520939,1.6629719168,1.4479434047
H,0,0.5970271722,1.9130917481,-1.0342562632
H,0,1.7794627605,1.1905281006,-2.1699897505
H,0,2.2462743135,2.5585416546,-1.1392883708
H,0,-3.4856981172,0.433710107,1.8752338656
H,0,-1.9829740017,-0.4454835913,2.322585322
H,0,-3.3294127434,-1.31860577,1.5207495405

Grid Structure C3 fixed at 1.9 / C2 fixed at 2.0

E(RB+HF-LYP) = -954.187662476

Zero-point correction=	0.220898 (Hartree/Particle)
Thermal correction to Energy=	0.235179
Thermal correction to Enthalpy=	0.236124
Thermal correction to Gibbs Free Energy=	0.179699
Sum of electronic and zero-point Energies=	-953.966765
Sum of electronic and thermal Energies=	-953.952483
Sum of electronic and thermal Enthalpies=	-953.951539
Sum of electronic and thermal Free Energies=	-954.007963

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.577	51.725	118.755

C,0,2.7020487657,-0.4876000837,-0.3354808502
C,0,2.1178708757,0.7789011141,-0.0653867869
O,0,0.8491643725,-0.7665419424,-0.0208142213
C,0,-0.0679937166,-1.054065316,-1.1514582316
N,0,-1.1960841871,-1.3498615494,-0.391364743
S,0,-2.1408530195,-0.0217838281,-0.0539429106
O,0,-3.3603034596,-0.0507131337,-0.882243849
O,0,-1.3755734305,1.2541388728,-0.0294201092
C,0,3.4317208222,-1.366351402,0.6285334092
C,0,1.9711612135,1.3453716072,1.3114339042
C,0,1.7089448122,1.684489812,-1.1845666021
C,0,-2.6307093623,-0.3882798075,1.63926167
H,0,2.8363582443,-0.7293623597,-1.3883266884
H,0,0.3014902796,-1.9403717158,-1.6788885079
H,0,-0.0938131682,-0.1854915352,-1.8206469588
H,0,3.2593243888,-2.4174874796,0.3787919257
H,0,3.1234685806,-1.2037594706,1.6625920307
H,0,4.5133425747,-1.1826764493,0.5570663591
H,0,2.6535038746,2.197879065,1.4346263073
H,0,2.1733536408,0.620239628,2.1002903452
H,0,0.9465851027,1.7172416733,1.4230510334
H,0,0.6448041683,1.9296269165,-1.0761393047
H,0,1.8869513048,1.2470779423,-2.1704782829
H,0,2.2734324285,2.6242386273,-1.1149060115
H,0,-3.331605624,0.3898679704,1.9498333036

```
 H,0,-1.7421354805,-0.3868098453,2.2722192932
 H,0,-3.1124738106,-1.3669772057,1.6552873157
```

Grid Structure C3 fixed at 1.9 / C2 fixed at 2.1

```
E(RB+HF-LYP) = -954.185979720

 Zero-point correction=                           0.221081 (Hartree/Particle)
 Thermal correction to Energy=                    0.236248
 Thermal correction to Enthalpy=                  0.237192
 Thermal correction to Gibbs Free Energy=         0.177703
 Sum of electronic and zero-point Energies=           -953.964899
 Sum of electronic and thermal Energies=              -953.949732
 Sum of electronic and thermal Enthalpies=            -953.948788
 Sum of electronic and thermal Free Energies=         -954.008276

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.248             53.581            125.204

C,0,2.6419876863,-0.4825936302,-0.3131661462
 C,0,2.1613733792,0.8190702483,-0.0623737891
 O,0,0.7825303027,-0.7647303625,-0.0433095956
 C,0,-0.0593572863,-1.0346509174,-1.2011478587
 N,0,-1.1859118249,-1.3785829942,-0.4410068348
 S,0,-2.1546108242,-0.0677156641,-0.0664444558
 O,0,-3.4112768075,-0.1681658611,-0.8294023446
 O,0,-1.4323092478,1.2295196,-0.1108688986
 C,0,3.3126972436,-1.3968359251,0.6651802238
 C,0,2.0010431494,1.3923151465,1.3090254651
 C,0,1.7671371725,1.7211250767,-1.1886564094
 C,0,-2.5367790235,-0.4178034173,1.6576686311
 H,0,2.7857525128,-0.7386598764,-1.3617477232
 H,0,0.3237875288,-1.899653711,-1.7551244105
 H,0,-0.1146680124,-0.1501383907,-1.8474205343
 H,0,3.0993357089,-2.4378071207,0.4057057672
 H,0,2.982187726,-1.228110627,1.6916048199
 H,0,4.4024263095,-1.2603776001,0.6254864714
 H,0,2.6484825247,2.2727203589,1.422784279
 H,0,2.2313368493,0.6854923919,2.1067388621
 H,0,0.964018627,1.7315136721,1.4217446785
 H,0,0.6971657052,1.9544721916,-1.1010307876
 H,0,1.963705566,1.2832285442,-2.1708614629
 H,0,2.3143661944,2.6704264401,-1.1137005448
 H,0,-3.2456315036,0.3424559517,1.9936608646
 H,0,-1.6140673223,-0.3739400073,2.2380178816
 H,0,-2.9827421434,-1.4116334119,1.7175666908
```

Grid Structure C3 fixed at 1.9 / C2 fixed at 2.2

```
E(RB+HF-LYP) = -954.184855473

 Zero-point correction=                           0.221235 (Hartree/Particle)
 Thermal correction to Energy=                    0.236347
 Thermal correction to Enthalpy=                  0.237292
 Thermal correction to Gibbs Free Energy=         0.178540
 Sum of electronic and zero-point Energies=           -953.963621
 Sum of electronic and thermal Energies=              -953.948508
 Sum of electronic and thermal Enthalpies=            -953.947564
 Sum of electronic and thermal Free Energies=         -954.006316

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

```
 Total                  148.310             53.491            123.653

C,0,2.5883202983,-0.4751553324,-0.2946559952
 C,0,2.2051216791,0.8539564483,-0.0612217425
 O,0,0.7267401473,-0.7752718527,-0.0613031918
 C,0,-0.0614417797,-1.0225395483,-1.2394499349
 N,0,-1.1818532445,-1.4032789117,-0.4740689994
 S,0,-2.1688012105,-0.1052547609,-0.0683956371
 O,0,-3.441124353,-0.2528438995,-0.7956767118
 O,0,-1.4789017932,1.2050438245,-0.145619955
 C,0,3.2137338278,-1.4128485041,0.6957532368
 C,0,2.0506271138,1.4399437878,1.3049576098
 C,0,1.8246731852,1.7520455082,-1.1952579801
 C,0,-2.4854353877,-0.4573090734,1.668131365
 H,0,2.7340288851,-0.7472126728,-1.3392787487
 H,0,0.3307295589,-1.8696985446,-1.8152609088
 H,0,-0.1401169463,-0.1246254696,-1.86442335
 H,0,2.9724233024,-2.445706324,0.4294735619
 H,0,2.8643361899,-1.238160081,1.7152242163
 H,0,4.3074007297,-1.3099051253,0.6820606284
 H,0,2.6557389237,2.3520695258,1.3954548645
 H,0,2.327196895,0.7566094219,2.1085432999
 H,0,1.0011555156,1.7357136344,1.436141277
 H,0,0.7542147671,1.9911309326,-1.1183618262
 H,0,2.0219219224,1.3046454033,-2.1731876178
 H,0,2.3721403755,2.7015462352,-1.1273106839
 H,0,-3.2001815328,0.2879955658,2.0246009829
 H,0,-1.5447020364,-0.3890342159,2.2161508409
 H,0,-2.9059648424,-1.4609158667,1.745904239
```

Grid Structure C3 fixed at 1.9 / C2 fixed at 2.3

```
E(RB+HF-LYP) = -954.183792099

 Zero-point correction=                           0.221137 (Hartree/Particle)
 Thermal correction to Energy=                    0.236348
 Thermal correction to Enthalpy=                  0.237292
 Thermal correction to Gibbs Free Energy=         0.177963
 Sum of electronic and zero-point Energies=           -953.962655
 Sum of electronic and thermal Energies=              -953.947444
 Sum of electronic and thermal Enthalpies=            -953.946500
 Sum of electronic and thermal Free Energies=         -954.005830

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.311             53.501            124.869


 C,0,2.5377477811,-0.4660829076,-0.2767100035
 C,0,2.2500188656,0.8854184126,-0.065925926
 O,0,0.6762869987,-0.7918343717,-0.0795932648
 C,0,-0.0740127464,-1.00441826,-1.273995583
 N,0,-1.1828171592,-1.4229301542,-0.5009975777
 S,0,-2.1877017644,-0.1406719183,-0.059365176
 O,0,-3.464979142,-0.3182013275,-0.7702398378
 O,0,-1.5244977684,1.1802994727,-0.1396052224
 C,0,3.1197434908,-1.4168530243,0.731729863
 C,0,2.1182587522,1.4939206436,1.2929553957
 C,0,1.8905510067,1.777972076,-1.2117144625
 C,0,-2.4626725702,-0.5199570079,1.6780269898
 H,0,2.6840066244,-0.7593728909,-1.3157439757
 H,0,0.3239514348,-1.8298511404,-1.8772857302
 H,0,-0.1739387367,-0.0890573901,-1.8696722432
 H,0,2.8639298102,-2.4444319075,0.4596989282
```

H,0,2.7421988111,-1.2355957718,1.7402222319
H,0,4.2149008993,-1.3361387384,0.7518370825
H,0,2.6977170708,2.4244184707,1.3537035174
H,0,2.4324095687,0.8328693785,2.1016600445
H,0,1.0641684684,1.764520144,1.4490738722
H,0,0.8255026686,2.0436634616,-1.1401735042
H,0,2.0726843385,1.310859918,-2.183508174
H,0,2.4575954749,2.7168675176,-1.16127403
H,0,-3.1861308309,0.205762805,2.0566140402
H,0,-1.5128322225,-0.4369993743,2.207833133
H,0,-2.8601089339,-1.5332360104,1.7513724517

Grid Structure C3 fixed at 2.0 / C2 fixed at 1.9

E(RB+HF-LYP) = -954.186683640

Zero-point correction=	0.221035 (Hartree/Particle)
Thermal correction to Energy=	0.235260
Thermal correction to Enthalpy=	0.236204
Thermal correction to Gibbs Free Energy=	0.180063
Sum of electronic and zero-point Energies=	-953.965649
Sum of electronic and thermal Energies=	-953.951424
Sum of electronic and thermal Enthalpies=	-953.950480
Sum of electronic and thermal Free Energies=	-954.006621

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.628	51.738	118.159

C,0,2.7987168718,-0.5914731864,-0.4234072266
C,0,2.1533497446,0.6012014705,-0.0019266194
O,0,0.8282780735,-0.7551405213,-0.1224423909
C,0,-0.1356095129,-0.8242276699,-1.24987159
N,0,-1.2561566088,-1.1297668353,-0.4818882945
S,0,-2.1003946828,0.2089681814,0.039293504
O,0,-3.3268459575,0.3659802605,-0.7636327357
O,0,-1.245210055,1.4136861831,0.2065436762
C,0,3.4620896231,-1.6146460006,0.4331591124
C,0,2.0395740388,1.0118365266,1.437197146
C,0,1.8398673536,1.6797348052,-0.9989728668
C,0,-2.5952434623,-0.336951714,1.6815750381
H,0,2.922822528,-0.71072956,-1.4981565661
H,0,0.1490213045,-1.660445824,-1.8966430076
H,0,-0.1161410038,0.12248174,-1.8012964354
H,0,3.237823858,-2.6210995584,0.0651393863
H,0,3.1609771713,-1.5512980969,1.4798609055
H,0,4.5540128899,-1.4875880378,0.3813728934
H,0,2.8174685449,1.7506673418,1.6733145965
H,0,2.1364037823,0.1723877792,2.1270548118
H,0,1.0627228862,1.4815539249,1.5872445132
H,0,0.8172857544,2.0385452051,-0.8411756868
H,0,1.9584234376,1.3451578081,-2.0333889513
H,0,2.5218837806,2.5247240475,-0.8337798979
H,0,-3.2341553144,0.44252457,2.1027424239
H,0,-1.7018213766,-0.4789529143,2.2913555848
H,0,-3.146538669,-1.2731709251,1.5830376771

Grid Structure C3 fixed at 2.0 / C2 fixed at 2.0

E(RB+HF-LYP) = -954.185103429

```
 Zero-point correction=                           0.221194 (Hartree/Particle)
 Thermal correction to Energy=                    0.236340
 Thermal correction to Enthalpy=                  0.237284
 Thermal correction to Gibbs Free Energy=         0.178017
 Sum of electronic and zero-point Energies=           -953.963909
 Sum of electronic and thermal Energies=              -953.948763
 Sum of electronic and thermal Enthalpies=            -953.947819
 Sum of electronic and thermal Free Energies=         -954.007087

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.306             53.626            124.739

 C,0,2.738997432,-0.5818147933,-0.4014426152
 C,0,2.1995929772,0.6487149671,0.0097460181
 O,0,0.7626022742,-0.7346983021,-0.1359541028
 C,0,-0.1155190114,-0.8066545746,-1.2953314465
 N,0,-1.2337068051,-1.1617382624,-0.5274747575
 S,0,-2.1133858467,0.1566154296,0.0151466342
 O,0,-3.3827495424,0.2177923438,-0.7301303427
 O,0,-1.3103662529,1.4017481631,0.1024560278
 C,0,3.341662051,-1.6446954006,0.4571320004
 C,0,2.0584317748,1.0562721359,1.4456414345
 C,0,1.8926821287,1.7229050212,-0.9915966489
 C,0,-2.4919364986,-0.3693168426,1.6944343577
 H,0,2.8677857646,-0.7115426043,-1.4747724731
 H,0,0.1914441605,-1.6236048769,-1.9575364706
 H,0,-0.1303212947,0.1502503746,-1.829705358
 H,0,3.0526195033,-2.6346918147,0.0902326168
 H,0,3.0429323195,-1.564752471,1.5036190476
 H,0,4.4388625479,-1.5865266967,0.4079877986
 H,0,2.8197393164,1.8086699148,1.6937746638
 H,0,2.1581970049,0.221291297,2.1403570809
 H,0,1.0740888147,1.5157499743,1.5838997745
 H,0,0.8582706489,2.0612356046,-0.8595800892
 H,0,2.040879537,1.3922430836,-2.0234748817
 H,0,2.5478582198,2.5859092054,-0.8108336163
 H,0,-3.1459404299,0.3888534239,2.1311612762
 H,0,-1.5604389443,-0.4504782444,2.2564130844
 H,0,-2.9996768494,-1.3337770553,1.6481399872
```

Grid Structure C3 fixed at 2.0 / C2 fixed at 2.1

```
E(RB+HF-LYP) = -954.184535262

 Zero-point correction=                           0.221341 (Hartree/Particle)
 Thermal correction to Energy=                    0.236443
 Thermal correction to Enthalpy=                  0.237387
 Thermal correction to Gibbs Free Energy=         0.178787
 Sum of electronic and zero-point Energies=           -953.963195
 Sum of electronic and thermal Energies=              -953.948092
 Sum of electronic and thermal Enthalpies=            -953.947148
 Sum of electronic and thermal Free Energies=         -954.005749

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.370             53.565            123.335

C,0,2.6869147216,-0.5742766064,-0.3820084092
 C,0,2.2469759049,0.6865172151,0.016679522
 O,0,0.7060322058,-0.7299153546,-0.1542253367
 C,0,-0.1078496178,-0.7883758745,-1.3365402042
 N,0,-1.2148119474,-1.1851672462,-0.5587249751
```

S,0,-2.121305321,0.1167504228,0.0091354988
O,0,-3.4115148114,0.1118775926,-0.7001470854
O,0,-1.3589979821,1.3862388633,0.0527272011
C,0,3.2294813693,-1.6682668769,0.4828647032
C,0,2.0915216562,1.1029343059,1.4476685906
C,0,1.9512962224,1.7550951922,-0.993624008
C,0,-2.421485792,-0.4071780461,1.7042822113
H,0,2.8186191639,-0.7189251786,-1.4534333039
H,0,0.2131108772,-1.5866070336,-2.0154154566
H,0,-0.1507268246,0.1791978466,-1.8496152688
H,0,2.8961360237,-2.6414559925,0.1093497046
H,0,2.9165142234,-1.5787648517,1.5246715209
H,0,4.328396374,-1.6637820836,0.4530168485
H,0,2.8171581589,1.8921798952,1.6878811505
H,0,2.2275894272,0.2833169239,2.1544474293
H,0,1.0889789132,1.5246201149,1.5839490434
H,0,0.9140085656,2.0933238953,-0.8768243861
H,0,2.1078778347,1.4173373758,-2.0220873734
H,0,2.5990145184,2.6241786632,-0.8149906284
H,0,-3.0867343798,0.3314541699,2.1572395149
H,0,-1.4681026894,-0.4488496392,2.232700065
H,0,-2.8954917949,-1.3894986929,1.6833324316

Grid Structure C3 fixed at 2.0 / C2 fixed at 2.2

E(RB+HF-LYP) = -954.184417553

Zero-point correction=	0.221250 (Hartree/Particle)
Thermal correction to Energy=	0.236455
Thermal correction to Enthalpy=	0.237399
Thermal correction to Gibbs Free Energy=	0.178266
Sum of electronic and zero-point Energies=	-953.963168
Sum of electronic and thermal Energies=	-953.947963
Sum of electronic and thermal Enthalpies=	-953.947019
Sum of electronic and thermal Free Energies=	-954.006151

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.377	53.592	124.455

C,0,2.6357380451,-0.5658062846,-0.3605493328
C,0,2.2898300551,0.7195150793,0.0219013527
O,0,0.6506976877,-0.7334924269,-0.1830623448
C,0,-0.113977885,-0.7662556794,-1.3833445958
N,0,-1.2029204057,-1.2050898046,-0.5919984845
S,0,-2.1338238586,0.0772855229,0.0102187691
O,0,-3.4400933293,0.0152616912,-0.6641776045
O,0,-1.4113157945,1.3673977245,0.0228141966
C,0,3.1214193698,-1.6808460491,0.5159226758
C,0,2.1276860174,1.1516208207,1.4472640043
C,0,2.018029438,1.7825306467,-1.0013505251
C,0,-2.3578761884,-0.4567523494,1.7134871491
H,0,2.7714776028,-0.7285330167,-1.4291978802
H,0,0.2179320332,-1.5429663865,-2.0817859027
H,0,-0.1831116592,0.2137722791,-1.868611255
H,0,2.7532415259,-2.6398474452,0.1390701666
H,0,2.7930946963,-1.5779107137,1.5521423077
H,0,4.2195939921,-1.7214946697,0.5070956989
H,0,2.8412040835,1.9531943423,1.6825322169
H,0,2.2708115926,0.3426655927,2.1649742764
H,0,1.1199402866,1.564981787,1.5789065279

```
 H,0,0.9814854777,2.1312612281,-0.9041276258
 H,0,2.1831738084,1.4327810481,-2.0246169952
 H,0,2.6669914703,2.6512575346,-0.8256163849
 H,0,-3.0319565811,0.259202738,2.1892163588
 H,0,-1.3857562945,-0.4652818461,2.2080862011
 H,0,-2.798910186,-1.4544923634,1.7071160293
```

Grid Structure C3 fixed at 2.0 / C2 fixed at 2.3

```
E(RB+HF-LYP) = -954.184409746

 Zero-point correction=                           0.221161 (Hartree/Particle)
 Thermal correction to Energy=                    0.236470
 Thermal correction to Enthalpy=                  0.237414
 Thermal correction to Gibbs Free Energy=         0.177542
 Sum of electronic and zero-point Energies=           -953.963249
 Sum of electronic and thermal Energies=              -953.947940
 Sum of electronic and thermal Enthalpies=            -953.946996
 Sum of electronic and thermal Free Energies=         -954.006868

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.387             53.614           126.011

C,0,2.5803693177,-0.5597890365,-0.3346306848
 C,0,2.3302117052,0.7466236779,0.0257630835
 O,0,0.592160355,-0.7404443061,-0.2146599725
 C,0,-0.1269250076,-0.7285566002,-1.4325518738
 N,0,-1.1965064064,-1.2177475739,-0.6358306534
 S,0,-2.1533157807,0.0361125717,0.0137300707
 O,0,-3.4711422852,-0.0747268231,-0.6290601149
 O,0,-1.4712079907,1.345283236,0.0141111355
 C,0,3.0074695348,-1.6867681881,0.5612684839
 C,0,2.1830703293,1.2083221791,1.4439868841
 C,0,2.0886589212,1.8011340612,-1.0149444116
 C,0,-2.3030238226,-0.5257545274,1.7157825598
 H,0,2.7160459706,-0.7476939274,-1.3994398402
 H,0,0.2183465914,-1.4741878697,-2.1576274101
 H,0,-0.218990959,0.2688432822,-1.8754740132
 H,0,2.6095525302,-2.633969284,0.1854686757
 H,0,2.6594849456,-1.5632181488,1.5891535535
 H,0,4.1028849693,-1.7696658411,0.5787965012
 H,0,2.8762333633,2.0350981317,1.6497295222
 H,0,2.3602082676,0.4214737167,2.1788042008
 H,0,1.166828675,1.599342367,1.587493183
 H,0,1.0606485295,2.1787860384,-0.9292743992
 H,0,2.2446879653,1.4291490364,-2.0319182766
 H,0,2.7568263912,2.6583108629,-0.8556790147
 H,0,-2.9837271208,0.1624066374,2.2220818434
 H,0,-1.31467523,-0.5071886051,2.1765990919
 H,0,-2.7115687595,-1.5372160675,1.7106308757
```

Grid Structure C3 fixed at 2.0 / C2 fixed at 2.4

