**SUPPORTING INFORMATION**

# Isotope Effects and the Mechanism of Epoxidation of Cyclohexenone with *tert*-Butylhydroperoxide

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## Theoretical Structures

All structures and energies were obtained using standard procedures in Gaussian 03.[1] All structures described as transition structures or TS have been verified to have one imaginary frequency. All other structures have been verified to have zero imaginary frequencies.

1. Gaussian 03, Revision B.04, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.

### Cyclohexenone – 6-31G* Gas Phase

E(RB+HF-LYP) = -308.666132412

| | |
|---|---|
| Zero-point correction= | 0.127949 (Hartree/Particle) |
| Thermal correction to Energy= | 0.134033 |
| Thermal correction to Enthalpy= | 0.134977 |
| Thermal correction to Gibbs Free Energy= | 0.098046 |
| Sum of electronic and zero-point Energies= | -308.538183 |
| Sum of electronic and thermal Energies= | -308.532099 |
| Sum of electronic and thermal Enthalpies= | -308.531155 |
| Sum of electronic and thermal Free Energies= | -308.568086 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 84.107 | 23.132 | 77.729 |

C,0,0.8708466997,-0.5288422935,-0.5196205762
C,0,1.0124466372,-0.0760027397,0.8829988402
O,0,1.816330977,-0.98870742,-1.1426269112
C,0,-0.0100588159,0.4588958475,1.572071204
H,0,1.9914400115,-0.2230833423,1.3320121427
C,0,-1.3722539208,0.7030131125,0.9789290195
H,0,0.1349273641,0.7340270057,2.6164555651
C,0,-1.3285643516,0.7450560069,-0.5555545179
H,0,-2.0552720062,-0.0927047033,1.3195251711
H,0,-1.7877856292,1.6367312192,1.3792727763
C,0,-0.5290477215,-0.4368434435,-1.1210719416
H,0,-2.3446792725,0.7518687794,-0.9664363125
H,0,-0.8527392544,1.6834186525,-0.8697032776
H,0,-1.0445367031,-1.3814643354,-0.8865215298
H,0,-0.4322134881,-0.3907928565,-2.2101014145

## Cyclohexenone – 6-31+G** Gas Phase

E(RB+HF-LYP) = -308.691053132

| | |
|---|---|
| Zero-point correction= | 0.127172 (Hartree/Particle) |
| Thermal correction to Energy= | 0.133281 |
| Thermal correction to Enthalpy= | 0.134225 |
| Thermal correction to Gibbs Free Energy= | 0.097244 |
| Sum of electronic and zero-point Energies= | -308.563881 |
| Sum of electronic and thermal Energies= | -308.557772 |
| Sum of electronic and thermal Enthalpies= | -308.556828 |
| Sum of electronic and thermal Free Energies= | -308.593809 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 83.635 | 23.290 | 77.833 |

C,0,0.868235807,-0.5298809526,-0.5177522614
C,0,1.01483359,-0.0753609898,0.8830726986
O,0,1.8137084455,-0.9988304991,-1.1407760611
C,0,-0.0095459014,0.4625554365,1.5716809331
H,0,1.9928973867,-0.2223423634,1.3330516872
C,0,-1.3717552965,0.7054866448,0.978909958
H,0,0.1378496644,0.7373224575,2.6154178884
C,0,-1.3301366163,0.7461552904,-0.5557364086
H,0,-2.05173598,-0.0912061497,1.321743631
H,0,-1.7866481758,1.6382948705,1.3800539316
C,0,-0.5268744671,-0.4328232947,-1.1235690551
H,0,-2.3462261653,0.7470191621,-0.96536197
H,0,-0.8598021729,1.686193953,-0.8722191044
H,0,-1.0390770816,-1.3800541646,-0.8947352825
H,0,-0.4254677332,-0.3813765806,-2.2113774799

## Cyclohexenone – 6-31G* - PCM Dichloroethane

E(RB+HF-LYP) = -308.674398820

| | |
|---|---|
| Zero-point correction= | 0.127369 (Hartree/Particle) |
| Thermal correction to Energy= | 0.133454 |
| Thermal correction to Enthalpy= | 0.134399 |
| Thermal correction to Gibbs Free Energy= | 0.097478 |
| Sum of electronic and zero-point Energies= | -308.547029 |
| Sum of electronic and thermal Energies= | -308.540944 |
| Sum of electronic and thermal Enthalpies= | -308.540000 |
| Sum of electronic and thermal Free Energies= | -308.576921 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 83.744 | 23.176 | 77.705 |

C,0,0.8674262741,-0.5267427725,-0.515352085
C,0,1.0143423955,-0.0751723776,0.8804868189
O,0,1.8149965079,-0.9981502295,-1.1412236964
C,0,-0.0109343567,0.459750182,1.5701165811
H,0,1.993227667,-0.2229341358,1.3349265448
C,0,-1.3710374722,0.7051518717,0.977749841
H,0,0.1347903473,0.7319182605,2.6170607355
C,0,-1.3297586335,0.7468403326,-0.5562512253
H,0,-2.0512028124,-0.0922199984,1.32172629
H,0,-1.7847533459,1.6383363885,1.3813420737
C,0,-0.5262692609,-0.4327774122,-1.1211987244
H,0,-2.3460671583,0.7445631686,-0.9663312309
H,0,-0.8589324774,1.687081044,-0.8733930961
H,0,-1.0406595377,-1.3792295771,-0.8878682748

H,0,-0.4289884241,-0.3846122576,-2.2109807083

## Cyclohexenone – 6-31+G** - PCM Dichloroethane

E(RB+HF-LYP) = -308.701464004

| | |
|---|---|
| Zero-point correction= | 0.126464 (Hartree/Particle) |
| Thermal correction to Energy= | 0.132570 |
| Thermal correction to Enthalpy= | 0.133514 |
| Thermal correction to Gibbs Free Energy= | 0.096559 |
| Sum of electronic and zero-point Energies= | -308.575000 |
| Sum of electronic and thermal Energies= | -308.568894 |
| Sum of electronic and thermal Enthalpies= | -308.567950 |
| Sum of electronic and thermal Free Energies= | -308.604905 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 83.189 | 23.331 | 77.780 |

C,0,0.8636677704,-0.5273862026,-0.5121933653
C,0,1.0172569278,-0.0738445916,0.8795792693
O,0,1.8120635641,-1.0117463208,-1.1386250137
C,0,-0.0106786424,0.4640271769,1.56887479
H,0,1.9951351289,-0.221482417,1.3366230651
C,0,-1.3700602963,0.7082240283,0.9774071295
H,0,0.1373911019,0.73490935,2.6160745163
C,0,-1.3315747902,0.7483494988,-0.5565166171
H,0,-2.0464762114,-0.0905589538,1.3248701252
H,0,-1.7831469249,1.6402934119,1.3826349413
C,0,-0.5232632516,-0.4274279256,-1.1238389479
H,0,-2.3479315193,0.7378892127,-0.96507092
H,0,-0.8677405295,1.6908920775,-0.8765341978
H,0,-1.0344005611,-1.3770070801,-0.8970031808
H,0,-0.4214253033,-0.3726169393,-2.2124677904

## t-Butyl Hydroperoxide – 6-31G* Gas Phase

E(RB+HF-LYP) = -308.802154705

| | |
|---|---|
| Zero-point correction= | 0.139541 (Hartree/Particle) |
| Thermal correction to Energy= | 0.147519 |
| Thermal correction to Enthalpy= | 0.148464 |
| Thermal correction to Gibbs Free Energy= | 0.108623 |
| Sum of electronic and zero-point Energies= | -308.662614 |
| Sum of electronic and thermal Energies= | -308.654635 |
| Sum of electronic and thermal Enthalpies= | -308.653691 |
| Sum of electronic and thermal Free Energies= | -308.693531 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 92.570 | 28.888 | 83.851 |

C,0,1.0054098095,-1.4491964527,0.4998789743
C,0,0.3564293,-0.1553038646,-0.0060246468
O,0,-1.0043670839,-0.306092839,0.4710581157
O,0,-1.7769892579,0.8720116109,0.0971905635
C,0,1.0030698891,1.0786874629,0.6315238378
C,0,0.3782940102,-0.0831582328,-1.537132013
H,0,2.065398675,-1.4671591457,0.225613265
H,0,0.9273801776,-1.5172220599,1.5894446744
H,0,0.5186745049,-2.3265737817,0.0616000974
H,0,2.0515090917,1.165730337,0.3244184116
H,0,0.4770576385,1.9879512293,0.3287606124