```
E(RB+HF-LYP) = -954.184428793

 Zero-point correction=                           0.221186 (Hartree/Particle)
 Thermal correction to Energy=                    0.236488
 Thermal correction to Enthalpy=                  0.237432
 Thermal correction to Gibbs Free Energy=         0.177365
 Sum of electronic and zero-point Energies=           -953.963242
 Sum of electronic and thermal Energies=              -953.947941
```

```
 Sum of electronic and thermal Enthalpies=            -953.946996
 Sum of electronic and thermal Free Energies=         -954.007064

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.399             53.615            126.422

 C,0,2.5227036122,-0.5709255187,-0.2873808616
 C,0,2.3847848185,0.7670175662,-0.0150119295
 O,0,0.5290603132,-0.7302719172,-0.287787632
 C,0,-0.1728128444,-0.5372743007,-1.4917434705
 N,0,-1.2045429175,-1.157985001,-0.728578036
 S,0,-2.1770626635,-0.0150610768,0.1045126881
 O,0,-3.5126223103,-0.1152935457,-0.4997672734
 O,0,-1.5382950187,1.3085031376,0.21900619
 C,0,2.8116150424,-1.6703239052,0.6974359833
 C,0,2.1780068306,1.3228774844,1.3629489645
 C,0,2.3033274472,1.7741545873,-1.1273578402
 C,0,-2.2246377264,-0.769636016,1.7359944597
 H,0,2.7017055002,-0.8370026346,-1.3289330893
 H,0,0.1667597734,-1.1655219251,-2.3224353898
 H,0,-0.2940818473,0.5127230163,-1.7750676322
 H,0,2.3767898225,-2.6104536018,0.346466477
 H,0,2.4016130956,-1.4641007703,1.6889011103
 H,0,3.8948741572,-1.8200041066,0.800783545
 H,0,2.7979649401,2.214997899,1.5185162287
 H,0,2.3990329222,0.608284988,2.1580656989
 H,0,1.129457935,1.6387902414,1.4634162744
 H,0,1.3448109639,2.3100644247,-1.0909959516
 H,0,2.412464969,1.3162726146,-2.1152265233
 H,0,3.089269959,2.5340038717,-1.0148921916
 H,0,-2.9041682865,-0.1695532353,2.3454396906
 H,0,-1.2163188476,-0.7604287364,2.1513583327
 H,0,-2.59709464,-1.7898945397,1.6346411779
```

Grid Structure C3 fixed at 2.0 / C2 fixed at 2.5

```
E(RB+HF-LYP) = -954.184168206

 Zero-point correction=                           0.221086 (Hartree/Particle)
 Thermal correction to Energy=                    0.235541
 Thermal correction to Enthalpy=                  0.236485
 Thermal correction to Gibbs Free Energy=         0.179510
 Sum of electronic and zero-point Energies=           -953.963082
 Sum of electronic and thermal Energies=              -953.948627
 Sum of electronic and thermal Enthalpies=            -953.947683
 Sum of electronic and thermal Free Energies=         -954.004658

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 147.804             51.664            119.915

C,0,2.4518506157,-0.5700664968,-0.2411012486
 C,0,2.4349870627,0.7860093614,-0.0622242301
 O,0,0.4604978424,-0.720013619,-0.3508083443
 C,0,-0.2281643091,-0.3292545484,-1.5075396243
 N,0,-1.2268461745,-1.0777122354,-0.8102004189
 S,0,-2.2033672452,-0.0784931223,0.2045725095
 O,0,-3.5517605448,-0.1466685324,-0.3724727762
 O,0,-1.5933575344,1.235137534,0.4680252002
 C,0,2.6081831807,-1.6150331508,0.832496336
 C,0,2.2080472526,1.449313764,1.2663245459
 C,0,2.5170405068,1.7184843632,-1.2399732229
 C,0,-2.1670766155,-1.0447358915,1.7200617728
```

H,0,2.6606389794,-0.9240699364,-1.2504373662
H,0,0.0998426952,-0.819216953,-2.4300701541
H,0,-0.3639413273,0.7507941414,-1.613623828
H,0,2.1339477164,-2.5492029111,0.5191803139
H,0,2.1545021416,-1.3126261445,1.7797486824
H,0,3.6708661608,-1.8224543277,1.0159913086
H,0,2.8406209275,2.3394529588,1.3720560572
H,0,2.3997520161,0.7907195391,2.1160070593
H,0,1.1626289286,1.7866036613,1.3278807896
H,0,1.6437175492,2.3843911007,-1.2802245864
H,0,2.5920461553,1.1829360198,-2.1916158724
H,0,3.3962062467,2.3724672946,-1.1495463859
H,0,-2.8393669381,-0.5527488393,2.426610277
H,0,-1.1441366693,-1.0560620959,2.0976494238
H,0,-2.5147536196,-2.0539919337,1.495542782

Grid Structure C3 fixed at 2.1 / C2 fixed at 1.9

E(RB+HF-LYP) = -954.184173881

Zero-point correction=	0.221328 (Hartree/Particle)
Thermal correction to Energy=	0.236334
Thermal correction to Enthalpy=	0.237278
Thermal correction to Gibbs Free Energy=	0.179048
Sum of electronic and zero-point Energies=	-953.962846
Sum of electronic and thermal Energies=	-953.947840
Sum of electronic and thermal Enthalpies=	-953.946896
Sum of electronic and thermal Free Energies=	-954.005126

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	148.302	53.618	122.557

C,0,2.8385424369,-0.576164802,-0.415526957
C,0,2.143152997,0.5787660076,-0.0059142656
O,0,0.7625579692,-0.7203350453,-0.1335703552
C,0,-0.1365314053,-0.7922838089,-1.2789418775
N,0,-1.248483926,-1.1259704989,-0.4917350085
S,0,-2.1243367072,0.2018931432,0.0309021797
O,0,-3.3780426202,0.2743909564,-0.7397554006
O,0,-1.3105390456,1.4383416078,0.1314095376
C,0,3.4633510816,-1.6171567157,0.4474321313
C,0,2.0009194173,0.9849888972,1.4350563298
C,0,1.8511681207,1.6709372708,-0.9990489554
C,0,-2.5396682677,-0.3189699107,1.7027124971
H,0,2.9816460439,-0.6938077418,-1.488516747
H,0,0.1523635639,-1.618999367,-1.9363422823
H,0,-0.1498673412,0.1584778659,-1.8230761061
H,0,3.2233074569,-2.618642713,0.0737146821
H,0,3.1504237436,-1.5506711591,1.4905374401
H,0,4.559127358,-1.5184742634,0.4118642298
H,0,2.7897273301,1.7028516133,1.6974000476
H,0,2.0613737715,0.1382301909,2.1206181673
H,0,1.0323180484,1.475674648,1.5678638676
H,0,0.8305692498,2.0399966011,-0.8558880901
H,0,1.9811509139,1.3428056735,-2.0345902927
H,0,2.5388371228,2.5085623929,-0.8208934591
H,0,-3.1933998004,0.4468281836,2.1262885052
H,0,-1.6201150355,-0.4094551084,2.2826820886
H,0,-3.0569474764,-1.2778549181,1.6476270934

Grid Structure C3 fixed at 2.1 / C2 fixed at 2.0

E(RB+HF-LYP) = -954.183768454

Zero-point correction=	0.221456 (Hartree/Particle)
Thermal correction to Energy=	0.236479
Thermal correction to Enthalpy=	0.237424
Thermal correction to Gibbs Free Energy=	0.179195
Sum of electronic and zero-point Energies=	-953.962312
Sum of electronic and thermal Energies=	-953.947289
Sum of electronic and thermal Enthalpies=	-953.946345
Sum of electronic and thermal Free Energies=	-954.004574

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.393	53.564	122.553

C,0,2.7845177473,-0.5650386918,-0.3959800425
C,0,2.1893558826,0.627185648,0.0101106893
O,0,0.7040338156,-0.7030329987,-0.1459008246
C,0,-0.1159727776,-0.7811022329,-1.3230049933
N,0,-1.2145087836,-1.158294205,-0.5230658077
S,0,-2.1305522337,0.1523806541,0.0092775119
O,0,-3.4107976856,0.130874786,-0.7172763962
O,0,-1.3706333075,1.4229654045,0.0395199495
C,0,3.3494154169,-1.6478454579,0.4625765076
C,0,2.0188744043,1.026096802,1.4484665277
C,0,1.8991392659,1.715904614,-0.9854708417
C,0,-2.4501361709,-0.3435428215,1.7089604472
H,0,2.9282966945,-0.6903002555,-1.4684395565
H,0,0.1974923474,-1.593387023,-1.9877293176
H,0,-0.1625123786,0.1761083753,-1.8540284451
H,0,3.0202374978,-2.6289755658,0.1033022547
H,0,3.0647580535,-1.5528989047,1.5118098522
H,0,4.44775663,-1.6363323115,0.4041927321
H,0,2.7916068457,1.7561752325,1.7256803464
H,0,2.0816319063,0.1811555219,2.1360350023
H,0,1.0431076643,1.5066525531,1.5709498916
H,0,0.8674918795,2.0649135427,-0.8653039428
H,0,2.0564121229,1.3924330386,-2.0187964324
H,0,2.5610907985,2.5712873833,-0.7934170791
H,0,-3.1209968158,0.4023079093,2.1412839073
H,0,-1.5031652794,-0.3753291594,2.2494816703
H,0,-2.9233385404,-1.3264028376,1.6990753892

Grid Structure C3 fixed at 2.1 / C2 fixed at 2.1

E(RB+HF-LYP) = -954.184311349

Zero-point correction=	0.221405 (Hartree/Particle)
Thermal correction to Energy=	0.236514
Thermal correction to Enthalpy=	0.237458
Thermal correction to Gibbs Free Energy=	0.178822
Sum of electronic and zero-point Energies=	-953.962907
Sum of electronic and thermal Energies=	-953.947797
Sum of electronic and thermal Enthalpies=	-953.946853
Sum of electronic and thermal Free Energies=	-954.005489

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.415	53.593	123.409

C,0,2.735291824,-0.5579527761,-0.3762200866
C,0,2.2345565765,0.6663992645,0.0186684373
O,0,0.6500058623,-0.698503563,-0.1716889179
C,0,-0.1102368595,-0.7629383329,-1.3717914734

N,0,-1.1837456911,-1.181294441,-0.5475775466
S,0,-2.1325882637,0.11171528,0.0076938038
O,0,-3.4285255507,0.0192527192,-0.6820801016
O,0,-1.4183623902,1.4056039959,-0.0067034954
C,0,3.2332354954,-1.6735878832,0.4870207077
C,0,2.0399400948,1.0736549482,1.4509472095
C,0,1.9592551833,1.7493318846,-0.9872844011
C,0,-2.371497788,-0.3794207465,1.7213148928
H,0,2.8852919903,-0.6964755738,-1.4465865371
H,0,0.2186421389,-1.5575390207,-2.0502771064
H,0,-0.18844335,0.203808661,-1.8807619493
H,0,2.8560654015,-2.6339621513,0.1196332188
H,0,2.9352239103,-1.5693170539,1.5319484611
H,0,4.3310199206,-1.7204026669,0.448662106
H,0,2.7778633676,1.8399397621,1.7255241033
H,0,2.1335768552,0.2426564774,2.1520458571
H,0,1.0451574687,1.5184430129,1.5642684396
H,0,0.925019523,2.0992442335,-0.8859726835
H,0,2.1283783071,1.4178476647,-2.016355814
H,0,2.6139603602,2.6105220145,-0.7958586057
H,0,-3.0534213117,0.3459905153,2.1707420251
H,0,-1.4047406913,-0.3701771807,2.2263353317
H,0,-2.8083173833,-1.378880044,1.7366631246

Grid Structure C3 fixed at 2.1 / C2 fixed at 2.2

E(RB+HF-LYP) = -954.185319565

Zero-point correction=	0.221243 (Hartree/Particle)
Thermal correction to Energy=	0.236487
Thermal correction to Enthalpy=	0.237431
Thermal correction to Gibbs Free Energy=	0.178028
Sum of electronic and zero-point Energies=	-953.964077
Sum of electronic and thermal Energies=	-953.948833
Sum of electronic and thermal Enthalpies=	-953.947889
Sum of electronic and thermal Free Energies=	-954.007292

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.398	53.672	125.024

C,0,2.6822387861,-0.5518268548,-0.3512490694
C,0,2.2709374493,0.699508679,0.0269541465
O,0,0.5921615246,-0.7019275304,-0.2132242378
C,0,-0.118014224,-0.7343874588,-1.4344444354
N,0,-1.1591654153,-1.2003761562,-0.58610657
S,0,-2.1396318968,0.0677513594,0.0108912924
O,0,-3.4533993787,-0.0966727653,-0.6267008095
O,0,-1.4774810601,1.3848409794,-0.0476812358
C,0,3.1093895855,-1.6910203991,0.523821192
C,0,2.0533717259,1.1233262855,1.4511531826
C,0,2.0303982818,1.777442921,-0.9939029294
C,0,-2.2749490198,-0.4256089023,1.7347758755
H,0,2.8421634852,-0.7082088771,-1.4180951616
H,0,0.22536574,-1.5045865253,-2.1328849274
H,0,-0.2270728716,0.2460291619,-1.9089306426
H,0,2.6954501405,-2.6325523041,0.1478597028
H,0,2.7896175582,-1.5741235832,1.5614052415
H,0,4.2040727799,-1.7891524644,0.5150553192
H,0,2.7779696786,1.9009464646,1.7294415853
H,0,2.1444292939,0.3031025679,2.1654268214
H,0,1.0530968798,1.5623183661,1.5477686826
H,0,0.9962327899,2.1374138608,-0.9243201784
H,0,2.2209503147,1.4345079378,-2.0156651955
H,0,2.6832806493,2.6389455864,-0.797452401

H,0,-2.965100096,0.2725571016,2.2137744075
H,0,-1.2860360848,-0.3717138139,2.1915765377
H,0,-2.6676716162,-1.4425746366,1.7730628066

Grid Structure C3 fixed at 2.1 / C2 fixed at 2.3

E(RB+HF-LYP) = -954.186567401

Zero-point correction=	0.221381 (Hartree/Particle)
Thermal correction to Energy=	0.236614
Thermal correction to Enthalpy=	0.237559
Thermal correction to Gibbs Free Energy=	0.178031
Sum of electronic and zero-point Energies=	-953.965186
Sum of electronic and thermal Energies=	-953.949953
Sum of electronic and thermal Enthalpies=	-953.949009
Sum of electronic and thermal Free Energies=	-954.008537

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.478	53.610	125.287

C,0,2.6351179076,-0.5576147565,-0.3163903056
C,0,2.3176161072,0.7273729516,0.0078507598
O,0,0.5410839017,-0.707542821,-0.2659126959
C,0,-0.1409693351,-0.6342056566,-1.4936134799
N,0,-1.1413845357,-1.1815842685,-0.6368715187
S,0,-2.138155241,0.0348543188,0.0672005894
O,0,-3.4546512356,-0.1182583037,-0.5650376352
O,0,-1.4944546372,1.3596549467,0.0845510511
C,0,2.9692099924,-1.6915203512,0.6087110162
C,0,2.0687378385,1.2139270488,1.4073671015
C,0,2.1573674856,1.7781744144,-1.0581619214
C,0,-2.2276009818,-0.5827624376,1.752966501
H,0,2.8151058362,-0.764891365,-1.3716637518
H,0,0.2001225707,-1.3432442999,-2.2542223299
H,0,-0.27417773,0.3811008167,-1.8779156872
H,0,2.50230861,-2.6172946899,0.2568573925
H,0,2.6330252683,-1.5168946133,1.6332208411
H,0,4.054812311,-1.859865066,0.6329212422
H,0,2.7294107493,2.0591649065,1.6427193651
H,0,2.2188346588,0.4451137365,2.1678255318
H,0,1.0368514269,1.5812375118,1.4824475845
H,0,1.1515807657,2.2165036657,-1.0162109478
H,0,2.3282071877,1.3812960742,-2.0640264258
H,0,2.8665210142,2.6014132067,-0.894590519
H,0,-2.9169333898,0.069552264,2.2937207907
H,0,-1.2298059019,-0.5439185879,2.1915293328
H,0,-2.6051756438,-1.6058096454,1.7270371183

Grid Structure C3 fixed at 2.1 / C2 fixed at 2.4

E(RB+HF-LYP) = -954.187655917

Zero-point correction=	0.221096 (Hartree/Particle)
Thermal correction to Energy=	0.235560
Thermal correction to Enthalpy=	0.236504
Thermal correction to Gibbs Free Energy=	0.179605
Sum of electronic and zero-point Energies=	-953.966560
Sum of electronic and thermal Energies=	-953.952096
Sum of electronic and thermal Enthalpies=	-953.951152
Sum of electronic and thermal Free Energies=	-954.008051

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

Total	147.816	51.737	119.755

```
C,0,2.5788785303,-0.5520723811,-0.2901988715
 C,0,2.3532717983,0.7521401298,0.010679529
 O,0,0.4858000279,-0.7217039596,-0.3060672792
 C,0,-0.1631174344,-0.5871240843,-1.5430039655
 N,0,-1.1305484105,-1.190295858,-0.6799335422
 S,0,-2.1578393804,-0.0131455207,0.0759370868
 O,0,-3.4797583556,-0.2159324547,-0.5273934041
 O,0,-1.5590421515,1.3305146876,0.0893915938
 C,0,2.8530026109,-1.686563973,0.6568788403
 C,0,2.1190976536,1.2735580665,1.4012641651
 C,0,2.2345582658,1.7893910449,-1.0751408409
 C,0,-2.1686480045,-0.6596252628,1.7531002726
 H,0,2.7530946832,-0.7900449673,-1.3402509375
 H,0,0.1874856064,-1.2582112611,-2.3320640242
 H,0,-0.3173522899,0.4434374524,-1.8719750496
 H,0,2.3515559894,-2.5971938907,0.3136139099
 H,0,2.5104569808,-1.4822311107,1.6742881102
 H,0,3.9298540228,-1.9001859836,0.7010060071
 H,0,2.7870899855,2.1184883206,1.6156645005
 H,0,2.2683510716,0.5204918692,2.1778065101
 H,0,1.0904264763,1.6516883203,1.4800817832
 H,0,1.2430488055,2.2622770855,-1.0505649432
 H,0,2.3968046422,1.3674955639,-2.0724660882
 H,0,2.967777408,2.594103753,-0.9258617026
 H,0,-2.8653748505,-0.0427397206,2.3250562681
 H,0,-1.159483164,-0.586332819,2.1601415531
 H,0,-2.5067855173,-1.6962240463,1.7223195191
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Grid Structure C3 fixed at 2.1 / C2 fixed at 2.5

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E(RB+HF-LYP) = -954.188469551
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Zero-point correction=	0.221045 (Hartree/Particle)
Thermal correction to Energy=	0.235551
Thermal correction to Enthalpy=	0.236495
Thermal correction to Gibbs Free Energy=	0.179197
Sum of electronic and zero-point Energies=	-953.967425
Sum of electronic and thermal Energies=	-953.952919
Sum of electronic and thermal Enthalpies=	-953.951975
Sum of electronic and thermal Free Energies=	-954.009273