H,0,0.9653967387,1.0054671145,1.7233615003
H,0,1.4083808716,-0.0401380237,-1.9074661385
H,0,-0.1035445462,-0.9673701836,-1.9702311188
H,0,-0.1453899668,0.8106576841,-1.8887327165
H,0,-2.3732305036,0.4751331774,-0.5622349344

## t-Butyl Hydroperoxide – 6-31+G** Gas Phase

E(RB+HF-LYP) = -308.834681482

| | |
|---|---|
| Zero-point correction= | 0.138618 (Hartree/Particle) |
| Thermal correction to Energy= | 0.146665 |
| Thermal correction to Enthalpy= | 0.147609 |
| Thermal correction to Gibbs Free Energy= | 0.107618 |
| Sum of electronic and zero-point Energies= | -308.696063 |
| Sum of electronic and thermal Energies= | -308.688017 |
| Sum of electronic and thermal Enthalpies= | -308.687073 |
| Sum of electronic and thermal Free Energies= | -308.727064 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 92.033 | 29.133 | 84.168 |

C,0,1.0031369474,-1.4501107255,0.5039101531
C,0,0.3598783529,-0.156265562,-0.0095138901
O,0,-1.0083646011,-0.3080614144,0.4595834763
O,0,-1.7780821509,0.8789136888,0.0933298143
C,0,0.9976739193,1.078846752,0.6349925469
C,0,0.3957718112,-0.0857648768,-1.540090363
H,0,2.0634764978,-1.4655183576,0.2331386343
H,0,0.9217825726,-1.5160980141,1.5926973372
H,0,0.5202878915,-2.327911859,0.0638667853
H,0,2.0501777641,1.1580905818,0.3424851343
H,0,0.4824068559,1.9894518293,0.3197383113
H,0,0.9437815146,1.0099859092,1.7257626
H,0,1.4315530144,-0.0582550816,-1.8944785008
H,0,-0.0921428589,-0.9637501777,-1.9768224775
H,0,-0.1087192716,0.8146792873,-1.9006928959
H,0,-2.4597961487,0.4722741618,-0.464791935

## t-Butyl Hydroperoxide – 6-31G* - PCM Dichloroethane

E(RB+HF-LYP) = -308.811124661

| | |
|---|---|
| Zero-point correction= | 0.138898 (Hartree/Particle) |
| Thermal correction to Energy= | 0.146779 |
| Thermal correction to Enthalpy= | 0.147723 |
| Thermal correction to Gibbs Free Energy= | 0.108084 |
| Sum of electronic and zero-point Energies= | -308.672226 |
| Sum of electronic and thermal Energies= | -308.664346 |
| Sum of electronic and thermal Enthalpies= | -308.663402 |
| Sum of electronic and thermal Free Energies= | -308.703041 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 92.105 | 28.762 | 83.428 |

C,0,1.0063701324,-1.4494773337,0.5001966755
C,0,0.3574599045,-0.1561776424,-0.0071999026
O,0,-1.0077924349,-0.3052290424,0.4675710025
O,0,-1.7816926358,0.8741080714,0.0982604124
C,0,1.0044948474,1.076586917,0.6322109616
C,0,0.3854357501,-0.0830082086,-1.5369375116

```
H,0,2.0641474703,-1.4694561366,0.2178332421
H,0,0.93846629,-1.5143745267,1.5911584277
H,0,0.5162888766,-2.3277059548,0.0667069666
H,0,2.0559482339,1.1544538094,0.3337194566
H,0,0.4891102159,1.9888452528,0.3192326426
H,0,0.9589757309,1.0085257092,1.7246176851
H,0,1.417777223,-0.0331685906,-1.9001262247
H,0,-0.0895298825,-0.9695063853,-1.9726353937
H,0,-0.1443310755,0.8065374775,-1.890178207
H,0,-2.4135363233,0.4772747192,-0.5466012519
```

## t-Butyl Hydroperoxide – 6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -308.844828851

 Zero-point correction=                           0.137794 (Hartree/Particle)
 Thermal correction to Energy=                    0.145733
 Thermal correction to Enthalpy=                  0.146677
 Thermal correction to Gibbs Free Energy=         0.106937
 Sum of electronic and zero-point Energies=           -308.707034
 Sum of electronic and thermal Energies=              -308.699096
 Sum of electronic and thermal Enthalpies=            -308.698152
 Sum of electronic and thermal Free Energies=         -308.737892

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  91.449             29.031             83.641

 C,0,1.0073197616,-1.4489379826,0.5009683424
 C,0,0.3620815294,-0.1554638795,-0.0101134438
 O,0,-1.0099576687,-0.3056331633,0.4645520825
 O,0,-1.7904760284,0.8738727355,0.100751611
 C,0,1.0044689718,1.0781572878,0.6315758026
 C,0,0.3942104805,-0.0848285034,-1.5395410371
 H,0,2.0689666534,-1.4567340671,0.2349754926
 H,0,0.9240434313,-1.5206268371,1.5898272596
 H,0,0.5328307694,-2.3275725531,0.052834591
 H,0,2.0562122293,1.1511344856,0.3351293493
 H,0,0.4943015896,1.9912315475,0.3140528458
 H,0,0.9564581326,1.0118690031,1.7233244263
 H,0,1.4302547718,-0.0587622801,-1.8930357872
 H,0,-0.095563335,-0.9621234619,-1.9756197495
 H,0,-0.1103980869,0.8156031361,-1.9004976346
 H,0,-2.4621210383,0.4765029153,-0.5007583258
```

## *t*-butanol 6-31G* Gas Phase

```
E(RB+HF-LYP) = -233.670971211

 Zero-point correction=                           0.136280 (Hartree/Particle)
 Thermal correction to Energy=                    0.142965
 Thermal correction to Enthalpy=                  0.143909
 Thermal correction to Gibbs Free Energy=         0.107336
 Sum of electronic and zero-point Energies=           -233.534691
 Sum of electronic and thermal Energies=              -233.528006
 Sum of electronic and thermal Enthalpies=            -233.527062
 Sum of electronic and thermal Free Energies=         -233.563636

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.712             24.726             76.975

 C,0,-0.0072890735,-0.0126250502,0.0026330234
```

```
C,0,-0.0344720364,-0.0597077787,1.5320596908
C,0,1.4363503487,-0.0437731575,-0.5217646529
O,0,-0.6961039782,-1.2056876921,-0.4132563957
C,0,-0.7560842819,1.2220291951,-0.5217642872
H,0,-0.6998903675,-1.2122456323,-1.3840623287
H,0,-0.766181848,1.2340697076,-1.6198905338
H,0,-1.7937393545,1.2120752889,-0.1722356373
H,0,-0.2842184664,2.1526741649,-0.1853777061
H,0,1.4518262474,-0.0464974874,-1.6198909037
H,0,2.0063794888,0.8301972071,-0.1853780882
H,0,1.9465578665,-0.9473856847,-0.1722362612
H,0,-1.0684655881,-0.077551149,1.8917892493
H,0,0.4670722473,-0.9640940714,1.8917889932
H,0,0.4696265512,0.8134167197,1.9602668708
```

### *t*-butanol 6-31+G** Gas Phase

```
E(RB+HF-LYP) = -233.701735701

 Zero-point correction=                           0.135395 (Hartree/Particle)
 Thermal correction to Energy=                    0.142132
 Thermal correction to Enthalpy=                  0.143076
 Thermal correction to Gibbs Free Energy=         0.106405
 Sum of electronic and zero-point Energies=           -233.566340
 Sum of electronic and thermal Energies=              -233.559604
 Sum of electronic and thermal Enthalpies=            -233.558660
 Sum of electronic and thermal Free Energies=         -233.595331

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  89.189             24.956             77.180