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.810	51.756	120.594

```
C,0,2.5156724615,-0.5536111017,-0.2475036132
 C,0,2.398420455,0.7755181147,-0.0188637352
 O,0,0.425235714,-0.7222364974,-0.3554162199
 C,0,-0.2071469768,-0.431351648,-1.5714200431
 N,0,-1.1431970512,-1.1493651331,-0.7570807596
 S,0,-2.1877519842,-0.0754227834,0.1410761131
 O,0,-3.5167835853,-0.2702025281,-0.4465059511
 O,0,-1.62456266,1.2771821213,0.2581302604
 C,0,2.6861114286,-1.6521674356,0.7666271788
 C,0,2.1590106918,1.3860346417,1.3356480675
 C,0,2.4020801138,1.7606164338,-1.1597959691
 C,0,-2.1199365391,-0.8766474497,1.7484601299
 H,0,2.7026851199,-0.8606847204,-1.2772689697
 H,0,0.1433421167,-1.0002092183,-2.4362021805
 H,0,-0.3773503418,0.6300109249,-1.763398892
 H,0,2.145701304,-2.5499765588,0.4503792733
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H,0,2.3189556583,-1.3751376654,1.7583736236
H,0,3.7461894898,-1.9230063264,0.8662316112
H,0,2.8411758132,2.2288935069,1.5092526301
H,0,2.2848866399,0.6780445804,2.1577309989
H,0,1.1365229311,1.7872033672,1.3840877786
H,0,1.4652398116,2.3350332668,-1.1884944328
H,0,2.5397417051,1.2717752535,-2.1300982517
H,0,3.2096081656,2.4959697288,-1.0366279163
H,0,-2.8133275261,-0.3384246925,2.3984523329
H,0,-1.099131414,-0.8076905551,2.1259326634
H,0,-2.4287865413,-1.9161886262,1.6306032723

Grid Structure C3 fixed at 2.2 / C2 fixed at 1.9

E(RB+HF-LYP) = -954.182350026

Zero-point correction=	0.221474 (Hartree/Particle)
Thermal correction to Energy=	0.236425
Thermal correction to Enthalpy=	0.237370
Thermal correction to Gibbs Free Energy=	0.179426
Sum of electronic and zero-point Energies=	-953.960876
Sum of electronic and thermal Energies=	-953.945925
Sum of electronic and thermal Enthalpies=	-953.944980
Sum of electronic and thermal Free Energies=	-954.002924

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.359	53.549	121.953

C,0,2.8826736138,-0.5580351034,-0.4152957143
C,0,2.1364179883,0.5537913054,-0.0040702354
O,0,0.7059952633,-0.6909277262,-0.1247686323
C,0,-0.1374043825,-0.7822729621,-1.2875224998
N,0,-1.241057538,-1.125829255,-0.4790746128
S,0,-2.1510868143,0.1994646201,0.0155149739
O,0,-3.4114192478,0.1920268103,-0.7462553648
O,0,-1.3751678793,1.4599314829,0.0582388319
C,0,3.4942525728,-1.6135541561,0.4391185268
C,0,1.9834194224,0.9469316831,1.4425598108
C,0,1.8445436723,1.6617040316,-0.984091647
C,0,-2.5247450605,-0.2789044012,1.7090233117
H,0,3.0387603701,-0.6637956832,-1.4882802907
H,0,0.1591237911,-1.6121419171,-1.9377874079
H,0,-0.1748300218,0.1629159267,-1.839960284
H,0,3.2227906508,-2.6107005521,0.0725576382
H,0,3.2027095669,-1.5381739639,1.4878449803
H,0,4.5915534296,-1.5470347826,0.3831410338
H,0,2.7825917631,1.6451834466,1.7248065366
H,0,2.0191109148,0.0899902506,2.1176317486
H,0,1.0235065153,1.454197494,1.5736207129
H,0,0.8225391598,2.0273795185,-0.8443199324
H,0,1.9810126928,1.3475573399,-2.0235335856
H,0,2.5290575084,2.4990769808,-0.7935520228
H,0,-3.1952307877,0.4806574077,2.1173691806
H,0,-1.5937024625,-0.3211053254,2.2759450884
H,0,-3.0128097011,-1.2543734697,1.6934488552

Grid Structure C3 fixed at 2.2 / C2 fixed at 2.0

E(RB+HF-LYP) = -954.183113434

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 Zero-point correction=                           0.221578 (Hartree/Particle)
 Thermal correction to Energy=                    0.236558
 Thermal correction to Enthalpy=                  0.237502
 Thermal correction to Gibbs Free Energy=         0.179433
 Sum of electronic and zero-point Energies=           -953.961535
 Sum of electronic and thermal Energies=              -953.946556
 Sum of electronic and thermal Enthalpies=            -953.945612
 Sum of electronic and thermal Free Energies=         -954.003681

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.442             53.538            122.217

 C,0,2.8383010911,-0.5603658042,-0.3901621039
 C,0,2.1865286494,0.5897340494,0.0184119408
 O,0,0.6561182033,-0.6878669944,-0.1415317409
 C,0,-0.1117471138,-0.7862075057,-1.3356116672
 N,0,-1.1894217615,-1.169037317,-0.4994050685
 S,0,-2.1430176102,0.1396639267,0.0023154137
 O,0,-3.4251033409,0.0353761818,-0.7115525563
 O,0,-1.4234756748,1.4301494449,-0.0287924408
 C,0,3.3823889409,-1.6612802009,0.4589940495
 C,0,1.9932232491,0.9713699413,1.4617652003
 C,0,1.899688524,1.695099955,-0.9642264759
 C,0,-2.4183486522,-0.3081011053,1.7221880401
 H,0,3.0005402694,-0.6707005332,-1.4621801313
 H,0,0.2100429186,-1.6042896869,-1.9887123593
 H,0,-0.1838634082,0.1636369645,-1.8761594879
 H,0,3.0236257624,-2.6338756434,0.1020509568
 H,0,3.1132512248,-1.5626670624,1.5121120605
 H,0,4.4797771846,-1.6825354422,0.3881810354
 H,0,2.7716152014,1.68405313,1.7663486554
 H,0,2.0302166966,0.1143632718,2.1367525907
 H,0,1.0232744231,1.4646920564,1.5770209816
 H,0,0.8665940169,2.0411769313,-0.8520710921
 H,0,2.0680797329,1.3862881767,-2.0007498073
 H,0,2.5578133858,2.5497601381,-0.7566063608
 H,0,-3.1040523436,0.4322975334,2.1403137709
 H,0,-1.4615465593,-0.2920343968,2.2457423216
 H,0,-2.8616560436,-1.3042920823,1.7536057273
```

Grid Structure C3 fixed at 2.2 / C2 fixed at 2.1

```
E(RB+HF-LYP) = -954.184837784

 Zero-point correction=                           0.221439 (Hartree/Particle)
 Thermal correction to Energy=                    0.236565
 Thermal correction to Enthalpy=                  0.237509
 Thermal correction to Gibbs Free Energy=         0.178772
 Sum of electronic and zero-point Energies=           -953.963399
 Sum of electronic and thermal Energies=              -953.948273
 Sum of electronic and thermal Enthalpies=            -953.947329
 Sum of electronic and thermal Free Energies=         -954.006066

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.447             53.622            123.623

 C,0,2.79246567,-0.5411080745,-0.3663386144
 C,0,2.2293860826,0.6423446962,0.0322998179
 O,0,0.6049941282,-0.6727517867,-0.1723173557
 C,0,-0.1032939672,-0.7567102355,-1.391385041
 N,0,-1.1419314861,-1.1791291694,-0.5166563015
 S,0,-2.1358628407,0.1104201715,0.0061293431
 O,0,-3.430446624,-0.0730303927,-0.6645528579
```

O,0,-1.467856538,1.4228654295,-0.0768252136
C,0,3.2631962153,-1.677727105,0.48538338
C,0,1.9999025205,1.0289693512,1.4683506649
C,0,1.9612479019,1.7432159504,-0.9605846753
C,0,-2.3222562188,-0.3250147346,1.7405329635
H,0,2.9653446314,-0.6623913687,-1.4359736341
H,0,0.2359264538,-1.5579150202,-2.0556174237
H,0,-0.2103071019,0.2021435611,-1.9083562137
H,0,2.8490004359,-2.6253372244,0.1218002519
H,0,2.9855335627,-1.5684057415,1.5356167734
H,0,4.3577497658,-1.7650214154,0.4314575033
H,0,2.7394080864,1.7804115179,1.7772631712
H,0,2.066507035,0.1841138274,2.1565273275
H,0,1.0083891233,1.4835503805,1.5683198176
H,0,0.9240344759,2.0871268683,-0.8748168158
H,0,2.1509371451,1.4288585852,-1.9919597382
H,0,2.6075271863,2.6056845885,-0.7473203537
H,0,-3.0195813856,0.3939328459,2.1764308623
H,0,-1.3463283318,-0.2628502263,2.2236312797
H,0,-2.7242321832,-1.3372048266,1.8015342567

Grid Structure C3 fixed at 2.2 / C2 fixed at 2.2

Zero-point correction= 0.221258 (Hartree/Particle)
Thermal correction to Energy= 0.236528
Thermal correction to Enthalpy= 0.237472
Thermal correction to Gibbs Free Energy= 0.177863
Sum of electronic and zero-point Energies= -953.965814
Sum of electronic and thermal Energies= -953.950544
Sum of electronic and thermal Enthalpies= -953.949600
Sum of electronic and thermal Free Energies= -954.009209

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.423	53.716	125.457

C,0,2.7461384257,-0.5232607993,-0.3401974675
C,0,2.2672293655,0.6892535758,0.0437359652
O,0,0.5544960843,-0.667284458,-0.213841241
C,0,-0.1043144414,-0.7182637033,-1.4554615288
N,0,-1.0979417196,-1.1846437459,-0.5439069961
S,0,-2.1302314899,0.0808297534,0.014625619
O,0,-3.4340850092,-0.1715354317,-0.6103503494
O,0,-1.5128015856,1.4120389718,-0.1074490126
C,0,3.1438630944,-1.6848550613,0.5197272445
C,0,2.0074317957,1.0911707089,1.4704484757
C,0,2.0324965658,1.7853351681,-0.9635853657
C,0,-2.2230069833,-0.3540631028,1.7563412383
H,0,2.9297049337,-0.6613315705,-1.4065533691
H,0,0.2496876548,-1.4966068229,-2.1373627034
H,0,-0.244345473,0.2536352229,-1.9366907791
H,0,2.6853748075,-2.6093676157,0.150023729
H,0,2.8522968561,-1.5621430628,1.5651816861
H,0,4.2328069163,-1.8302635443,0.4883827616
H,0,2.7183008037,1.8693036246,1.7808108115
H,0,2.0886021119,0.2606427774,2.1747300052
H,0,1.0021624422,1.5212219195,1.5527276336
H,0,0.996084868,2.1404887032,-0.9075956127
H,0,2.2415245722,1.4589601374,-1.9877017059
H,0,2.6777418709,2.6480219566,-0.7473665553
H,0,-2.9271517206,0.3407139123,2.2195430512
H,0,-1.2295777337,-0.2514667874,2.1947409747
H,0,-2.5838198855,-1.3802320566,1.8375425954

Grid Structure C3 fixed at 2.2 / C2 fixed at 2.3

E(RB+HF-LYP) = -954.189428451

Zero-point correction=	0.221135 (Hartree/Particle)
Thermal correction to Energy=	0.235569
Thermal correction to Enthalpy=	0.236513
Thermal correction to Gibbs Free Energy=	0.179874
Sum of electronic and zero-point Energies=	-953.968293
Sum of electronic and thermal Energies=	-953.953860
Sum of electronic and thermal Enthalpies=	-953.952915
Sum of electronic and thermal Free Energies=	-954.009554

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.822	51.773	119.206

```
C,0,2.7013196633,-0.5102184747,-0.3164387686
 C,0,2.3041565583,0.7288535497,0.0503955651
 O,0,0.5086022203,-0.6765961619,-0.2507552327
 C,0,-0.1106080802,-0.6776581579,-1.5104559317
 N,0,-1.0687430169,-1.1868994498,-0.5781422948
 S,0,-2.1288492969,0.0547263117,0.0242219646
 O,0,-3.4362098438,-0.2378201489,-0.5719053044
 O,0,-1.5459906928,1.3986296366,-0.1071192167
 C,0,3.0406499506,-1.6823661858,0.5575659843
 C,0,2.0360879604,1.1565338259,1.4684258262
 C,0,2.1009220418,1.8165881141,-0.9736618884
 C,0,-2.1524446017,-0.4005819907,1.7628092146
 H,0,2.8830731622,-0.672695692,-1.380135942
 H,0,0.252906673,-1.429983036,-2.2146339733
 H,0,-0.2689089432,0.3106128448,-1.9479858532
 H,0,2.5419658207,-2.5884197058,0.1944543181
 H,0,2.7471706148,-1.5372110188,1.6000651045
 H,0,4.1218310503,-1.8781185847,0.537877162
 H,0,2.729002453,1.9556325737,1.7659306135
 H,0,2.1321141872,0.3436926785,2.1915683148
 H,0,1.0221578468,1.570176999,1.5431244928
 H,0,1.067285916,2.1856151877,-0.9431547768
 H,0,2.3232932693,1.4750116865,-1.9902597204
 H,0,2.7494485126,2.6774280332,-0.7595437367
 H,0,-2.8572116307,0.2725658061,2.2559705364
 H,0,-1.1474175427,-0.2762488576,2.1679296182
 H,0,-2.4856359447,-1.4359944419,1.8446364936
```

Grid Structure C3 fixed at 2.2 / C2 fixed at 2.4

E(RB+HF-LYP) = -954.191493447

Zero-point correction=	0.221002 (Hartree/Particle)
Thermal correction to Energy=	0.235540
Thermal correction to Enthalpy=	0.236484
Thermal correction to Gibbs Free Energy=	0.179032
Sum of electronic and zero-point Energies=	-953.970491
Sum of electronic and thermal Energies=	-953.955953
Sum of electronic and thermal Enthalpies=	-953.955009
Sum of electronic and thermal Free Energies=	-954.012461

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	147.804	51.806	120.918

```
C,0,2.6611057938,-0.504446407,-0.2890990137
 C,0,2.3465804119,0.7637420036,0.0434135187
```

O,0,0.4691402111,-0.6921662744,-0.2965047052
C,0,-0.1267230829,-0.6053463125,-1.5627972539
N,0,-1.0602407665,-1.1786876531,-0.6379158684
S,0,-2.1336365724,0.0257449314,0.0433554671
O,0,-3.4459190281,-0.2712747789,-0.5372175717
O,0,-1.5724920541,1.3808967114,-0.0496001949
C,0,2.9406608832,-1.6690448692,0.6178596389
C,0,2.0767623429,1.238237981,1.4466411905
C,0,2.1947668913,1.8315269616,-1.0109598555
C,0,-2.1010858475,-0.5008595249,1.7613496029
H,0,2.8412552534,-0.7066482916,-1.3464610971
H,0,0.2401119408,-1.3107277357,-2.3113515865
H,0,-0.2965109826,0.4088514919,-1.9287443491
H,0,2.3871591259,-2.5551940351,0.286974127
H,0,2.6660603593,-1.4760901991,1.6580317428
H,0,4.0086531104,-1.9266721952,0.5971342987
H,0,2.7537589264,2.0607401108,1.71526039
H,0,2.1894304889,0.4539370277,2.1985784503
H,0,1.0546715532,1.6352255267,1.5124297526
H,0,1.1792700899,2.250788162,-0.9954536605
H,0,2.4012562861,1.4519207601,-2.0175559044
H,0,2.8809611435,2.6687324985,-0.8214857867
H,0,-2.8063246977,0.1364615611,2.2993766447
H,0,-1.0881285273,-0.3690283891,2.1436938168
H,0,-2.4099909331,-1.5459058841,1.8094295736

Grid Structure C3 fixed at 2.2 / C2 fixed at 2.5

E(RB+HF-LYP) = -954.193044592

Zero-point correction=	0.221260 (Hartree/Particle)
Thermal correction to Energy=	0.236519
Thermal correction to Enthalpy=	0.237464
Thermal correction to Gibbs Free Energy=	0.178302
Sum of electronic and zero-point Energies=	-953.971784
Sum of electronic and thermal Energies=	-953.956525
Sum of electronic and thermal Enthalpies=	-953.955581
Sum of electronic and thermal Free Energies=	-954.014743

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.418	53.718	124.516

C,0,-2.5679578172,0.6206200147,-0.4855119709
C,0,-2.474802947,-0.5165323409,0.2298874187
O,0,-0.3711971021,0.5588664496,-0.5876443267
C,0,0.1857180228,-0.1431178202,-1.665231889
N,0,1.1615791944,0.7123010702,-1.0504677445
S,0,2.1414394017,-0.1541902381,0.1256692274
O,0,3.4687597052,-0.2355410975,-0.4887720871
O,0,1.4699185132,-1.367589746,0.6098542282
C,0,-2.6446264043,2.0361865987,0.0144223494
C,0,-2.2456791999,-0.576099273,1.7173247468
C,0,-2.5219792749,-1.8656566569,-0.4440281219
C,0,2.1560484126,1.0707164133,1.4409046331
H,0,-2.7341551438,0.5172565397,-1.5592258213
H,0,-0.1242869045,0.1814217113,-2.6602117962
H,0,0.2658045954,-1.2224263128,-1.528769354
H,0,-1.9680504347,2.6823957064,-0.5558439868
H,0,-2.3826930718,2.131144648,1.0716126719
H,0,-3.6604434544,2.4350504958,-0.1135135939
H,0,-2.9893777665,-1.2234499279,2.2014634156
H,0,-2.289012106,0.4018901695,2.202464794
H,0,-1.2595791334,-1.0160554927,1.9230105994
H,0,-1.5975040414,-2.4306993786,-0.2577829259

```
 H,0,-2.6670969055,-1.7833249767,-1.5266972906
 H,0,-3.3426308334,-2.4763548591,-0.0420986437
 H,0,2.8059300533,0.6799511371,2.2270165487
 H,0,1.1364635532,1.1970174563,1.8070051727
 H,0,2.5523749887,2.0045534817,1.0400252006
```

Grid Structure C3 fixed at 2.3 / C2 fixed at 1.9

```
E(RB+HF-LYP) = -954.180739213

 Zero-point correction=                           0.221473 (Hartree/Particle)
 Thermal correction to Energy=                    0.236442
 Thermal correction to Enthalpy=                  0.237386
 Thermal correction to Gibbs Free Energy=         0.179257
 Sum of electronic and zero-point Energies=           -953.959266
 Sum of electronic and thermal Energies=              -953.944297
 Sum of electronic and thermal Enthalpies=            -953.943353
 Sum of electronic and thermal Free Energies=         -954.001483

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.370             53.541           122.344


C,0,2.9282311605,-0.5413213976,-0.4213559511
 C,0,2.1311846271,0.5242399573,-0.002033115
 O,0,0.6528999587,-0.6645710873,-0.1088316703
 C,0,-0.1439889245,-0.7841462456,-1.2859729567
 N,0,-1.2385542738,-1.1240049029,-0.4534735952
 S,0,-2.179959914,0.2031139039,0.0000551372
 O,0,-3.4383799873,0.123480481,-0.759467843
 O,0,-1.4357010169,1.4803378666,-0.011382086
 C,0,3.5408495439,-1.6072644557,0.4196821286
 C,0,1.9746266957,0.8999152173,1.4518423145
 C,0,1.8320421544,1.6488915747,-0.9650071704
 C,0,-2.5295291472,-0.2244934497,1.7114950273
 H,0,3.1006565017,-0.6255463468,-1.4942377105
 H,0,0.1602006789,-1.6244609554,-1.9191560156
 H,0,-0.1991596833,0.1501016897,-1.855176014
 H,0,3.2884501938,-2.6013173108,0.0297658453
 H,0,3.233897027,-1.5574853143,1.4656725296
 H,0,4.6381998247,-1.5288660409,0.3813828674
 H,0,2.7781660943,1.5868437033,1.7482328394
 H,0,2.0002028643,0.0328644056,2.114854437
 H,0,1.0188337741,1.4130726574,1.5885203857
 H,0,0.8087343792,2.0090029903,-0.8223060083
 H,0,1.9694707762,1.3503802227,-2.009290857
 H,0,2.5132771577,2.486536953,-0.7645935416
 H,0,-3.2144986803,0.5336035117,2.0979114035
 H,0,-1.5930900503,-0.2239492119,2.2710019775
 H,0,-2.9944567346,-1.2109994155,1.7341766417
```

Grid Structure C3 fixed at 2.3 / C2 fixed at 2.0

```
E(RB+HF-LYP) = -954.182706418

 Zero-point correction=                           0.221574 (Hartree/Particle)
 Thermal correction to Energy=                    0.236581
 Thermal correction to Enthalpy=                  0.237525
 Thermal correction to Gibbs Free Energy=         0.179293
 Sum of electronic and zero-point Energies=           -953.961133
 Sum of electronic and thermal Energies=              -953.946126
```

```
 Sum of electronic and thermal Enthalpies=           -953.945182
 Sum of electronic and thermal Free Energies=        -954.003413

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.457             53.564           122.559

 C,0,2.8941506415,-0.5407106647,-0.3860790161
 C,0,2.185212502,0.5629715653,0.0314256299
 O,0,0.6114602154,-0.6604926981,-0.1311851483
 C,0,-0.1075390586,-0.788877686,-1.3417893476
 N,0,-1.1652508385,-1.1641263507,-0.468763142
 S,0,-2.1560183103,0.1457973676,-0.0101442544
 O,0,-3.4381798947,-0.0447392428,-0.7033932974
 O,0,-1.4762858185,1.4508315412,-0.1160701845
 C,0,3.4309992654,-1.6585106196,0.4465074826
 C,0,1.9724414174,0.9177618554,1.4819219176
 C,0,1.8945767316,1.6880430381,-0.9315763642
 C,0,-2.3869142977,-0.2331722162,1.7321629722
 H,0,3.0792939004,-0.6250448312,-1.4572634063
 H,0,0.2248575238,-1.619498888,-1.9726129621
 H,0,-0.199271099,0.1486724281,-1.8997030334
 H,0,3.0696900228,-2.6253821009,0.0743079083
 H,0,3.1590116809,-1.5761743651,1.5004774104
 H,0,4.528348042,-1.6864635733,0.3795371813
 H,0,2.7496751776,1.6194694273,1.8131391458
 H,0,1.9960460987,0.046476131,2.1395825864
 H,0,1.0038506798,1.4135655664,1.5968979181
 H,0,0.8582490517,2.0248570829,-0.8245576259
 H,0,2.0743417544,1.3998470734,-1.9724996509
 H,0,2.5442086653,2.5443374016,-0.7048117934
 H,0,-3.0902342609,0.5029494691,2.1279697475
 H,0,-1.4226142943,-0.1604233115,2.2368132411
 H,0,-2.7959233375,-1.2408893729,1.8161227919
```