 C,0,-0.0061612474,-0.0106715974,0.002531389
 C,0,-0.0347622342,-0.0602104161,1.5317081305
 C,0,1.4373481277,-0.0417679284,-0.5222267876
 O,0,-0.6971158344,-1.207440278,-0.416855266
 C,0,-0.7548465926,1.223895912,-0.522226422
 H,0,-0.7123284076,-1.2337889563,-1.3834382483
 H,0,-0.7636169962,1.2384086432,-1.6194039649
 H,0,-1.7917096252,1.2161215542,-0.1721469571
 H,0,-0.2792506769,2.1505867552,-0.1820784003
 H,0,1.454301449,-0.0421067923,-1.6194043348
 H,0,2.0020878442,0.8334557326,-0.1820787808
 H,0,1.9490471695,-0.9436047543,-0.1721475811
 H,0,-1.0682353246,-0.0772907108,1.8911466897
 H,0,0.4671826615,-0.9637644381,1.8911464336
 H,0,0.4694274415,0.8130718521,1.9581551296
```

### *t*-butanol 6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -233.677778544

 Zero-point correction=                           0.135675 (Hartree/Particle)
 Thermal correction to Energy=                    0.142328
 Thermal correction to Enthalpy=                  0.143272
 Thermal correction to Gibbs Free Energy=         0.106764
 Sum of electronic and zero-point Energies=           -233.542104
 Sum of electronic and thermal Energies=              -233.535451
 Sum of electronic and thermal Enthalpies=            -233.534506
 Sum of electronic and thermal Free Energies=         -233.571015

                    E (Thermal)             CV                S
```

| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 89.312 | 24.694 | 76.838 |

C,0,-0.0075548914,-0.0130854601,0.0015282374
C,0,-0.0340388579,-0.0589574909,1.5313570009
C,0,1.4365307052,-0.0418314307,-0.5209689151
O,0,-0.6970087405,-1.2072547853,-0.4188190157
C,0,-0.7544928755,1.2231562522,-0.5209685497
H,0,-0.7062079124,-1.22318794,-1.3989476587
H,0,-0.7665009197,1.233051654,-1.618631744
H,0,-1.7917539048,1.2175282695,-0.1685049756
H,0,-0.2783851894,2.1513535239,-0.1837090162
H,0,1.4511041235,-0.0472828388,-1.6186321139
H,0,2.0023191408,0.8345886514,-0.1837093966
H,0,1.9502875612,-0.942939744,-0.1685055997
H,0,-1.0676991815,-0.0740365707,1.894091225
H,0,0.469732758,-0.9616730543,1.8940909685
H,0,0.4705089662,0.8149451086,1.9573237955

## *t*-butanol 6-31+G** - PCM Dichloroethane

E(RB+HF-LYP) = -233.709837511

| | |
|---|---|
| Zero-point correction= | 0.134555 (Hartree/Particle) |
| Thermal correction to Energy= | 0.141293 |
| Thermal correction to Enthalpy= | 0.142237 |
| Thermal correction to Gibbs Free Energy= | 0.105558 |
| Sum of electronic and zero-point Energies= | -233.575282 |
| Sum of electronic and thermal Energies= | -233.568545 |
| Sum of electronic and thermal Enthalpies= | -233.567601 |
| Sum of electronic and thermal Free Energies= | -233.604279 |

| | E (Thermal) | CV | S |
|---|---|---|---|
| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
| Total | 88.662 | 24.983 | 77.197 |

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.006792 | 0.000000 | 0.012382 |
| 2 | 6 | 0 | 1.500934 | -0.000003 | -0.317293 |
| 3 | 6 | 0 | -0.674273 | -1.264296 | -0.531925 |
| 4 | 8 | 0 | -0.061865 | -0.000001 | 1.458813 |
| 5 | 6 | 0 | -0.674268 | 1.264300 | -0.531923 |
| 6 | 1 | 0 | -0.998366 | 0.000000 | 1.743478 |
| 7 | 1 | 0 | -1.735902 | 1.282640 | -0.256947 |
| 8 | 1 | 0 | -0.197535 | 2.160804 | -0.122266 |
| 9 | 1 | 0 | -0.610939 | 1.305839 | -1.624999 |
| 10 | 1 | 0 | -1.735908 | -1.282632 | -0.256948 |
| 11 | 1 | 0 | -0.610945 | -1.305834 | -1.625001 |
| 12 | 1 | 0 | -0.197543 | -2.160803 | -0.122269 |
| 13 | 1 | 0 | 1.984438 | 0.887623 | 0.103801 |
| 14 | 1 | 0 | 1.984435 | -0.887632 | 0.103799 |
| 15 | 1 | 0 | 1.658079 | -0.000002 | -1.400594 |