Grid Structure C3 fixed at 2.3 / C2 fixed at 2.1

```
E(RB+HF-LYP) = -954.185713273

 Zero-point correction=                           0.221490 (Hartree/Particle)
 Thermal correction to Energy=                    0.236630
 Thermal correction to Enthalpy=                  0.237575
 Thermal correction to Gibbs Free Energy=         0.178628
 Sum of electronic and zero-point Energies=           -953.964223
 Sum of electronic and thermal Energies=              -953.949083
 Sum of electronic and thermal Enthalpies=            -953.948139
 Sum of electronic and thermal Free Energies=         -954.007085

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.488             53.631           124.063

C,0,2.8460491535,-0.5169444572,-0.3652150818
 C,0,2.221038862,0.6186854139,0.0517781107
 O,0,0.5593402458,-0.6483977361,-0.1562010042
 C,0,-0.0944535377,-0.7732694995,-1.3948974196
 N,0,-1.1035321677,-1.1763685325,-0.4700176592
 S,0,-2.1462211175,0.1165898066,-0.0111267235
 O,0,-3.4324453708,-0.1655293358,-0.6599059698
 O,0,-1.5231251394,1.4394613874,-0.184030243
 C,0,3.3166049922,-1.6741151477,0.4600787187
 C,0,1.9714144157,0.9673554834,1.4972279628
 C,0,1.9399040605,1.7433409171,-0.9141578118
 C,0,-2.2917226071,-0.2246011444,1.7474980589
 H,0,3.0383735703,-0.605986139,-1.4353379861
```

```
 H,0,0.2597002204,-1.5935855185,-2.0254979965
 H,0,-0.2217126428,0.1683176617,-1.9366111259
 H,0,2.8920608763,-2.6141873073,0.0860219408
 H,0,3.0515921354,-1.5823563268,1.5155355753
 H,0,4.4094898963,-1.7717684234,0.3939695761
 H,0,2.7173298333,1.6960977275,1.8427227716
 H,0,2.0133054633,0.1004812535,2.1600993786
 H,0,0.9865138743,1.4353194803,1.5994363397
 H,0,0.8952439771,2.065195161,-0.8360068492
 H,0,2.1496829927,1.4601358465,-1.9510843661
 H,0,2.5657011777,2.613392302,-0.67214477
 H,0,-3.0110748511,0.4917274743,2.1506298195
 H,0,-1.3125516476,-0.0944004947,2.2101257907
 H,0,-2.6525617413,-1.2462237926,1.8735156002
```

Grid Structure C3 fixed at 2.3 / C2 fixed at 2.2

```
E(RB+HF-LYP) = -954.189182691

 Zero-point correction=                           0.221251 (Hartree/Particle)
 Thermal correction to Energy=                    0.236579
 Thermal correction to Enthalpy=                  0.237523
 Thermal correction to Gibbs Free Energy=         0.177188
 Sum of electronic and zero-point Energies=           -953.967932
 Sum of electronic and thermal Energies=              -953.952604
 Sum of electronic and thermal Enthalpies=            -953.951660
 Sum of electronic and thermal Free Energies=         -954.011995

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.455             53.740            126.985

C,0,2.8013673343,-0.49548213,-0.3451822445
 C,0,2.2543080051,0.6687720099,0.0692959512
 O,0,0.5124017585,-0.6511747139,-0.1826954643
 C,0,-0.089276778,-0.7585433595,-1.4455665104
 N,0,-1.0554232375,-1.1874232442,-0.4806650754
 S,0,-2.1400289059,0.0894428989,-0.0102843474
 O,0,-3.4272308241,-0.2595597224,-0.6193616295
 O,0,-1.5614618586,1.4233604604,-0.2300685822
 C,0,3.211855335,-1.6806531958,0.4769823817
 C,0,1.9814229061,1.0206746641,1.5094247643
 C,0,1.9889280007,1.7927936981,-0.9019046798
 C,0,-2.2111618834,-0.2280379481,1.7571254136
 H,0,2.9960594127,-0.5945484737,-1.4145890206
 H,0,0.2825381512,-1.5662746209,-2.0801073538
 H,0,-0.2434372161,0.1900014407,-1.965109935
 H,0,2.7319817078,-2.594897881,0.105562744
 H,0,2.95613229,-1.577136495,1.5341137479
 H,0,4.2969941441,-1.8404809759,0.4087958688
 H,0,2.7021339946,1.7723043108,1.8600268908
 H,0,2.0396373035,0.1614115969,2.1812223242
 H,0,0.9840204833,1.4663879962,1.6021829434
 H,0,0.9389391523,2.1064639986,-0.8516157427
 H,0,2.2251601137,1.5112686723,-1.9338052687
 H,0,2.597057338,2.6721011987,-0.6479029655
 H,0,-2.9351347805,0.4750076523,2.1750300943
 H,0,-1.2194832131,-0.0618443827,2.1799973702
 H,0,-2.5385038512,-1.2570383333,1.9113583408
```

Grid Structure C3 fixed at 2.3 / C2 fixed at 2.3

```
E(RB+HF-LYP) = -954.192427254
```

```
 Zero-point correction=                           0.221247 (Hartree/Particle)
 Thermal correction to Energy=                    0.236560
 Thermal correction to Enthalpy=                  0.237504
 Thermal correction to Gibbs Free Energy=         0.177691
 Sum of electronic and zero-point Energies=           -953.971181
 Sum of electronic and thermal Energies=              -953.955868
 Sum of electronic and thermal Enthalpies=            -953.954923
 Sum of electronic and thermal Free Energies=         -954.014737

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.443             53.751            125.888


C,0,2.7552493249,-0.5515222101,-0.3098797807
 C,0,2.3038956263,0.6820039967,-0.0142269185
 O,0,0.4641897305,-0.6904144461,-0.1623758612
 C,0,-0.1282005836,-0.8627136276,-1.4213150754
 N,0,-1.0574485105,-1.2204270113,-0.3892136305
 S,0,-2.1372120267,0.0978328498,0.0171507628
 O,0,-3.4372354366,-0.3000582962,-0.5290987365
 O,0,-1.5607570863,1.4065903249,-0.3204437325
 C,0,3.1037146027,-1.6732356046,0.6246894197
 C,0,2.03719737,1.1878368636,1.3799637876
 C,0,2.0705807106,1.7069785217,-1.0970534433
 C,0,-2.150749529,-0.0904533692,1.8044376101
 H,0,2.9346725574,-0.7709761885,-1.3643041715
 H,0,0.2304023422,-1.7112745104,-2.0068642482
 H,0,-0.2914583015,0.0553181003,-1.9888358538
 H,0,2.5591090642,-2.586414532,0.3537416124
 H,0,2.8720903672,-1.4480146165,1.6686720391
 H,0,4.1751070577,-1.9096355274,0.5637248756
 H,0,2.7363884704,1.9961559406,1.6352646938
 H,0,2.1277333402,0.4137776336,2.1454247544
 H,0,1.027320107,1.6138795795,1.4359916319
 H,0,1.0285521178,2.0524986564,-1.0848668935
 H,0,2.2984931245,1.3131083237,-2.0935654057
 H,0,2.699179147,2.5939529252,-0.9363311011
 H,0,-2.8574693669,0.6460780447,2.1931340317
 H,0,-1.144895753,0.1002726342,2.1811810232
 H,0,-2.4773933491,-1.1033948031,2.0433716701
```

Grid Structure C3 fixed at 2.3 / C2 fixed at 2.4

```
E(RB+HF-LYP) = -954.195059136

 Zero-point correction=                           0.221481 (Hartree/Particle)
 Thermal correction to Energy=                    0.236555
 Thermal correction to Enthalpy=                  0.237499
 Thermal correction to Gibbs Free Energy=         0.179249
 Sum of electronic and zero-point Energies=           -953.973578
 Sum of electronic and thermal Energies=              -953.958504
 Sum of electronic and thermal Enthalpies=            -953.957560
 Sum of electronic and thermal Free Energies=         -954.015810

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.440             53.635            122.597

C,0,2.7231183304,-0.5579352,-0.2791047385
 C,0,2.3495729412,0.7108773755,-0.039041716
 O,0,0.4294127807,-0.7174653141,-0.2202013475
 C,0,-0.1525612782,-0.7675720154,-1.4943413576
 N,0,-1.0633971548,-1.2126389734,-0.476901473
 S,0,-2.1400459636,0.0751045358,0.0535848389
```

O,0,-3.4513087984,-0.2931991453,-0.484796047
O,0,-1.5723853564,1.4042311506,-0.2091628053
C,0,2.9981984504,-1.6593755773,0.7039955463
C,0,2.0584224303,1.2795739792,1.3255006952
C,0,2.1834543071,1.7010411849,-1.1662248152
C,0,-2.0993059676,-0.2375081642,1.8230078923
H,0,2.9109395966,-0.8290196437,-1.3200623375
H,0,0.2007568293,-1.5620177956,-2.1534442667
H,0,-0.3185676388,0.1997601891,-1.9700945075
H,0,2.409206773,-2.5517598825,0.4592538197
H,0,2.7638283737,-1.3814217189,1.7347889199
H,0,4.056460306,-1.9531694324,0.6705888271
H,0,2.7259957393,2.1245454257,1.5437903901
H,0,2.169361627,0.550514786,2.1316948335
H,0,1.0331160281,1.6720619511,1.3530145378
H,0,1.1607646018,2.102023368,-1.1854413559
H,0,2.40326087,1.256133157,-2.142997122
H,0,2.8532297391,2.5622926312,-1.0335123743
H,0,-2.7953302764,0.4677558713,2.282543667
H,0,-1.0828246305,-0.0682197071,2.1807700779
H,0,-2.4168267255,-1.2658219836,2.0005923403

Grid Structure C3 fixed at 2.3 / C2 fixed at 2.5

E(RB+HF-LYP) = -954.196944633

Zero-point correction=	0.221478 (Hartree/Particle)
Thermal correction to Energy=	0.236594
Thermal correction to Enthalpy=	0.237539
Thermal correction to Gibbs Free Energy=	0.178537
Sum of electronic and zero-point Energies=	-953.975467
Sum of electronic and thermal Energies=	-953.960350
Sum of electronic and thermal Enthalpies=	-953.959406
Sum of electronic and thermal Free Energies=	-954.018407

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.465	53.548	124.179

C,0,2.6918550222,-0.5438699781,-0.2595381026
C,0,2.3960156421,0.7481455792,-0.0397719174
O,0,0.4005555215,-0.7434181725,-0.2480328788
C,0,-0.1716867793,-0.740249407,-1.5275035248
N,0,-1.0735894135,-1.2221305781,-0.5168741783
S,0,-2.1510599802,0.0514907264,0.0625118131
O,0,-3.4654832282,-0.3083670354,-0.4729492033
O,0,-1.5881592063,1.3875804702,-0.1708702579
C,0,2.9358074006,-1.6362169145,0.7429706852
C,0,2.1323735098,1.3498849465,1.3161671354
C,0,2.2501664414,1.7201751673,-1.1851557534
C,0,-2.0869338187,-0.3100473315,1.821909917
H,0,2.8574872125,-0.843926773,-1.2963586461
H,0,0.1809086243,-1.5103305367,-2.2148128279
H,0,-0.3394636938,0.2451529816,-1.9632378298
H,0,2.3221530798,-2.5154574577,0.5132715651
H,0,2.7097384352,-1.334179979,1.7690406875
H,0,3.9856821593,-1.9595454115,0.7156593816
H,0,2.8112909188,2.1920326047,1.5086141931
H,0,2.2458016828,0.6364904452,2.1358597394
H,0,1.1111995919,1.7541150249,1.3513541651
H,0,1.2365826753,2.1446692404,-1.2092867243
H,0,2.4542951018,1.2505673278,-2.1537679041
H,0,2.9397076133,2.5686302454,-1.0730923835

```
H,0,-2.7781470253,0.3808727574,2.309611736
H,0,-1.0660266174,-0.1476919071,2.1701507464
H,0,-2.400013385,-1.3436306074,1.9752724242
```

Grid Structure C3 fixed at 2.4 / C2 fixed at 2.0

```
E(RB+HF-LYP) = -954.182298629

 Zero-point correction=                           0.221289 (Hartree/Particle)
 Thermal correction to Energy=                    0.236455
 Thermal correction to Enthalpy=                  0.237400
 Thermal correction to Gibbs Free Energy=         0.178485
 Sum of electronic and zero-point Energies=           -953.961009
 Sum of electronic and thermal Energies=              -953.945843
 Sum of electronic and thermal Enthalpies=            -953.944899
 Sum of electronic and thermal Free Energies=         -954.003813

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.378             53.700            123.995

 C,0,2.9448117623,-0.5034223205,-0.3966468438
 C,0,2.1894668605,0.5417816656,0.069118244
 O,0,0.5702114092,-0.6238466737,-0.0698963838
 C,0,-0.0870766574,-0.8426690606,-1.2938951573
 N,0,-1.1348887191,-1.1699158021,-0.3830576527
 S,0,-2.1814475755,0.1477196781,-0.0528618976
 O,0,-3.4461583274,-0.1712897276,-0.7283469726
 O,0,-1.5504767936,1.457392284,-0.2894277212
 C,0,3.5151618343,-1.6442661107,0.3826437251
 C,0,2.001448431,0.8357624937,1.5396266376
 C,0,1.8598713153,1.7011840606,-0.8427494939
 C,0,-2.3983073747,-0.0725138874,1.7177688636
 H,0,3.1259810946,-0.5371096238,-1.4717186879
 H,0,0.2692890632,-1.7102940168,-1.8573960957
 H,0,-0.1930879351,0.0540270761,-1.9128135438
 H,0,3.1663653874,-2.6042136642,-0.0204128036
 H,0,3.2590397105,-1.6087378701,1.4434118428
 H,0,4.6115840781,-1.6518909591,0.2985933452
 H,0,2.7995833232,1.5015200022,1.8938362532
 H,0,2.0107669854,-0.0660547471,2.1556156327
 H,0,1.0480429628,1.3493197063,1.6960039471
 H,0,0.8138589211,2.0016558362,-0.7250702515
 H,0,2.0465293088,1.4635825505,-1.8955329896
 H,0,2.4840437625,2.5669209764,-0.582306007
 H,0,-3.1278886453,0.6722368432,2.0436273885
 H,0,-1.4371331723,0.0835998677,2.2093617897
 H,0,-2.7704599364,-1.0818543159,1.8981668788
```

Grid Structure C3 fixed at 2.4 / C2 fixed at 2.1

```
E(RB+HF-LYP) = -954.186638158

 Zero-point correction=                           0.221268 (Hartree/Particle)
 Thermal correction to Energy=                    0.236530
 Thermal correction to Enthalpy=                  0.237474
 Thermal correction to Gibbs Free Energy=         0.177884
 Sum of electronic and zero-point Energies=           -953.965370
 Sum of electronic and thermal Energies=              -953.950108
 Sum of electronic and thermal Enthalpies=            -953.949164
 Sum of electronic and thermal Free Energies=         -954.008754

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

Total	148.425	53.740	125.418

```
C,0,2.8990333427,-0.4738143334,-0.3821053149
 C,0,2.2205751588,0.60226507,0.0875018093
 O,0,0.5199651099,-0.6155253054,-0.0993368509
 C,0,-0.0754531946,-0.8465624467,-1.3475157453
 N,0,-1.0646793228,-1.1818748286,-0.3692795447
 S,0,-2.1662410834,0.1200569173,-0.0507779007
 O,0,-3.4278507893,-0.2852653137,-0.6794118263
 O,0,-1.5861962506,1.4361689581,-0.3562684778
 C,0,3.3990485797,-1.6608736401,0.3833418593
 C,0,1.9836665453,0.8793227525,1.5529556271
 C,0,1.8978661951,1.7644744337,-0.8222456299
 C,0,-2.3113260789,-0.0511603322,1.7323433802
 H,0,3.0941462331,-0.5035110359,-1.455483331
 H,0,0.3024393303,-1.7109137896,-1.8988548906
 H,0,-0.2197776194,0.0468510673,-1.9607376822
 H,0,2.9970563552,-2.5929629554,-0.0354320358
 H,0,3.1333887978,-1.6289336081,1.4423601779
 H,0,4.4937084797,-1.7324216025,0.3133308728
 H,0,2.7418311346,1.5784925169,1.931040284
 H,0,2.0179482128,-0.0215745602,2.1696714742
 H,0,1.0069706319,1.3551413461,1.6920529102
 H,0,0.8416273838,2.0437156226,-0.7385452373
 H,0,2.1223124601,1.5401505592,-1.8707290722
 H,0,2.489863007,2.6452636061,-0.537018995
 H,0,-3.0566132881,0.6772949005,2.0594157546
 H,0,-1.3404740972,0.1575286226,2.1839641322
 H,0,-2.6396222772,-1.0668432998,1.9568501876
```

Grid Structure C3 fixed at 2.4 / C2 fixed at 2.2

```
E(RB+HF-LYP) = -954.191116605
```

Zero-point correction=	0.221126 (Hartree/Particle)
Thermal correction to Energy=	0.236471
Thermal correction to Enthalpy=	0.237415
Thermal correction to Gibbs Free Energy=	0.176874
Sum of electronic and zero-point Energies=	-953.969991
Sum of electronic and thermal Energies=	-953.954646
Sum of electronic and thermal Enthalpies=	-953.953701
Sum of electronic and thermal Free Energies=	-954.014243

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.388	53.815	127.420

```
C,0,2.8629856219,-0.4563857665,-0.368673527
 C,0,2.2576024437,0.6533214262,0.0990903954
 O,0,0.4819035214,-0.6267308185,-0.120808404
 C,0,-0.072820203,-0.8406235659,-1.3893058599
 N,0,-1.0255152819,-1.1928260991,-0.3762987686
 S,0,-2.1607847131,0.0974363064,-0.0465490735
 O,0,-3.4184846369,-0.3478120793,-0.6523776554
 O,0,-1.6081787493,1.4185071,-0.374534233
 C,0,3.3065608567,-1.6701164488,0.3935297577
 C,0,1.991785121,0.933249325,1.5578890516
 C,0,1.9472344348,1.8124360752,-0.8179475063
 C,0,-2.2634653978,-0.0664818985,1.7402364861
 H,0,3.0585887892,-0.4966727174,-1.4421042015
 H,0,0.3181691586,-1.6945052608,-1.9455149123
 H,0,-0.2377487828,0.0609708845,-1.9828109825
```

```
 H,0,2.839936396,-2.5780045361,-0.0114680418
 H,0,3.0626094953,-1.619788528,1.4573743315
 H,0,4.3932088135,-1.808640803,0.3056502764
 H,0,2.7141950186,1.667038758,1.9411368717
 H,0,2.0537940787,0.0416420085,2.1859427211
 H,0,0.9952675097,1.3732237,1.6818565478
 H,0,0.8853217769,2.0809687415,-0.7607510877
 H,0,2.1977295522,1.5896909775,-1.8609611256
 H,0,2.5188835274,2.7030705734,-0.5214433524
 H,0,-3.0118594511,0.6532481785,2.0793115118
 H,0,-1.2860178047,0.1600117386,2.1686289993
 H,0,-2.5721340391,-1.0855604212,1.9768785534
```

Grid Structure C3 fixed at 2.4 / C2 fixed at 2.3

```
E(RB+HF-LYP) = -954.194937885

 Zero-point correction=                           0.221438 (Hartree/Particle)
 Thermal correction to Energy=                    0.236555
 Thermal correction to Enthalpy=                  0.237499
 Thermal correction to Gibbs Free Energy=         0.179028
 Sum of electronic and zero-point Energies=           -953.973500
 Sum of electronic and thermal Energies=              -953.958383
 Sum of electronic and thermal Enthalpies=            -953.957439
 Sum of electronic and thermal Free Energies=         -954.015910

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.440             53.667            123.063

C,0,2.8349292395,-0.469668457,-0.3373756205
 C,0,2.2966285519,0.6861239397,0.0885172935
 O,0,0.4475770194,-0.6558181476,-0.1764260128
 C,0,-0.092836046,-0.7674721639,-1.4643010275
 N,0,-1.0238975727,-1.1910100347,-0.4555863975
 S,0,-2.1574855989,0.0821438241,-0.0201066959
 O,0,-3.4273914411,-0.3299888423,-0.6220698265
 O,0,-1.606347454,1.4178148341,-0.2832043847
 C,0,3.2136027096,-1.6798963975,0.4659258394
 C,0,1.9996185629,1.0179578274,1.5294209877
 C,0,2.0260770435,1.8194262061,-0.8718517835
 C,0,-2.2104631627,-0.1896048095,1.7556672476
 H,0,3.0386946137,-0.5558376652,-1.4068523025
 H,0,0.2961584141,-1.578707084,-2.0811444984
 H,0,-0.2637981461,0.1776582559,-1.9817925546
 H,0,2.6836971489,-2.5702689611,0.1024166271
 H,0,2.98865248,-1.5747735683,1.530220146
 H,0,4.2880370253,-1.8894463242,0.3711195127
 H,0,2.6871481132,1.7945072712,1.892629677
 H,0,2.0847619688,0.1576946293,2.1973869489
 H,0,0.9856270096,1.4269283995,1.6207490898
 H,0,0.9689531905,2.1132287334,-0.838555252
 H,0,2.2845594196,1.5552062109,-1.9032476105
 H,0,2.6099397232,2.7098612477,-0.5994597852
 H,0,-2.9411390907,0.5146095576,2.1596974483
 H,0,-1.2182007743,0.0034838539,2.165888355
 H,0,-2.5220848896,-1.2186351248,1.9393402863
```

Grid Structure C3 fixed at 2.4 / C2 fixed at 2.4

```
E(RB+HF-LYP) = -954.197917260

 Zero-point correction=                           0.221623 (Hartree/Particle)
 Thermal correction to Energy=                    0.236667
```

```
 Thermal correction to Enthalpy=                  0.237611
 Thermal correction to Gibbs Free Energy=         0.179288
 Sum of electronic and zero-point Energies=           -953.976294
 Sum of electronic and thermal Energies=              -953.961251
 Sum of electronic and thermal Enthalpies=            -953.960307
 Sum of electronic and thermal Free Energies=         -954.018629

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 148.510             53.507           122.751

C,0,2.806906593,-0.4674649797,-0.3186771719
 C,0,2.3344965819,0.7229525543,0.0843427934
 O,0,0.419494517,-0.6916192433,-0.2185602587
 C,0,-0.11701333,-0.7397260384,-1.5118548199
 N,0,-1.0342873964,-1.2002448702,-0.5046004053
 S,0,-2.155955073,0.067126153,-0.0023924894
 O,0,-3.4364385317,-0.3153958509,-0.600552019
 O,0,-1.5966172159,1.4065518514,-0.2240786967
 C,0,3.1376025521,-1.6768654092,0.5078306511
 C,0,2.0221649748,1.0871336316,1.5134275517
 C,0,2.0996692881,1.8425048362,-0.9010338288
 C,0,-2.179964122,-0.2728183289,1.7623995943
 H,0,3.0108531691,-0.5831185087,-1.3855005475
 H,0,0.2636104108,-1.5266736159,-2.1637694291
 H,0,-0.288118838,0.2281319168,-1.9843235585
 H,0,2.5774915346,-2.5530177865,0.1562753627
 H,0,2.9106317222,-1.5457334544,1.5689655753
 H,0,4.2045654109,-1.9256337603,0.4237111595
 H,0,2.6808255256,1.8964500274,1.8581473281
 H,0,2.1314468412,0.2500749093,2.2069400302
 H,0,0.9941736009,1.4654008719,1.5882689935
 H,0,1.0484252733,2.1602231053,-0.8849781526
 H,0,2.361460237,1.5517570474,-1.9244096093
 H,0,2.6984285045,2.7268699851,-0.6414866998
 H,0,-2.8971789982,0.4211724449,2.2062332094
 H,0,-1.1788454896,-0.1030982466,2.1614372486
 H,0,-2.4971613445,-1.3057009469,1.9118909326
```

Interpolated Grid of Non-Stationary Point Structures

*The predicted KIEs were calculated from the non-stationary point structures listed aboved. From the predicted KIEs and C-O bond distances a grid was used to calculate 2800 geometries and predicted KIEs.

Predicted KIE at C3

	C2 C-O Bond Disance→								
C3 C-O Bond Distance ↓	1.90	1.91	1.92	1.93	1.94	1.95	1.96	1.97	1.98
1.90	1.0225	1.0226	1.0227	1.0228	1.0228	1.0229	1.0230	1.0231	1.0232
1.91	1.0222	1.0222	1.0223	1.0224	1.0224	1.0225	1.0226	1.0226	1.0227
1.92	1.0218	1.0218	1.0219	1.0219	1.0220	1.0221	1.0221	1.0222	1.0222
1.93	1.0214	1.0215	1.0215	1.0215	1.0216	1.0216	1.0217	1.0217	1.0217
1.94	1.0211	1.0211	1.0211	1.0211	1.0212	1.0212	1.0212	1.0212	1.0213
1.95	1.0207	1.0207	1.0207	1.0207	1.0207	1.0207	1.0208	1.0208	1.0208
1.96	1.0203	1.0203	1.0203	1.0203	1.0203	1.0203	1.0203	1.0203	1.0203
1.97	1.0199	1.0199	1.0199	1.0199	1.0199	1.0199	1.0199	1.0198	1.0198
1.98	1.0196	1.0195	1.0195	1.0195	1.0195	1.0194	1.0194	1.0194	1.0194
1.99	1.0192	1.0192	1.0191	1.0191	1.0190	1.0190	1.0190	1.0189	1.0189

2.00	1.0188	1.0188	1.0187	1.0187	1.0186	1.0186	1.0185	1.0185	1.0184
2.01	1.0184	1.0183	1.0183	1.0182	1.0182	1.0181	1.0181	1.0180	1.0179
2.02	1.0180	1.0179	1.0179	1.0178	1.0177	1.0177	1.0176	1.0175	1.0175
2.03	1.0176	1.0175	1.0174	1.0174	1.0173	1.0172	1.0171	1.0171	1.0170
2.04	1.0172	1.0171	1.0170	1.0169	1.0168	1.0168	1.0167	1.0166	1.0165
2.05	1.0167	1.0167	1.0166	1.0165	1.0164	1.0163	1.0162	1.0161	1.0160
2.06	1.0163	1.0162	1.0161	1.0160	1.0159	1.0158	1.0157	1.0157	1.0156
2.07	1.0159	1.0158	1.0157	1.0156	1.0155	1.0154	1.0153	1.0152	1.0151
2.08	1.0155	1.0154	1.0153	1.0152	1.0151	1.0149	1.0148	1.0147	1.0146
2.09	1.0151	1.0150	1.0148	1.0147	1.0146	1.0145	1.0144	1.0142	1.0141
2.10	1.0147	1.0145	1.0144	1.0143	1.0142	1.0140	1.0139	1.0138	1.0137
2.11	1.0143	1.0142	1.0141	1.0139	1.0138	1.0137	1.0135	1.0134	1.0133
2.12	1.0140	1.0139	1.0137	1.0136	1.0134	1.0133	1.0132	1.0130	1.0129
2.13	1.0137	1.0135	1.0134	1.0132	1.0131	1.0129	1.0128	1.0126	1.0125
2.14	1.0133	1.0132	1.0130	1.0129	1.0127	1.0126	1.0124	1.0123	1.0121
2.15	1.0130	1.0128	1.0127	1.0125	1.0124	1.0122	1.0120	1.0119	1.0117
2.16	1.0127	1.0125	1.0123	1.0122	1.0120	1.0118	1.0117	1.0115	1.0113
2.17	1.0123	1.0122	1.0120	1.0118	1.0116	1.0115	1.0113	1.0111	1.0110
2.18	1.0120	1.0118	1.0116	1.0115	1.0113	1.0111	1.0109	1.0108	1.0106
2.19	1.0117	1.0115	1.0113	1.0111	1.0109	1.0107	1.0106	1.0104	1.0102
2.20	1.0113	1.0111	1.0110	1.0108	1.0106	1.0104	1.0102	1.0100	1.0098
2.21	1.0111	1.0109	1.0107	1.0105	1.0103	1.0101	1.0099	1.0097	1.0095
2.22	1.0109	1.0107	1.0105	1.0103	1.0101	1.0099	1.0097	1.0095	1.0093
2.23	1.0107	1.0105	1.0103	1.0101	1.0098	1.0096	1.0094	1.0092	1.0090
2.24	1.0105	1.0102	1.0100	1.0098	1.0096	1.0094	1.0092	1.0090	1.0088
2.25	1.0102	1.0100	1.0098	1.0096	1.0094	1.0091	1.0089	1.0087	1.0085
2.26	1.0100	1.0098	1.0096	1.0093	1.0091	1.0089	1.0087	1.0085	1.0082
2.27	1.0098	1.0096	1.0093	1.0091	1.0089	1.0087	1.0084	1.0082	1.0080
2.28	1.0096	1.0093	1.0091	1.0089	1.0086	1.0084	1.0082	1.0079	1.0077
2.29	1.0094	1.0091	1.0089	1.0086	1.0084	1.0082	1.0079	1.0077	1.0074
2.30	1.0091	1.0089	1.0086	1.0084	1.0082	1.0079	1.0077	1.0074	1.0072

C3 C-O Bond Distance ↓	**C2 C-O Bond Disance→**								
	1.99	**2.00**	**2.01**	**2.02**	**2.03**	**2.04**	**2.05**	**2.06**	**2.07**
1.90	1.0232	1.0233	1.0234	1.0236	1.0237	1.0239	1.0240	1.0241	1.0243
1.91	1.0227	1.0228	1.0229	1.0231	1.0232	1.0233	1.0234	1.0235	1.0237
1.92	1.0223	1.0223	1.0224	1.0225	1.0226	1.0227	1.0229	1.0230	1.0231
1.93	1.0218	1.0218	1.0219	1.0220	1.0221	1.0222	1.0223	1.0224	1.0225
1.94	1.0213	1.0213	1.0214	1.0215	1.0216	1.0216	1.0217	1.0218	1.0219
1.95	1.0208	1.0208	1.0209	1.0209	1.0210	1.0211	1.0212	1.0212	1.0213
1.96	1.0203	1.0203	1.0204	1.0204	1.0205	1.0205	1.0206	1.0206	1.0207
1.97	1.0198	1.0198	1.0198	1.0199	1.0199	1.0200	1.0200	1.0201	1.0201
1.98	1.0193	1.0193	1.0193	1.0194	1.0194	1.0194	1.0195	1.0195	1.0195
1.99	1.0188	1.0188	1.0188	1.0188	1.0189	1.0189	1.0189	1.0189	1.0189
2.00	1.0184	1.0183	1.0183	1.0183	1.0183	1.0183	1.0183	1.0183	1.0183
2.01	1.0179	1.0178	1.0178	1.0178	1.0178	1.0178	1.0178	1.0178	1.0178
2.02	1.0174	1.0173	1.0173	1.0173	1.0173	1.0173	1.0172	1.0172	1.0172
2.03	1.0169	1.0168	1.0168	1.0168	1.0168	1.0167	1.0167	1.0167	1.0166
2.04	1.0164	1.0163	1.0163	1.0163	1.0162	1.0162	1.0162	1.0161	1.0161
2.05	1.0159	1.0159	1.0158	1.0158	1.0157	1.0157	1.0156	1.0156	1.0155
2.06	1.0155	1.0154	1.0153	1.0152	1.0152	1.0151	1.0151	1.0150	1.0150
2.07	1.0150	1.0149	1.0148	1.0147	1.0147	1.0146	1.0145	1.0145	1.0144
2.08	1.0145	1.0144	1.0143	1.0142	1.0141	1.0141	1.0140	1.0139	1.0138
2.09	1.0140	1.0139	1.0138	1.0137	1.0136	1.0135	1.0135	1.0134	1.0133
2.10	1.0135	1.0134	1.0133	1.0132	1.0131	1.0130	1.0129	1.0128	1.0127
2.11	1.0131	1.0130	1.0129	1.0128	1.0127	1.0126	1.0125	1.0124	1.0123
2.12	1.0127	1.0126	1.0125	1.0124	1.0123	1.0122	1.0120	1.0119	1.0118

2.13	1.0124	1.0122	1.0121	1.0120	1.0118	1.0117	1.0116	1.0115	1.0114
2.14	1.0120	1.0118	1.0117	1.0116	1.0114	1.0113	1.0112	1.0110	1.0109
2.15	1.0116	1.0114	1.0113	1.0111	1.0110	1.0109	1.0107	1.0106	1.0105
2.16	1.0112	1.0110	1.0109	1.0107	1.0106	1.0104	1.0103	1.0102	1.0100
2.17	1.0108	1.0106	1.0105	1.0103	1.0102	1.0100	1.0099	1.0097	1.0096
2.18	1.0104	1.0102	1.0101	1.0099	1.0097	1.0096	1.0094	1.0093	1.0091
2.19	1.0100	1.0098	1.0097	1.0095	1.0093	1.0092	1.0090	1.0088	1.0087
2.20	1.0096	1.0094	1.0092	1.0091	1.0089	1.0087	1.0086	1.0084	1.0082
2.21	1.0093	1.0091	1.0090	1.0088	1.0086	1.0084	1.0083	1.0081	1.0079
2.22	1.0091	1.0089	1.0087	1.0085	1.0083	1.0082	1.0080	1.0078	1.0076
2.23	1.0088	1.0086	1.0084	1.0082	1.0080	1.0079	1.0077	1.0075	1.0073
2.24	1.0085	1.0083	1.0081	1.0080	1.0078	1.0076	1.0074	1.0072	1.0070
2.25	1.0083	1.0081	1.0079	1.0077	1.0075	1.0073	1.0071	1.0069	1.0067
2.26	1.0080	1.0078	1.0076	1.0074	1.0072	1.0070	1.0068	1.0066	1.0064
2.27	1.0077	1.0075	1.0073	1.0071	1.0069	1.0067	1.0065	1.0063	1.0061
2.28	1.0075	1.0072	1.0070	1.0068	1.0066	1.0064	1.0062	1.0060	1.0058
2.29	1.0072	1.0070	1.0068	1.0065	1.0063	1.0061	1.0059	1.0057	1.0055
2.30	1.0069	1.0067	1.0065	1.0063	1.0061	1.0058	1.0056	1.0054	1.0052
2.31		1.0065	1.0063	1.0061	1.0059	1.0057	1.0055	1.0053	1.0050
2.32		1.0063	1.0061	1.0059	1.0057	1.0055	1.0053	1.0051	1.0049
2.33		1.0062	1.0060	1.0058	1.0056	1.0053	1.0051	1.0049	1.0047
2.34		1.0060	1.0058	1.0056	1.0054	1.0052	1.0050	1.0048	1.0046
2.35		1.0058	1.0056	1.0054	1.0052	1.0050	1.0048	1.0046	1.0044
2.36		1.0057	1.0055	1.0053	1.0051	1.0049	1.0046	1.0044	1.0042
2.37		1.0055	1.0053	1.0051	1.0049	1.0047	1.0045	1.0043	1.0041
2.38		1.0053	1.0051	1.0049	1.0047	1.0045	1.0043	1.0041	1.0039
2.39		1.0052	1.0050	1.0048	1.0046	1.0044	1.0042	1.0040	1.0038
2.40		1.0050	1.0048	1.0046	1.0044	1.0042	1.0040	1.0038	1.0036

C3 C-O Bond Distance ↓	**C2 C-O Bond Disance→**								
	2.08	**2.09**	**2.10**	**2.11**	**2.12**	**2.13**	**2.14**	**2.15**	**2.16**
1.90	1.0244	1.0245	1.0247	1.0248	1.0248	1.0249	1.0250	1.0251	1.0252
1.91	1.0238	1.0239	1.0240	1.0241	1.0242	1.0242	1.0243	1.0244	1.0245
1.92	1.0232	1.0233	1.0234	1.0235	1.0235	1.0236	1.0236	1.0237	1.0238
1.93	1.0226	1.0227	1.0228	1.0228	1.0229	1.0229	1.0229	1.0230	1.0230
1.94	1.0220	1.0220	1.0221	1.0222	1.0222	1.0222	1.0223	1.0223	1.0223
1.95	1.0214	1.0214	1.0215	1.0215	1.0215	1.0216	1.0216	1.0216	1.0216
1.96	1.0208	1.0208	1.0209	1.0209	1.0209	1.0209	1.0209	1.0209	1.0209
1.97	1.0201	1.0202	1.0202	1.0202	1.0202	1.0202	1.0202	1.0202	1.0202
1.98	1.0195	1.0196	1.0196	1.0196	1.0195	1.0195	1.0195	1.0195	1.0195
1.99	1.0189	1.0189	1.0190	1.0189	1.0189	1.0189	1.0188	1.0188	1.0187
2.00	1.0183	1.0183	1.0183	1.0183	1.0182	1.0182	1.0181	1.0181	1.0180
2.01	1.0178	1.0177	1.0177	1.0177	1.0176	1.0176	1.0175	1.0174	1.0174
2.02	1.0172	1.0172	1.0171	1.0171	1.0170	1.0169	1.0169	1.0168	1.0167
2.03	1.0166	1.0166	1.0166	1.0165	1.0164	1.0163	1.0162	1.0162	1.0161
2.04	1.0160	1.0160	1.0160	1.0159	1.0158	1.0157	1.0156	1.0155	1.0154
2.05	1.0155	1.0154	1.0154	1.0153	1.0152	1.0151	1.0150	1.0149	1.0148
2.06	1.0149	1.0148	1.0148	1.0147	1.0146	1.0145	1.0143	1.0142	1.0141
2.07	1.0143	1.0143	1.0142	1.0141	1.0140	1.0138	1.0137	1.0136	1.0135
2.08	1.0138	1.0137	1.0136	1.0135	1.0133	1.0132	1.0131	1.0130	1.0128
2.09	1.0132	1.0131	1.0130	1.0129	1.0127	1.0126	1.0125	1.0123	1.0122
2.10	1.0126	1.0125	1.0124	1.0123	1.0121	1.0120	1.0118	1.0117	1.0115
2.11	1.0122	1.0121	1.0119	1.0118	1.0116	1.0115	1.0113	1.0112	1.0110
2.12	1.0117	1.0116	1.0115	1.0113	1.0112	1.0110	1.0109	1.0107	1.0106
2.13	1.0112	1.0111	1.0110	1.0108	1.0107	1.0105	1.0104	1.0102	1.0101
2.14	1.0108	1.0107	1.0105	1.0104	1.0102	1.0101	1.0099	1.0098	1.0096
2.15	1.0103	1.0102	1.0101	1.0099	1.0097	1.0096	1.0094	1.0093	1.0091

2.16	1.0099	1.0097	1.0096	1.0094	1.0093	1.0091	1.0090	1.0088	1.0086
2.17	1.0094	1.0093	1.0091	1.0090	1.0088	1.0086	1.0085	1.0083	1.0082
2.18	1.0090	1.0088	1.0086	1.0085	1.0083	1.0082	1.0080	1.0078	1.0077
2.19	1.0085	1.0083	1.0082	1.0080	1.0078	1.0077	1.0075	1.0074	1.0072
2.20	1.0080	1.0079	1.0077	1.0075	1.0074	1.0072	1.0070	1.0069	1.0067
2.21	1.0077	1.0076	1.0074	1.0072	1.0071	1.0069	1.0067	1.0066	1.0064
2.22	1.0074	1.0072	1.0071	1.0069	1.0068	1.0066	1.0065	1.0063	1.0062
2.23	1.0071	1.0069	1.0068	1.0066	1.0065	1.0063	1.0062	1.0060	1.0059
2.24	1.0068	1.0066	1.0064	1.0063	1.0062	1.0060	1.0059	1.0058	1.0056
2.25	1.0065	1.0063	1.0061	1.0060	1.0059	1.0057	1.0056	1.0055	1.0053
2.26	1.0062	1.0060	1.0058	1.0057	1.0056	1.0054	1.0053	1.0052	1.0051
2.27	1.0059	1.0057	1.0055	1.0054	1.0053	1.0051	1.0050	1.0049	1.0048
2.28	1.0056	1.0054	1.0052	1.0051	1.0050	1.0049	1.0047	1.0046	1.0045
2.29	1.0053	1.0051	1.0049	1.0048	1.0047	1.0046	1.0045	1.0044	1.0042
2.30	1.0050	1.0048	1.0046	1.0045	1.0044	1.0043	1.0042	1.0041	1.0040
2.31	1.0048	1.0046	1.0044	1.0043	1.0042	1.0041	1.0040	1.0039	1.0038
2.32	1.0047	1.0045	1.0043	1.0042	1.0041	1.0040	1.0039	1.0038	1.0037
2.33	1.0045	1.0043	1.0041	1.0040	1.0039	1.0038	1.0037	1.0036	1.0035
2.34	1.0044	1.0041	1.0039	1.0038	1.0037	1.0036	1.0036	1.0035	1.0034
2.35	1.0042	1.0040	1.0038	1.0037	1.0036	1.0035	1.0034	1.0033	1.0032
2.36	1.0040	1.0038	1.0036	1.0035	1.0034	1.0033	1.0032	1.0031	1.0030
2.37	1.0039	1.0037	1.0035	1.0034	1.0033	1.0032	1.0031	1.0030	1.0029
2.38	1.0037	1.0035	1.0033	1.0032	1.0031	1.0030	1.0029	1.0028	1.0027
2.39	1.0036	1.0034	1.0032	1.0031	1.0030	1.0029	1.0028	1.0027	1.0026
2.40	1.0034	1.0032	1.0030	1.0029	1.0028	1.0027	1.0026	1.0025	1.0024

	C2 C-O Bond Disance→								
C3 C-O Bond Distance ↓	**2.17**	**2.18**	**2.19**	**2.20**	**2.21**	**2.22**	**2.23**	**2.24**	**2.25**
1.90	1.0253	1.0254	1.0254	1.0255	1.0255	1.0256	1.0256	1.0256	1.0256
1.91	1.0245	1.0246	1.0247	1.0248	1.0248	1.0248	1.0248	1.0248	1.0248
1.92	1.0238	1.0239	1.0239	1.0240	1.0240	1.0240	1.0240	1.0240	1.0240
1.93	1.0231	1.0231	1.0232	1.0232	1.0232	1.0232	1.0232	1.0232	1.0231
1.94	1.0224	1.0224	1.0224	1.0224	1.0224	1.0224	1.0224	1.0223	1.0223
1.95	1.0216	1.0216	1.0217	1.0217	1.0216	1.0216	1.0216	1.0215	1.0215
1.96	1.0209	1.0209	1.0209	1.0209	1.0209	1.0208	1.0208	1.0207	1.0207
1.97	1.0202	1.0202	1.0201	1.0201	1.0201	1.0200	1.0200	1.0199	1.0199
1.98	1.0194	1.0194	1.0194	1.0194	1.0193	1.0192	1.0192	1.0191	1.0190
1.99	1.0187	1.0187	1.0186	1.0186	1.0185	1.0184	1.0184	1.0183	1.0182
2.00	1.0180	1.0179	1.0179	1.0178	1.0177	1.0177	1.0176	1.0175	1.0174
2.01	1.0173	1.0173	1.0172	1.0171	1.0170	1.0170	1.0169	1.0168	1.0167
2.02	1.0167	1.0166	1.0165	1.0164	1.0164	1.0163	1.0162	1.0161	1.0160
2.03	1.0160	1.0159	1.0158	1.0158	1.0157	1.0156	1.0155	1.0154	1.0153
2.04	1.0153	1.0152	1.0152	1.0151	1.0150	1.0149	1.0148	1.0147	1.0146
2.05	1.0147	1.0146	1.0145	1.0144	1.0143	1.0142	1.0141	1.0140	1.0138
2.06	1.0140	1.0139	1.0138	1.0137	1.0136	1.0135	1.0134	1.0132	1.0131
2.07	1.0134	1.0132	1.0131	1.0130	1.0129	1.0128	1.0127	1.0125	1.0124
2.08	1.0127	1.0126	1.0124	1.0123	1.0122	1.0121	1.0120	1.0118	1.0117
2.09	1.0120	1.0119	1.0118	1.0116	1.0115	1.0114	1.0113	1.0111	1.0110
2.10	1.0114	1.0112	1.0111	1.0109	1.0108	1.0107	1.0106	1.0104	1.0103
2.11	1.0109	1.0107	1.0106	1.0104	1.0103	1.0102	1.0101	1.0100	1.0098
2.12	1.0104	1.0103	1.0101	1.0100	1.0098	1.0097	1.0096	1.0095	1.0094
2.13	1.0099	1.0098	1.0096	1.0095	1.0094	1.0092	1.0091	1.0090	1.0089
2.14	1.0094	1.0093	1.0091	1.0090	1.0089	1.0088	1.0086	1.0085	1.0084
2.15	1.0090	1.0088	1.0086	1.0085	1.0084	1.0083	1.0082	1.0081	1.0080
2.16	1.0085	1.0083	1.0082	1.0080	1.0079	1.0078	1.0077	1.0076	1.0075
2.17	1.0080	1.0078	1.0077	1.0075	1.0074	1.0073	1.0072	1.0071	1.0070
2.18	1.0075	1.0073	1.0072	1.0070	1.0069	1.0068	1.0067	1.0066	1.0065

2.19	1.0070	1.0069	1.0067	1.0065	1.0064	1.0064	1.0063	1.0062	1.0061
2.20	1.0065	1.0064	1.0062	1.0060	1.0060	1.0059	1.0058	1.0057	1.0056
2.21	1.0063	1.0061	1.0060	1.0058	1.0057	1.0056	1.0055	1.0055	1.0054
2.22	1.0060	1.0059	1.0057	1.0056	1.0055	1.0054	1.0053	1.0052	1.0051
2.23	1.0057	1.0056	1.0055	1.0053	1.0052	1.0051	1.0051	1.0050	1.0049
2.24	1.0055	1.0053	1.0052	1.0051	1.0050	1.0049	1.0048	1.0048	1.0047
2.25	1.0052	1.0051	1.0049	1.0048	1.0047	1.0047	1.0046	1.0045	1.0045
2.26	1.0049	1.0048	1.0047	1.0046	1.0045	1.0044	1.0044	1.0043	1.0042
2.27	1.0047	1.0046	1.0044	1.0043	1.0043	1.0042	1.0041	1.0041	1.0040
2.28	1.0044	1.0043	1.0042	1.0041	1.0040	1.0039	1.0039	1.0038	1.0038
2.29	1.0041	1.0040	1.0039	1.0038	1.0038	1.0037	1.0037	1.0036	1.0035
2.30	1.0039	1.0038	1.0037	1.0036	1.0035	1.0035	1.0034	1.0034	1.0033
2.31	1.0037	1.0036	1.0035	1.0034	1.0034	1.0033	1.0033	1.0033	1.0032
2.32	1.0036	1.0035	1.0034	1.0033	1.0032	1.0032	1.0032	1.0031	1.0031
2.33	1.0034	1.0033	1.0032	1.0031	1.0031	1.0031	1.0031	1.0030	1.0030
2.34	1.0033	1.0032	1.0031	1.0030	1.0030	1.0029	1.0029	1.0029	1.0029
2.35	1.0031	1.0030	1.0029	1.0028	1.0028	1.0028	1.0028	1.0028	1.0028
2.36	1.0029	1.0029	1.0028	1.0027	1.0027	1.0027	1.0027	1.0027	1.0027
2.37	1.0028	1.0027	1.0026	1.0025	1.0025	1.0025	1.0026	1.0026	1.0026
2.38	1.0026	1.0025	1.0024	1.0024	1.0024	1.0024	1.0024	1.0025	1.0025
2.39	1.0025	1.0024	1.0023	1.0022	1.0022	1.0023	1.0023	1.0024	1.0024
2.40	1.0023	1.0022	1.0021	1.0020	1.0021	1.0021	1.0022	1.0022	1.0023

C3 C-O Bond Distance ↓	**C2 C-O Bond Disance→** **2.26**	**2.27**	**2.28**	**2.29**	**2.30**	**2.31**	**2.32**	**2.33**	**2.34**
1.90	1.0256	1.0256	1.0257	1.0257	1.0257				
1.91	1.0248	1.0248	1.0248	1.0248	1.0248				
1.92	1.0240	1.0240	1.0240	1.0239	1.0239				
1.93	1.0231	1.0231	1.0231	1.0231	1.0231				
1.94	1.0223	1.0223	1.0222	1.0222	1.0222				
1.95	1.0215	1.0214	1.0214	1.0214	1.0213				
1.96	1.0206	1.0206	1.0205	1.0205	1.0205				
1.97	1.0198	1.0197	1.0197	1.0196	1.0196				
1.98	1.0190	1.0189	1.0188	1.0188	1.0187				
1.99	1.0181	1.0181	1.0180	1.0179	1.0178				
2.00	1.0173	1.0172	1.0171	1.0170	1.0170	1.0168	1.0167	1.0166	1.0164
2.01	1.0166	1.0165	1.0164	1.0163	1.0162	1.0161	1.0160	1.0158	1.0157
2.02	1.0159	1.0158	1.0157	1.0156	1.0155	1.0154	1.0152	1.0151	1.0150
2.03	1.0152	1.0151	1.0150	1.0149	1.0148	1.0146	1.0145	1.0144	1.0143
2.04	1.0145	1.0144	1.0142	1.0141	1.0140	1.0139	1.0138	1.0137	1.0135
2.05	1.0137	1.0136	1.0135	1.0134	1.0133	1.0132	1.0131	1.0129	1.0128
2.06	1.0130	1.0129	1.0128	1.0127	1.0126	1.0125	1.0123	1.0122	1.0121
2.07	1.0123	1.0122	1.0121	1.0120	1.0119	1.0117	1.0116	1.0115	1.0113
2.08	1.0116	1.0115	1.0114	1.0112	1.0111	1.0110	1.0109	1.0107	1.0106
2.09	1.0109	1.0108	1.0106	1.0105	1.0104	1.0103	1.0101	1.0100	1.0099
2.10	1.0102	1.0100	1.0099	1.0098	1.0097	1.0095	1.0094	1.0093	1.0092
2.11	1.0097	1.0096	1.0095	1.0093	1.0092	1.0091	1.0090	1.0089	1.0088
2.12	1.0092	1.0091	1.0090	1.0089	1.0088	1.0087	1.0086	1.0085	1.0084
2.13	1.0088	1.0087	1.0085	1.0084	1.0083	1.0082	1.0082	1.0081	1.0080
2.14	1.0083	1.0082	1.0081	1.0080	1.0079	1.0078	1.0077	1.0077	1.0076
2.15	1.0078	1.0077	1.0076	1.0075	1.0074	1.0074	1.0073	1.0073	1.0073
2.16	1.0074	1.0073	1.0072	1.0071	1.0070	1.0069	1.0069	1.0069	1.0069
2.17	1.0069	1.0068	1.0067	1.0066	1.0065	1.0065	1.0065	1.0065	1.0065
2.18	1.0064	1.0063	1.0062	1.0062	1.0061	1.0061	1.0061	1.0061	1.0061
2.19	1.0060	1.0059	1.0058	1.0057	1.0056	1.0056	1.0057	1.0057	1.0057
2.20	1.0055	1.0054	1.0053	1.0052	1.0052	1.0052	1.0053	1.0053	1.0054
2.21	1.0053	1.0052	1.0051	1.0050	1.0049	1.0050	1.0050	1.0051	1.0051

2.22	1.0051	1.0050	1.0049	1.0048	1.0047	1.0048	1.0048	1.0049	1.0049
2.23	1.0048	1.0048	1.0047	1.0046	1.0045	1.0046	1.0046	1.0046	1.0047
2.24	1.0046	1.0045	1.0045	1.0044	1.0043	1.0043	1.0044	1.0044	1.0044
2.25	1.0044	1.0043	1.0042	1.0042	1.0041	1.0041	1.0042	1.0042	1.0042
2.26	1.0042	1.0041	1.0040	1.0040	1.0039	1.0039	1.0039	1.0040	1.0040
2.27	1.0039	1.0039	1.0038	1.0037	1.0037	1.0037	1.0037	1.0037	1.0037
2.28	1.0037	1.0036	1.0036	1.0035	1.0035	1.0035	1.0035	1.0035	1.0035
2.29	1.0035	1.0034	1.0034	1.0033	1.0033	1.0033	1.0033	1.0033	1.0033
2.30	1.0033	1.0032	1.0031	1.0031	1.0030	1.0030	1.0030	1.0031	1.0031
2.31	1.0032	1.0031	1.0031	1.0030	1.0030	1.0030	1.0030	1.0030	1.0030
2.32	1.0031	1.0030	1.0030	1.0030	1.0029	1.0029	1.0029	1.0029	1.0029
2.33	1.0030	1.0030	1.0029	1.0029	1.0029	1.0029	1.0029	1.0029	1.0029
2.34	1.0029	1.0029	1.0029	1.0029	1.0028	1.0028	1.0028	1.0028	1.0028
2.35	1.0028	1.0028	1.0028	1.0028	1.0028	1.0028	1.0028	1.0028	1.0028
2.36	1.0027	1.0027	1.0027	1.0027	1.0027	1.0027	1.0027	1.0027	1.0027
2.37	1.0026	1.0026	1.0027	1.0027	1.0027	1.0027	1.0027	1.0027	1.0027
2.38	1.0025	1.0026	1.0026	1.0026	1.0027	1.0026	1.0026	1.0026	1.0026
2.39	1.0024	1.0025	1.0025	1.0026	1.0026	1.0026	1.0026	1.0026	1.0026
2.40	1.0024	1.0024	1.0025	1.0025	1.0026	1.0025	1.0025	1.0025	1.0025

C3 C-O Bond Distance ↓	**C2 C-O Bond Disance→**								
	2.35	**2.36**	**2.37**	**2.38**	**2.39**	**2.40**	**2.41**	**2.42**	**2.43**
2.00	1.0163	1.0162	1.0161	1.0159	1.0158	1.0157	1.0155	1.0153	1.0152
2.01	1.0156	1.0155	1.0153	1.0152	1.0151	1.0149	1.0148	1.0146	1.0145
2.02	1.0149	1.0147	1.0146	1.0145	1.0143	1.0142	1.0141	1.0139	1.0137
2.03	1.0141	1.0140	1.0139	1.0137	1.0136	1.0135	1.0133	1.0132	1.0130
2.04	1.0134	1.0133	1.0131	1.0130	1.0129	1.0128	1.0126	1.0125	1.0123
2.05	1.0127	1.0125	1.0124	1.0123	1.0122	1.0120	1.0119	1.0118	1.0116
2.06	1.0119	1.0118	1.0117	1.0116	1.0114	1.0113	1.0112	1.0110	1.0109
2.07	1.0112	1.0111	1.0110	1.0108	1.0107	1.0106	1.0104	1.0103	1.0102
2.08	1.0105	1.0104	1.0102	1.0101	1.0100	1.0098	1.0097	1.0096	1.0095
2.09	1.0098	1.0096	1.0095	1.0094	1.0092	1.0091	1.0090	1.0089	1.0088
2.10	1.0090	1.0089	1.0088	1.0086	1.0085	1.0084	1.0083	1.0082	1.0081
2.11	1.0087	1.0086	1.0084	1.0083	1.0082	1.0081	1.0080	1.0079	1.0078
2.12	1.0083	1.0082	1.0081	1.0080	1.0079	1.0078	1.0077	1.0076	1.0075
2.13	1.0079	1.0079	1.0078	1.0077	1.0076	1.0076	1.0075	1.0073	1.0072
2.14	1.0076	1.0075	1.0075	1.0074	1.0073	1.0073	1.0072	1.0071	1.0070
2.15	1.0072	1.0072	1.0071	1.0071	1.0071	1.0070	1.0069	1.0068	1.0067
2.16	1.0069	1.0068	1.0068	1.0068	1.0068	1.0067	1.0066	1.0065	1.0064
2.17	1.0065	1.0065	1.0065	1.0065	1.0065	1.0065	1.0064	1.0062	1.0061
2.18	1.0061	1.0061	1.0062	1.0062	1.0062	1.0062	1.0061	1.0060	1.0059
2.19	1.0058	1.0058	1.0058	1.0059	1.0059	1.0059	1.0058	1.0057	1.0056
2.20	1.0054	1.0055	1.0055	1.0056	1.0056	1.0057	1.0055	1.0054	1.0053
2.21	1.0052	1.0052	1.0053	1.0053	1.0053	1.0054	1.0053	1.0052	1.0051
2.22	1.0049	1.0050	1.0050	1.0051	1.0051	1.0051	1.0050	1.0050	1.0049
2.23	1.0047	1.0047	1.0048	1.0048	1.0048	1.0049	1.0048	1.0047	1.0046
2.24	1.0045	1.0045	1.0045	1.0046	1.0046	1.0046	1.0046	1.0045	1.0044
2.25	1.0042	1.0043	1.0043	1.0043	1.0043	1.0044	1.0043	1.0043	1.0042
2.26	1.0040	1.0040	1.0040	1.0041	1.0041	1.0041	1.0041	1.0040	1.0040
2.27	1.0038	1.0038	1.0038	1.0038	1.0038	1.0039	1.0038	1.0038	1.0038
2.28	1.0035	1.0035	1.0036	1.0036	1.0036	1.0036	1.0036	1.0036	1.0036
2.29	1.0033	1.0033	1.0033	1.0033	1.0033	1.0033	1.0033	1.0033	1.0033
2.30	1.0031	1.0031	1.0031	1.0031	1.0031	1.0031	1.0031	1.0031	1.0031
2.31	1.0030	1.0030	1.0030	1.0030	1.0030	1.0030			
2.32	1.0029	1.0029	1.0029	1.0029	1.0029	1.0029			
2.33	1.0029	1.0029	1.0029	1.0029	1.0029	1.0029			
2.34	1.0028	1.0028	1.0028	1.0028	1.0028	1.0028			

2.35	1.0028	1.0028	1.0028	1.0028	1.0027	1.0027
2.36	1.0027	1.0027	1.0027	1.0027	1.0027	1.0027
2.37	1.0027	1.0026	1.0026	1.0026	1.0026	1.0026
2.38	1.0026	1.0026	1.0026	1.0026	1.0026	1.0025
2.39	1.0025	1.0025	1.0025	1.0025	1.0025	1.0025
2.40	1.0025	1.0025	1.0025	1.0024	1.0024	1.0024

C3 C-O Bond Distance ↓	**C2 C-O Bond Disance→**						
	2.44	**2.45**	**2.46**	**2.47**	**2.48**	**2.49**	**2.50**
2.00	1.0150	1.0148	1.0147	1.0145	1.0143	1.0142	1.0140
2.01	1.0143	1.0141	1.0140	1.0138	1.0137	1.0135	1.0133
2.02	1.0136	1.0134	1.0133	1.0131	1.0130	1.0128	1.0127
2.03	1.0129	1.0127	1.0126	1.0125	1.0123	1.0122	1.0120
2.04	1.0122	1.0120	1.0119	1.0118	1.0116	1.0115	1.0113
2.05	1.0115	1.0114	1.0112	1.0111	1.0109	1.0108	1.0107
2.06	1.0108	1.0107	1.0105	1.0104	1.0103	1.0101	1.0100
2.07	1.0101	1.0100	1.0098	1.0097	1.0096	1.0095	1.0093
2.08	1.0094	1.0093	1.0091	1.0090	1.0089	1.0088	1.0087
2.09	1.0087	1.0086	1.0085	1.0083	1.0082	1.0081	1.0080
2.10	1.0080	1.0079	1.0078	1.0077	1.0076	1.0075	1.0074
2.11	1.0077	1.0076	1.0075	1.0074	1.0073	1.0072	1.0071
2.12	1.0074	1.0073	1.0072	1.0071	1.0070	1.0069	1.0068
2.13	1.0071	1.0070	1.0069	1.0068	1.0067	1.0066	1.0065
2.14	1.0069	1.0067	1.0066	1.0065	1.0064	1.0063	1.0062
2.15	1.0066	1.0065	1.0064	1.0062	1.0061	1.0060	1.0059
2.16	1.0063	1.0062	1.0061	1.0060	1.0058	1.0057	1.0056
2.17	1.0060	1.0059	1.0058	1.0057	1.0056	1.0055	1.0053
2.18	1.0057	1.0056	1.0055	1.0054	1.0053	1.0052	1.0050
2.19	1.0055	1.0053	1.0052	1.0051	1.0050	1.0049	1.0048
2.20	1.0052	1.0051	1.0049	1.0048	1.0047	1.0046	1.0045
2.21	1.0050	1.0049	1.0048	1.0047	1.0046	1.0045	1.0044
2.22	1.0048	1.0047	1.0046	1.0045	1.0044	1.0043	1.0042
2.23	1.0046	1.0045	1.0044	1.0043	1.0043	1.0042	1.0041
2.24	1.0044	1.0043	1.0042	1.0042	1.0041	1.0040	1.0040
2.25	1.0042	1.0041	1.0041	1.0040	1.0040	1.0039	1.0039
2.26	1.0040	1.0039	1.0039	1.0038	1.0038	1.0038	1.0037
2.27	1.0038	1.0037	1.0037	1.0037	1.0037	1.0036	1.0036
2.28	1.0036	1.0035	1.0035	1.0035	1.0035	1.0035	1.0035
2.29	1.0033	1.0034	1.0034	1.0034	1.0034	1.0034	1.0034
2.30	1.0031	1.0032	1.0032	1.0032	1.0032	1.0032	1.0032

Predicted KIE at C2

C3 C-O Bond Distance ↓	**C2 C-O Bond Disance→**								
	1.90	**1.91**	**1.92**	**1.93**	**1.94**	**1.95**	**1.96**	**1.97**	**1.98**
1.90	**1.0216**	1.0212	1.0209	1.0205	1.0202	1.0199	1.0195	1.0192	1.0188
1.91	1.0217	1.0213	1.0210	1.0206	1.0203	1.0199	1.0195	1.0192	1.0188
1.92	1.0218	1.0214	1.0211	1.0207	1.0203	1.0199	1.0195	1.0192	1.0188
1.93	1.0220	1.0216	1.0212	1.0208	1.0204	1.0200	1.0196	1.0192	1.0188
1.94	1.0221	1.0217	1.0212	1.0208	1.0204	1.0200	1.0196	1.0191	1.0187
1.95	1.0222	1.0218	1.0213	1.0209	1.0205	1.0200	1.0196	1.0191	1.0187
1.96	1.0223	1.0219	1.0214	1.0210	1.0205	1.0200	1.0196	1.0191	1.0187
1.97	1.0225	1.0220	1.0215	1.0210	1.0206	1.0201	1.0196	1.0191	1.0187
1.98	1.0226	1.0221	1.0216	1.0211	1.0206	1.0201	1.0196	1.0191	1.0186

1.99	1.0227	1.0222	1.0217	1.0212	1.0207	1.0201	1.0196	1.0191	1.0186
2.00	1.0228	1.0223	1.0218	1.0212	1.0207	1.0202	1.0196	1.0191	1.0186
2.01	1.0229	1.0224	1.0218	1.0213	1.0207	1.0202	1.0196	1.0191	1.0185
2.02	1.0230	1.0224	1.0219	1.0213	1.0208	1.0202	1.0196	1.0191	1.0185
2.03	1.0231	1.0225	1.0219	1.0214	1.0208	1.0202	1.0196	1.0191	1.0185
2.04	1.0232	1.0226	1.0220	1.0214	1.0208	1.0202	1.0196	1.0191	1.0185
2.05	1.0233	1.0227	1.0221	1.0215	1.0209	1.0202	1.0196	1.0190	1.0184
2.06	1.0234	1.0227	1.0221	1.0215	1.0209	1.0203	1.0196	1.0190	1.0184
2.07	1.0234	1.0228	1.0222	1.0215	1.0209	1.0203	1.0196	1.0190	1.0184
2.08	1.0235	1.0229	1.0222	1.0216	1.0209	1.0203	1.0196	1.0190	1.0184
2.09	1.0236	1.0230	1.0223	1.0216	1.0210	1.0203	1.0196	1.0190	1.0183
2.10	1.0237	1.0230	1.0224	1.0217	1.0210	1.0203	1.0196	1.0190	1.0183
2.11	1.0238	1.0231	1.0224	1.0217	1.0210	1.0203	1.0196	1.0190	1.0183
2.12	1.0238	1.0231	1.0224	1.0217	1.0210	1.0203	1.0196	1.0189	1.0182
2.13	1.0239	1.0232	1.0225	1.0218	1.0211	1.0204	1.0196	1.0189	1.0182
2.14	1.0240	1.0233	1.0225	1.0218	1.0211	1.0204	1.0196	1.0189	1.0182
2.15	1.0241	1.0233	1.0226	1.0218	1.0211	1.0204	1.0196	1.0189	1.0182
2.16	1.0241	1.0234	1.0226	1.0219	1.0211	1.0204	1.0196	1.0189	1.0181
2.17	1.0242	1.0234	1.0227	1.0219	1.0211	1.0204	1.0196	1.0189	1.0181
2.18	1.0243	1.0235	1.0227	1.0219	1.0212	1.0204	1.0196	1.0188	1.0181
2.19	1.0243	1.0235	1.0228	1.0220	1.0212	1.0204	1.0196	1.0188	1.0180
2.20	1.0244	1.0236	1.0228	1.0220	1.0212	1.0204	1.0196	1.0188	1.0180
2.21	1.0245	1.0237	1.0228	1.0220	1.0212	1.0204	1.0196	1.0188	1.0180
2.22	1.0245	1.0237	1.0229	1.0221	1.0212	1.0204	1.0196	1.0188	1.0180
2.23	1.0246	1.0238	1.0229	1.0221	1.0213	1.0204	1.0196	1.0188	1.0179
2.24	1.0247	1.0238	1.0230	1.0221	1.0213	1.0204	1.0196	1.0187	1.0179
2.25	1.0247	1.0239	1.0230	1.0221	1.0213	1.0204	1.0196	1.0187	1.0179
2.26	1.0248	1.0239	1.0230	1.0222	1.0213	1.0204	1.0196	1.0187	1.0178
2.27	1.0248	1.0240	1.0231	1.0222	1.0213	1.0204	1.0196	1.0187	1.0178
2.28	1.0249	1.0240	1.0231	1.0222	1.0213	1.0204	1.0196	1.0187	1.0178
2.29	1.0250	1.0241	1.0232	1.0223	1.0214	1.0204	1.0195	1.0186	1.0177
2.30	1.0250	1.0241	1.0232	1.0223	1.0214	1.0205	1.0195	1.0186	1.0177

C3 C-O Bond Distance ↓	**C2 C-O Bond Disance→**								
	1.99	**2.00**	**2.01**	**2.02**	**2.03**	**2.04**	**2.05**	**2.06**	**2.07**
1.90	1.0185	1.0182	1.0177	1.0173	1.0168	1.0164	1.0159	1.0155	1.0150
1.91	1.0184	1.0181	1.0176	1.0172	1.0167	1.0163	1.0158	1.0154	1.0149
1.92	1.0184	1.0180	1.0176	1.0171	1.0166	1.0162	1.0157	1.0152	1.0148
1.93	1.0184	1.0180	1.0175	1.0170	1.0165	1.0161	1.0156	1.0151	1.0147
1.94	1.0183	1.0179	1.0174	1.0169	1.0165	1.0160	1.0155	1.0150	1.0145
1.95	1.0183	1.0178	1.0173	1.0168	1.0164	1.0159	1.0154	1.0149	1.0144
1.96	1.0182	1.0178	1.0173	1.0168	1.0163	1.0158	1.0153	1.0148	1.0143
1.97	1.0182	1.0177	1.0172	1.0167	1.0162	1.0157	1.0152	1.0147	1.0141
1.98	1.0181	1.0176	1.0171	1.0166	1.0161	1.0156	1.0150	1.0145	1.0140
1.99	1.0181	1.0176	1.0170	1.0165	1.0160	1.0155	1.0149	1.0144	1.0139
2.00	1.0180	1.0175	1.0170	1.0164	1.0159	1.0154	1.0148	1.0143	1.0138
2.01	1.0180	1.0174	1.0169	1.0164	1.0158	1.0153	1.0147	1.0142	1.0136
2.02	1.0180	1.0174	1.0168	1.0163	1.0157	1.0152	1.0146	1.0141	1.0135
2.03	1.0179	1.0173	1.0168	1.0162	1.0157	1.0151	1.0145	1.0140	1.0134
2.04	1.0179	1.0173	1.0167	1.0161	1.0156	1.0150	1.0144	1.0139	1.0133
2.05	1.0178	1.0172	1.0166	1.0161	1.0155	1.0149	1.0143	1.0138	1.0132
2.06	1.0178	1.0172	1.0166	1.0160	1.0154	1.0148	1.0142	1.0137	1.0131
2.07	1.0177	1.0171	1.0165	1.0159	1.0153	1.0147	1.0142	1.0136	1.0130
2.08	1.0177	1.0171	1.0165	1.0159	1.0153	1.0147	1.0141	1.0135	1.0129
2.09	1.0177	1.0170	1.0164	1.0158	1.0152	1.0146	1.0140	1.0133	1.0127
2.10	1.0176	1.0169	1.0163	1.0157	1.0151	1.0145	1.0139	1.0132	1.0126
2.11	1.0176	1.0169	1.0163	1.0156	1.0150	1.0144	1.0138	1.0131	1.0125
2.12	1.0175	1.0168	1.0162	1.0156	1.0149	1.0143	1.0137	1.0130	1.0124
2.13	1.0175	1.0168	1.0161	1.0155	1.0149	1.0142	1.0136	1.0129	1.0123

2.14	1.0175	1.0167	1.0161	1.0154	1.0148	1.0141	1.0135	1.0128	1.0122
2.15	1.0174	1.0167	1.0160	1.0154	1.0147	1.0141	1.0134	1.0127	1.0121
2.16	1.0174	1.0166	1.0160	1.0153	1.0146	1.0140	1.0133	1.0126	1.0120
2.17	1.0173	1.0166	1.0159	1.0152	1.0146	1.0139	1.0132	1.0125	1.0119
2.18	1.0173	1.0165	1.0158	1.0152	1.0145	1.0138	1.0131	1.0124	1.0118
2.19	1.0173	1.0165	1.0158	1.0151	1.0144	1.0137	1.0130	1.0123	1.0116
2.20	1.0172	1.0164	1.0157	1.0150	1.0143	1.0136	1.0129	1.0122	1.0115
2.21	1.0172	1.0164	1.0157	1.0150	1.0143	1.0135	1.0128	1.0121	1.0114
2.22	1.0171	1.0163	1.0156	1.0149	1.0142	1.0135	1.0128	1.0120	1.0113
2.23	1.0171	1.0163	1.0155	1.0148	1.0141	1.0134	1.0127	1.0120	1.0112
2.24	1.0171	1.0162	1.0155	1.0148	1.0140	1.0133	1.0126	1.0119	1.0111
2.25	1.0170	1.0162	1.0154	1.0147	1.0140	1.0132	1.0125	1.0118	1.0110
2.26	1.0170	1.0161	1.0154	1.0146	1.0139	1.0131	1.0124	1.0117	1.0109
2.27	1.0169	1.0160	1.0153	1.0146	1.0138	1.0131	1.0123	1.0116	1.0108
2.28	1.0169	1.0160	1.0152	1.0145	1.0137	1.0130	1.0122	1.0115	1.0107
2.29	1.0168	1.0159	1.0152	1.0144	1.0137	1.0129	1.0121	1.0114	1.0106
2.30	1.0168	1.0159	1.0151	1.0144	1.0136	1.0128	1.0121	1.0113	1.0105
2.31		1.0158	1.0150	1.0142	1.0135	1.0127	1.0119	1.0112	1.0104
2.32		1.0157	1.0149	1.0141	1.0134	1.0126	1.0118	1.0111	1.0103
2.33		1.0155	1.0148	1.0140	1.0132	1.0125	1.0117	1.0109	1.0102
2.34		1.0154	1.0147	1.0139	1.0131	1.0124	1.0116	1.0108	1.0101
2.35		1.0153	1.0146	1.0138	1.0130	1.0123	1.0115	1.0107	1.0100
2.36		1.0152	1.0144	1.0137	1.0129	1.0121	1.0114	1.0106	1.0098
2.37		1.0151	1.0143	1.0136	1.0128	1.0120	1.0113	1.0105	1.0097
2.38		1.0150	1.0142	1.0134	1.0127	1.0119	1.0111	1.0104	1.0096
2.39		1.0149	1.0141	1.0133	1.0126	1.0118	1.0110	1.0103	1.0095
2.40		1.0147	1.0140	1.0132	1.0125	1.0117	1.0109	1.0102	1.0094

C3 C-O Bond Distance ↓	**C2 C-O Bond Disance→**								
	2.08	**2.09**	**2.10**	**2.11**	**2.12**	**2.13**	**2.14**	**2.15**	**2.16**
1.90	1.0146	1.0142	1.0137	1.0134	1.0130	1.0127	1.0124	1.0121	1.0117
1.91	1.0145	1.0140	1.0136	1.0132	1.0129	1.0125	1.0122	1.0119	1.0115
1.92	1.0143	1.0139	1.0134	1.0131	1.0127	1.0124	1.0120	1.0117	1.0114
1.93	1.0142	1.0137	1.0132	1.0129	1.0126	1.0122	1.0119	1.0115	1.0112
1.94	1.0140	1.0136	1.0131	1.0127	1.0124	1.0120	1.0117	1.0113	1.0110
1.95	1.0139	1.0134	1.0129	1.0126	1.0122	1.0119	1.0115	1.0112	1.0108
1.96	1.0138	1.0133	1.0128	1.0124	1.0121	1.0117	1.0113	1.0110	1.0106
1.97	1.0136	1.0131	1.0126	1.0123	1.0119	1.0115	1.0112	1.0108	1.0104
1.98	1.0135	1.0130	1.0125	1.0121	1.0117	1.0114	1.0110	1.0106	1.0102
1.99	1.0134	1.0128	1.0123	1.0119	1.0116	1.0112	1.0108	1.0104	1.0101
2.00	1.0132	1.0127	1.0122	1.0118	1.0114	1.0110	1.0106	1.0103	1.0099
2.01	1.0131	1.0126	1.0120	1.0116	1.0112	1.0109	1.0105	1.0101	1.0097
2.02	1.0130	1.0124	1.0119	1.0115	1.0111	1.0107	1.0103	1.0099	1.0095
2.03	1.0129	1.0123	1.0117	1.0113	1.0109	1.0105	1.0102	1.0098	1.0094
2.04	1.0127	1.0122	1.0116	1.0112	1.0108	1.0104	1.0100	1.0096	1.0092
2.05	1.0126	1.0120	1.0115	1.0111	1.0106	1.0102	1.0098	1.0094	1.0090
2.06	1.0125	1.0119	1.0113	1.0109	1.0105	1.0101	1.0097	1.0093	1.0088
2.07	1.0124	1.0118	1.0112	1.0108	1.0104	1.0099	1.0095	1.0091	1.0087
2.08	1.0123	1.0117	1.0111	1.0106	1.0102	1.0098	1.0094	1.0089	1.0085
2.09	1.0121	1.0115	1.0109	1.0105	1.0101	1.0096	1.0092	1.0088	1.0083
2.10	1.0120	1.0114	1.0108	1.0103	1.0099	1.0095	1.0090	1.0086	1.0082
2.11	1.0119	1.0113	1.0106	1.0102	1.0098	1.0093	1.0089	1.0084	1.0080
2.12	1.0118	1.0111	1.0105	1.0101	1.0096	1.0092	1.0087	1.0083	1.0079
2.13	1.0117	1.0110	1.0104	1.0099	1.0095	1.0090	1.0086	1.0081	1.0077
2.14	1.0115	1.0109	1.0102	1.0098	1.0093	1.0089	1.0084	1.0080	1.0075
2.15	1.0114	1.0108	1.0101	1.0097	1.0092	1.0088	1.0083	1.0079	1.0074
2.16	1.0113	1.0106	1.0100	1.0095	1.0091	1.0086	1.0082	1.0077	1.0072
2.17	1.0112	1.0105	1.0098	1.0094	1.0089	1.0085	1.0080	1.0076	1.0071
2.18	1.0111	1.0104	1.0097	1.0092	1.0088	1.0083	1.0079	1.0074	1.0069

2.19	1.0110	1.0103	1.0096	1.0091	1.0086	1.0082	1.0077	1.0073	1.0068
2.20	1.0108	1.0101	1.0094	1.0090	1.0085	1.0080	1.0076	1.0071	1.0066
2.21	1.0107	1.0100	1.0093	1.0089	1.0084	1.0079	1.0075	1.0070	1.0065
2.22	1.0106	1.0099	1.0092	1.0087	1.0083	1.0078	1.0074	1.0069	1.0064
2.23	1.0105	1.0098	1.0091	1.0086	1.0082	1.0077	1.0073	1.0068	1.0063
2.24	1.0104	1.0097	1.0090	1.0085	1.0081	1.0076	1.0071	1.0067	1.0062
2.25	1.0103	1.0096	1.0088	1.0084	1.0079	1.0075	1.0070	1.0066	1.0061
2.26	1.0102	1.0095	1.0087	1.0083	1.0078	1.0074	1.0069	1.0065	1.0060
2.27	1.0101	1.0093	1.0086	1.0082	1.0077	1.0073	1.0068	1.0064	1.0059
2.28	1.0100	1.0092	1.0085	1.0080	1.0076	1.0072	1.0067	1.0063	1.0058
2.29	1.0099	1.0091	1.0083	1.0079	1.0075	1.0070	1.0066	1.0062	1.0058
2.30	1.0098	1.0090	1.0082	1.0078	1.0074	1.0069	1.0065	1.0061	1.0057
2.31	1.0096	1.0089	1.0081	1.0077	1.0073	1.0069	1.0065	1.0061	1.0057
2.32	1.0095	1.0088	1.0080	1.0076	1.0072	1.0068	1.0064	1.0060	1.0057
2.33	1.0094	1.0087	1.0079	1.0075	1.0071	1.0068	1.0064	1.0060	1.0057
2.34	1.0093	1.0085	1.0078	1.0074	1.0071	1.0067	1.0064	1.0060	1.0057
2.35	1.0092	1.0084	1.0077	1.0073	1.0070	1.0067	1.0063	1.0060	1.0057
2.36	1.0091	1.0083	1.0075	1.0072	1.0069	1.0066	1.0063	1.0060	1.0057
2.37	1.0090	1.0082	1.0074	1.0071	1.0068	1.0066	1.0063	1.0060	1.0057
2.38	1.0089	1.0081	1.0073	1.0070	1.0068	1.0065	1.0062	1.0059	1.0057
2.39	1.0087	1.0080	1.0072	1.0070	1.0067	1.0064	1.0062	1.0059	1.0057
2.40	1.0086	1.0079	1.0071	1.0069	1.0066	1.0064	1.0061	1.0059	1.0057

C2 C-O Bond Disance→

C3 C-O Bond Distance ↓

	2.17	**2.18**	**2.19**	**2.20**	**2.21**	**2.22**	**2.23**	**2.24**	**2.25**
1.90	1.0114	1.0111	1.0107	1.0104	1.0102	1.0100	1.0097	1.0095	1.0093
1.91	1.0112	1.0109	1.0105	1.0102	1.0100	1.0097	1.0095	1.0093	1.0091
1.92	1.0110	1.0107	1.0103	1.0100	1.0098	1.0095	1.0093	1.0091	1.0088
1.93	1.0108	1.0105	1.0101	1.0098	1.0096	1.0093	1.0091	1.0088	1.0086
1.94	1.0106	1.0103	1.0099	1.0096	1.0093	1.0091	1.0089	1.0086	1.0084
1.95	1.0104	1.0101	1.0097	1.0094	1.0091	1.0089	1.0086	1.0084	1.0082
1.96	1.0103	1.0099	1.0095	1.0092	1.0089	1.0087	1.0084	1.0082	1.0079
1.97	1.0101	1.0097	1.0093	1.0090	1.0087	1.0085	1.0082	1.0080	1.0077
1.98	1.0099	1.0095	1.0091	1.0088	1.0085	1.0083	1.0080	1.0077	1.0075
1.99	1.0097	1.0093	1.0089	1.0086	1.0083	1.0080	1.0078	1.0075	1.0073
2.00	1.0095	1.0091	1.0087	**1.0084**	1.0081	1.0078	1.0076	1.0073	1.0070
2.01	1.0093	1.0089	1.0085	1.0082	1.0079	1.0076	1.0074	1.0071	1.0069
2.02	1.0091	1.0087	1.0084	1.0080	1.0077	1.0074	1.0072	1.0069	1.0067
2.03	1.0090	1.0086	1.0082	1.0078	1.0075	1.0073	1.0070	1.0067	1.0065
2.04	1.0088	1.0084	1.0080	1.0076	1.0073	1.0071	1.0068	1.0065	1.0063
2.05	1.0086	1.0082	1.0078	1.0074	1.0071	1.0069	1.0066	1.0064	1.0061
2.06	1.0084	1.0080	1.0076	1.0072	1.0069	1.0067	1.0064	1.0062	1.0059
2.07	1.0083	1.0078	1.0074	1.0070	1.0067	1.0065	1.0062	1.0060	1.0057
2.08	1.0081	1.0076	1.0072	1.0068	1.0065	1.0063	1.0060	1.0058	1.0055
2.09	1.0079	1.0075	1.0070	1.0066	1.0064	1.0061	1.0059	1.0056	1.0054
2.10	1.0077	1.0073	1.0068	1.0064	1.0062	1.0059	1.0057	1.0054	1.0052
2.11	1.0076	1.0071	1.0067	1.0062	1.0060	1.0057	1.0055	1.0053	1.0050
2.12	1.0074	1.0070	1.0065	1.0061	1.0058	1.0056	1.0053	1.0051	1.0048
2.13	1.0073	1.0068	1.0064	1.0059	1.0057	1.0054	1.0052	1.0049	1.0047
2.14	1.0071	1.0067	1.0062	1.0058	1.0055	1.0053	1.0050	1.0048	1.0045
2.15	1.0069	1.0065	1.0060	1.0056	1.0053	1.0051	1.0049	1.0046	1.0044
2.16	1.0068	1.0063	1.0059	1.0054	1.0052	1.0049	1.0047	1.0044	1.0042
2.17	1.0066	1.0062	1.0057	1.0053	1.0050	1.0048	1.0045	1.0043	1.0040
2.18	1.0065	1.0060	1.0056	1.0051	1.0049	1.0046	1.0044	1.0041	1.0039
2.19	1.0063	1.0059	1.0054	1.0049	1.0047	1.0044	1.0042	1.0040	1.0037
2.20	1.0062	1.0057	1.0052	1.0048	1.0045	1.0043	1.0040	1.0038	1.0035
2.21	1.0061	1.0056	1.0052	1.0047	1.0045	1.0042	1.0040	1.0038	1.0035
2.22	1.0060	1.0055	1.0051	1.0046	1.0044	1.0042	1.0040	1.0038	1.0035
2.23	1.0059	1.0054	1.0050	1.0045	1.0043	1.0041	1.0039	1.0037	1.0035
2.24	1.0058	1.0053	1.0049	1.0044	1.0043	1.0041	1.0039	1.0037	1.0035

2.25	1.0057	1.0053	1.0048	1.0044	1.0042	1.0040	1.0039	1.0037	1.0035
2.26	1.0056	1.0052	1.0047	1.0043	1.0041	1.0040	1.0038	1.0037	1.0035
2.27	1.0055	1.0051	1.0046	1.0042	1.0041	1.0039	1.0038	1.0037	1.0035
2.28	1.0054	1.0050	1.0045	1.0041	1.0040	1.0039	1.0038	1.0036	1.0035
2.29	1.0053	1.0049	1.0045	1.0040	1.0039	1.0038	1.0037	1.0036	1.0035
2.30	1.0052	1.0048	1.0044	1.0039	1.0039	1.0038	1.0037	1.0036	1.0035
2.31	1.0052	1.0048	1.0044	1.0040	1.0039	1.0038	1.0037	1.0036	1.0036
2.32	1.0053	1.0049	1.0045	1.0041	1.0040	1.0039	1.0038	1.0037	1.0036
2.33	1.0053	1.0049	1.0045	1.0042	1.0041	1.0039	1.0038	1.0037	1.0036
2.34	1.0053	1.0050	1.0046	1.0042	1.0041	1.0040	1.0039	1.0037	1.0036
2.35	1.0053	1.0050	1.0047	1.0043	1.0042	1.0041	1.0039	1.0038	1.0036
2.36	1.0053	1.0050	1.0047	1.0044	1.0043	1.0041	1.0040	1.0038	1.0037
2.37	1.0054	1.0051	1.0048	1.0045	1.0043	1.0042	1.0040	1.0038	1.0037
2.38	1.0054	1.0051	1.0048	1.0046	1.0044	1.0042	1.0040	1.0039	1.0037
2.39	1.0054	1.0052	1.0049	1.0046	1.0045	1.0043	1.0041	1.0039	1.0037
2.40	1.0054	1.0052	1.0050	1.0047	1.0045	1.0043	1.0041	1.0039	1.0037

C3 C-O Bond Distance ↓	**C2 C-O Bond Disance→** **2.26**	**2.27**	**2.28**	**2.29**	**2.30**	**2.31**	**2.32**	**2.33**	**2.34**
1.90	1.0091	1.0088	1.0086	1.0084	1.0082				
1.91	1.0088	1.0086	1.0084	1.0081	1.0079				
1.92	1.0086	1.0084	1.0081	1.0079	1.0077				
1.93	1.0084	1.0081	1.0079	1.0077	1.0074				
1.94	1.0081	1.0079	1.0077	1.0074	1.0072				
1.95	1.0079	1.0077	1.0074	1.0072	1.0069				
1.96	1.0077	1.0074	1.0072	1.0069	1.0067				
1.97	1.0075	1.0072	1.0070	1.0067	1.0065				
1.98	1.0072	1.0070	1.0067	1.0065	1.0062				
1.99	1.0070	1.0067	1.0065	1.0062	1.0060				
2.00	1.0068	1.0065	1.0062	1.0060	1.0057	1.0056	1.0054	1.0053	1.0051
2.01	1.0066	1.0063	1.0061	1.0058	1.0055	1.0054	1.0052	1.0051	1.0049
2.02	1.0064	1.0061	1.0059	1.0056	1.0054	1.0052	1.0051	1.0049	1.0048
2.03	1.0062	1.0060	1.0057	1.0054	1.0052	1.0050	1.0049	1.0047	1.0046
2.04	1.0060	1.0058	1.0055	1.0053	1.0050	1.0049	1.0047	1.0045	1.0044
2.05	1.0059	1.0056	1.0053	1.0051	1.0048	1.0047	1.0045	1.0044	1.0042
2.06	1.0057	1.0054	1.0052	1.0049	1.0047	1.0045	1.0043	1.0042	1.0040
2.07	1.0055	1.0052	1.0050	1.0047	1.0045	1.0043	1.0042	1.0040	1.0038
2.08	1.0053	1.0050	1.0048	1.0045	1.0043	1.0041	1.0040	1.0038	1.0037
2.09	1.0051	1.0049	1.0046	1.0044	1.0041	1.0040	1.0038	1.0036	1.0035
2.10	1.0049	1.0047	1.0044	1.0042	1.0039	1.0038	1.0036	1.0035	1.0033
2.11	1.0048	1.0045	1.0043	1.0040	1.0038	1.0036	1.0035	1.0033	1.0032
2.12	1.0046	1.0044	1.0041	1.0039	1.0036	1.0035	1.0033	1.0032	1.0031
2.13	1.0044	1.0042	1.0039	1.0037	1.0035	1.0033	1.0032	1.0031	1.0029
2.14	1.0043	1.0040	1.0038	1.0035	1.0033	1.0032	1.0031	1.0029	1.0028
2.15	1.0041	1.0039	1.0036	1.0034	1.0031	1.0030	1.0029	1.0028	1.0027
2.16	1.0040	1.0037	1.0035	1.0032	1.0030	1.0029	1.0028	1.0027	1.0026
2.17	1.0038	1.0035	1.0033	1.0031	1.0028	1.0027	1.0026	1.0026	1.0025
2.18	1.0036	1.0034	1.0031	1.0029	1.0026	1.0026	1.0025	1.0024	1.0024
2.19	1.0035	1.0032	1.0030	1.0027	1.0025	1.0024	1.0024	1.0023	1.0022
2.20	1.0033	1.0031	1.0028	1.0026	1.0023	1.0023	1.0022	1.0022	1.0021
2.21	1.0033	1.0031	1.0029	1.0026	1.0024	1.0023	1.0023	1.0022	1.0022
2.22	1.0033	1.0031	1.0029	1.0027	1.0025	1.0024	1.0024	1.0023	1.0023
2.23	1.0033	1.0031	1.0030	1.0028	1.0026	1.0025	1.0024	1.0024	1.0023
2.24	1.0034	1.0032	1.0030	1.0028	1.0026	1.0026	1.0025	1.0025	1.0024
2.25	1.0034	1.0032	1.0030	1.0029	1.0027	1.0027	1.0026	1.0025	1.0025
2.26	1.0034	1.0032	1.0031	1.0029	1.0028	1.0027	1.0027	1.0026	1.0025
2.27	1.0034	1.0033	1.0031	1.0030	1.0029	1.0028	1.0027	1.0027	1.0026
2.28	1.0034	1.0033	1.0032	1.0031	1.0030	1.0029	1.0028	1.0027	1.0027
2.29	1.0034	1.0033	1.0032	1.0031	1.0030	1.0030	1.0029	1.0028	1.0027
2.30	1.0035	1.0034	1.0033	1.0032	1.0031	1.0030	1.0030	1.0029	1.0028

2.31	1.0035	1.0034	1.0033	1.0032	1.0031	1.0030	1.0029	1.0029	1.0028
2.32	1.0035	1.0034	1.0033	1.0032	1.0031	1.0030	1.0029	1.0028	1.0028
2.33	1.0035	1.0034	1.0033	1.0031	1.0030	1.0030	1.0029	1.0028	1.0028
2.34	1.0035	1.0034	1.0032	1.0031	1.0030	1.0029	1.0029	1.0028	1.0027
2.35	1.0035	1.0034	1.0032	1.0031	1.0030	1.0029	1.0028	1.0028	1.0027
2.36	1.0035	1.0034	1.0032	1.0031	1.0029	1.0029	1.0028	1.0027	1.0027
2.37	1.0035	1.0034	1.0032	1.0030	1.0029	1.0028	1.0028	1.0027	1.0027
2.38	1.0035	1.0034	1.0032	1.0030	1.0028	1.0028	1.0028	1.0027	1.0027
2.39	1.0035	1.0034	1.0032	1.0030	1.0028	1.0028	1.0027	1.0027	1.0026
2.40	1.0036	1.0034	1.0032	1.0030	1.0028	1.0027	1.0027	1.0027	1.0026

C3 C-O Bond Distance ↓	**C2 C-O Bond Disance→** **2.35**	**2.36**	**2.37**	**2.38**	**2.39**	**2.40**	**2.41**	**2.42**	**2.43**
2.00	1.0050	1.0048	1.0047	1.0045	1.0044	1.0042	1.0042	1.0041	1.0040
2.01	1.0048	1.0046	1.0045	1.0043	1.0042	1.0040	1.0040	1.0039	1.0038
2.02	1.0046	1.0045	1.0043	1.0042	1.0040	1.0039	1.0038	1.0037	1.0037
2.03	1.0044	1.0043	1.0041	1.0040	1.0038	1.0037	1.0036	1.0035	1.0035
2.04	1.0042	1.0041	1.0039	1.0038	1.0036	1.0035	1.0034	1.0034	1.0033
2.05	1.0041	1.0039	1.0037	1.0036	1.0034	1.0033	1.0032	1.0032	1.0031
2.06	1.0039	1.0037	1.0036	1.0034	1.0032	1.0031	1.0030	1.0030	1.0029
2.07	1.0037	1.0035	1.0034	1.0032	1.0031	1.0029	1.0028	1.0028	1.0027
2.08	1.0035	1.0033	1.0032	1.0030	1.0029	1.0027	1.0027	1.0026	1.0026
2.09	1.0033	1.0032	1.0030	1.0028	1.0027	1.0025	1.0025	1.0024	1.0024
2.10	1.0031	1.0030	1.0028	1.0027	1.0025	1.0023	1.0023	1.0022	1.0022
2.11	1.0030	1.0029	1.0027	1.0026	1.0024	1.0023	1.0022	1.0022	1.0022
2.12	1.0029	1.0028	1.0026	1.0025	1.0024	1.0022	1.0022	1.0022	1.0022
2.13	1.0028	1.0027	1.0026	1.0024	1.0023	1.0022	1.0022	1.0022	1.0022
2.14	1.0027	1.0026	1.0025	1.0024	1.0022	1.0021	1.0021	1.0021	1.0021
2.15	1.0026	1.0025	1.0024	1.0023	1.0022	1.0021	1.0021	1.0021	1.0021
2.16	1.0025	1.0024	1.0023	1.0022	1.0021	1.0020	1.0021	1.0021	1.0021
2.17	1.0024	1.0023	1.0022	1.0021	1.0021	1.0020	1.0020	1.0021	1.0021
2.18	1.0023	1.0022	1.0021	1.0021	1.0020	1.0019	1.0020	1.0020	1.0021
2.19	1.0022	1.0021	1.0021	1.0020	1.0019	1.0019	1.0019	1.0020	1.0021
2.20	1.0021	1.0020	1.0020	1.0019	1.0019	1.0018	1.0019	1.0020	1.0021
2.21	1.0021	1.0021	1.0020	1.0020	1.0019	1.0019	1.0020	1.0020	1.0021
2.22	1.0022	1.0021	1.0021	1.0020	1.0020	1.0019	1.0020	1.0021	1.0021
2.23	1.0023	1.0022	1.0022	1.0021	1.0020	1.0020	1.0020	1.0021	1.0022
2.24	1.0023	1.0023	1.0022	1.0022	1.0021	1.0020	1.0021	1.0021	1.0022
2.25	1.0024	1.0023	1.0023	1.0022	1.0022	1.0021	1.0021	1.0022	1.0022
2.26	1.0025	1.0024	1.0023	1.0023	1.0022	1.0021	1.0022	1.0022	1.0023
2.27	1.0025	1.0025	1.0024	1.0023	1.0023	1.0022	1.0022	1.0023	1.0023
2.28	1.0026	1.0025	1.0025	1.0024	1.0023	1.0022	1.0023	1.0023	1.0023
2.29	1.0027	1.0026	1.0025	1.0024	1.0024	1.0023	1.0023	1.0023	1.0023
2.30	1.0027	1.0027	1.0026	1.0025	1.0024	1.0023	1.0024	1.0024	1.0024
2.31	1.0027	1.0026	1.0026	1.0025	1.0024	1.0023			
2.32	1.0027	1.0026	1.0026	1.0025	1.0024	1.0023			
2.33	1.0027	1.0026	1.0026	1.0025	1.0024	1.0024			
2.34	1.0027	1.0026	1.0025	1.0025	1.0024	1.0024			
2.35	1.0027	1.0026	1.0025	1.0025	1.0024	1.0024			
2.36	1.0026	1.0026	1.0025	1.0025	1.0024	1.0024			
2.37	1.0026	1.0026	1.0025	1.0025	1.0024	1.0024			
2.38	1.0026	1.0026	1.0025	1.0025	1.0024	1.0024			
2.39	1.0026	1.0025	1.0025	1.0024	1.0024	1.0024			
2.40	1.0026	1.0025	1.0025	1.0024	1.0024	1.0024			

C3 C-O Bond Distance	**C2 C-O Bond Disance→** **2.44**	**2.45**	**2.46**	**2.47**	**2.48**	**2.49**	**2.50**

↓

2.00	1.0040	1.0039	1.0038	1.0037	1.0037	1.0036	1.0035
2.01	1.0038	1.0037	1.0036	1.0036	1.0035	1.0034	1.0034
2.02	1.0036	1.0035	1.0035	1.0034	1.0033	1.0033	1.0032
2.03	1.0034	1.0033	1.0033	1.0032	1.0031	1.0031	1.0030
2.04	1.0032	1.0032	1.0031	1.0030	1.0030	1.0029	1.0029
2.05	1.0030	1.0030	1.0029	1.0029	1.0028	1.0027	1.0027
2.06	1.0029	1.0028	1.0028	1.0027	1.0026	1.0026	1.0025
2.07	1.0027	1.0026	1.0026	1.0025	1.0025	1.0024	1.0024
2.08	1.0025	1.0025	1.0024	1.0023	1.0023	1.0022	1.0022
2.09	1.0023	1.0023	1.0022	1.0022	1.0021	1.0021	1.0020
2.10	1.0021	1.0021	1.0020	1.0020	1.0020	1.0019	1.0019
2.11	1.0021	1.0021	1.0021	1.0020	1.0020	1.0020	1.0019
2.12	1.0021	1.0021	1.0021	1.0021	1.0021	1.0020	1.0020
2.13	1.0021	1.0021	1.0021	1.0021	1.0021	1.0021	1.0021
2.14	1.0021	1.0022	1.0022	1.0022	1.0022	1.0022	1.0022
2.15	1.0021	1.0022	1.0022	1.0022	1.0022	1.0022	1.0023
2.16	1.0021	1.0022	1.0022	1.0022	1.0023	1.0023	1.0023
2.17	1.0022	1.0022	1.0022	1.0023	1.0023	1.0024	1.0024
2.18	1.0022	1.0022	1.0023	1.0023	1.0024	1.0024	1.0025
2.19	1.0022	1.0022	1.0023	1.0024	1.0024	1.0025	1.0026
2.20	1.0022	1.0022	1.0023	1.0024	1.0025	1.0026	1.0026
2.21	1.0022	1.0023	1.0023	1.0024	1.0025	1.0026	1.0026
2.22	1.0022	1.0023	1.0023	1.0024	1.0025	1.0025	1.0026
2.23	1.0022	1.0023	1.0023	1.0024	1.0025	1.0025	1.0026
2.24	1.0022	1.0023	1.0024	1.0024	1.0025	1.0025	1.0026
2.25	1.0023	1.0023	1.0024	1.0024	1.0024	1.0025	1.0025
2.26	1.0023	1.0023	1.0024	1.0024	1.0024	1.0025	1.0025
2.27	1.0023	1.0023	1.0024	1.0024	1.0024	1.0025	1.0025
2.28	1.0023	1.0024	1.0024	1.0024	1.0024	1.0025	1.0025
2.29	1.0024	1.0024	1.0024	1.0024	1.0024	1.0024	1.0025
2.30	1.0024	1.0024	1.0024	1.0024	1.0024	1.0024	1.0024

Geometry Predictions from Non-Stationary Point Grid

GAS	Predicted C-O Bond Distances from Non-Stationary Point Grid		C-O Bond Distance Difference between Stationary and Non-Stationary Point Geometries	
b3lyp/6-31+G**	C3	C2	C3	C2
ts 2	2.04	2.19	-0.01	0.05
ts 3	2.05	2.18	0.03	0.03
ts 4	2.10	2.12	0.01	0.04
ts 5	1.99	2.24	0.01	0.00
ts 6	2.04	2.21	0.01	0.03
ts 7	2.00	2.21	-0.02	0.03
ts 8	2.02	2.20	0.01	-0.01
ts 9	2.05	2.14	-0.02	0.02

PCM	Predicted C-O Bond Distances from Non-Stationary Point Grid		C-O Bond Distance Difference between Stationary and Non-Stationary Point Geometries	
b3lyp/6-31+G**	C3	C2	C3	C2
ts 2	2.10	2.21	0.06	0.13
ts 3	2.09	2.25	0.08	0.09
ts 4	2.12	2.19	0.06	0.13
ts 5	2.09	2.22	0.06	0.10
ts 6	2.10	2.21	0.07	0.12

ts 7	2.11	2.18	0.03	0.13
ts 8	2.09	2.20	0.06	0.12
ts 9	2.11	2.19	0.05	0.11

GAS PHASE TRANS **b3lyp/6-31+G****	Predicted C-O Bond Distances from Non-Stationary Point Grid		C-O Bond Distance Difference between Stationary and Non-Stationary Point Geometries	
ts 3	2.04	2.17	0.02	0.02
ts 5	1.95	2.30	0.01	0.00
ts 7	1.95	2.27	-0.02	0.02
ts 8	2.00	2.20	-0.01	-0.02
ts 9	2.12	2.04	-0.03	0.02

GAS PHASE CIS **b3lyp/6-31+G****	Predicted C-O Bond Distances from Non-Stationary Point Grid		C-O Bond Distance Difference between Stationary and Non-Stationary Point Geometries	
ts 3	1.94	2.30	0.02	0.04
ts 5	2.00	2.19	-0.02	0.02
ts 7	2.23	1.97	-0.07	0.01
ts 8	1.94	2.30	0.02	0.04
ts 9	1.95	2.28	0.00	0.00

PCM TRANS **b3lyp/6-31+G****	Predicted C-O Bond Distances from Non-Stationary Point Grid		C-O Bond Distance Difference between Stationary and Non-Stationary Point Geometries	
ts 3	2.08	2.20	0.05	0.09
ts 5	2.02	2.27	0.06	0.07
ts 7	2.02	2.26	0.03	0.11
ts 8	2.07	2.20	0.04	0.07
ts 9	2.11	2.13	0.03	0.08

PCM CIS **b3lyp/6-31+G****	Predicted C-O Bond Distances from Non-Stationary Point Grid		C-O Bond Distance Difference between Stationary and Non-Stationary Point Geometries	
ts 3	2.00	2.35	0.09	0.03
ts 5	2.06	2.20	0.03	0.09
ts 7	2.21	2.04	0.03	0.06
ts 8	2.00	2.31	0.06	0.07
ts 9	2.01	2.28	0.04	0.13

Experimental NMR Results.

The integrations of the C4 methyl carbon of 2-methyl-2-butene was in each spectrum set to 1000. The average integrations for the other carbons for each reaction are shown in Table A, along with the standard results for starting material that had not been subjected to the reaction conditions. In each case the averages are based on 6 spectra. Table A also shows the relative isotopic enhancements (R/R_0), calculated as the ratio of integrations for the recovered versus standard materials. The standard deviations ($\Delta R/R_0$) were calculated from eq 1, where IntSample is the

average integration for each sample peak (listed in the table), IntStandard is the average integration for the corresponding peak in the standard (listed in the table), and ΔIntSample and ΔIntStandard are the standard deviations in the sample and standard peaks, respectively. From the R/R_0's, $\Delta R/R_0$'s, and uncertainties in the % conversion, the KIEs and errors were calculated as previously described. (Singleton, D. A.; Thomas, A. A. *J. Am. Chem. Soc.* **1995**, *117*, 9357.)

$$\Delta R/R_0 = R/R_0 * ((\Delta \text{IntSample}/\text{IntSample})^2 + (\Delta \text{IntStandard}/\text{IntStandard})^2)^{1/2} \quad (1)$$

Table A. Average ^{13}C Integration and R/Ro's for epoxidation of 2-methyl-2-butene.

	C1	C2	C3	C4	C5
standard	977.62	1047.54	1032.90	1000.00	978.23
exp 1	989.17	1067.17	1033.90	1000.00	977.67
R/R_0	1.012	1.019	1.001	1.000	0.999
$\Delta R/R_0$	0.005	0.004	0.003		0.003
standard	977.62	1047.54	1032.90	1000.00	978.23
exp 2	989.29	1067.62	1032.70	1000.00	978.75
R/R_0	1.012	1.019	1.000	1.000	1.001
$\Delta R/R_0$	0.004	0.002	0.003	0.000	0.003