## Cyclohexenone oxide (8) – chair conformation –6-31G* Gas Phase

E(RB+HF-LYP) = -383.859478756

| | |
|---|---|
| Zero-point correction= | 0.133075 (Hartree/Particle) |
| Thermal correction to Energy= | 0.139741 |
| Thermal correction to Enthalpy= | 0.140685 |
| Thermal correction to Gibbs Free Energy= | 0.102147 |
| Sum of electronic and zero-point Energies= | -383.726404 |
| Sum of electronic and thermal Energies= | -383.719738 |
| Sum of electronic and thermal Enthalpies= | -383.718794 |

```
 Sum of electronic and thermal Free Energies=         -383.757332

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  87.689             25.550             81.110

 C,0,-0.6045766941,-0.518910548,-1.2398618435
 C,0,0.8412500082,-0.433703324,-0.7858382871
 C,0,1.0268284283,-0.1330359383,0.6762269034
 C,0,-0.0677546986,0.5616651699,1.4068962299
 C,0,-1.3642378863,0.9621791914,0.7191646707
 C,0,-1.346241832,0.7658253488,-0.8092617904
 O,0,1.7994951422,-0.5352088227,-1.5289431598
 H,0,2.0605905327,-0.0455938837,1.0085879313
 H,0,0.2208494845,1.1439447293,2.2839893776
 H,0,-2.1657861511,0.3631681093,1.1708608084
 H,0,-1.5858668258,2.0101162159,0.9540437145
 H,0,-2.3719415197,0.7492850431,-1.1947629817
 H,0,-0.851681,1.6258053634,-1.2797840941
 H,0,-1.0759746325,-1.3954690189,-0.7770648261
 H,0,-0.618307848,-0.6460895806,-2.3256578132
 O,0,0.1409908253,-0.8418551366,1.563550549
```

## Cyclohexenone oxide (8) – chair conformation –6-31+G** Gas Phase

```
E(RB+HF-LYP) = -383.886499281

 Zero-point correction=                           0.132263 (Hartree/Particle)
 Thermal correction to Energy=                    0.138965
 Thermal correction to Enthalpy=                  0.139909
 Thermal correction to Gibbs Free Energy=         0.101292
 Sum of electronic and zero-point Energies=           -383.754237
 Sum of electronic and thermal Energies=              -383.747534
 Sum of electronic and thermal Enthalpies=            -383.746590
 Sum of electronic and thermal Free Energies=         -383.785208

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  87.202             25.743             81.278

 C,0,-0.6045772909,-0.5157307556,-1.2443877773
 C,0,0.8365557346,-0.4394771646,-0.7819168619
 C,0,1.0282426321,-0.131037038,0.6775867094
 C,0,-0.0670398077,0.5660750875,1.4071897237
 C,0,-1.3653751867,0.9597820869,0.720024052
 C,0,-1.347882313,0.7671607311,-0.8089066613
 O,0,1.7980670532,-0.5538154687,-1.5238932034
 H,0,2.062294642,-0.0429663712,1.0058947496
 H,0,0.2226468187,1.1513644402,2.2809416287
 H,0,-2.1637761844,0.3572469196,1.1718032214
 H,0,-1.5890703062,2.0061263502,0.9573769332
 H,0,-2.3732420686,0.7480544786,-1.1936590267
 H,0,-0.8561614163,1.6289190382,-1.2780482559
 H,0,-1.0788580313,-1.3951519957,-0.7906221213
 H,0,-0.6112402176,-0.6356175591,-2.3304637254
 O,0,0.1470512754,-0.8388098611,1.5732260041
```

## Cyclohexenone oxide (8) – chair conformation –6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -383.868521401

 Zero-point correction=                           0.132560 (Hartree/Particle)
 Thermal correction to Energy=                    0.139245
```

```
 Thermal correction to Enthalpy=                  0.140189
 Thermal correction to Gibbs Free Energy=         0.101601
 Sum of electronic and zero-point Energies=           -383.735961
 Sum of electronic and thermal Energies=              -383.729277
 Sum of electronic and thermal Enthalpies=            -383.728333
 Sum of electronic and thermal Free Energies=         -383.766920

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   87.377             25.628             81.215

 C,0,-0.6044732118,-0.5174500049,-1.2411186827
 C,0,0.8355989136,-0.4357692707,-0.7821713307
 C,0,1.0271924725,-0.1299329593,0.675361243
 C,0,-0.0686982434,0.5633506437,1.4063929749
 C,0,-1.365489616,0.9594923953,0.7189531316
 C,0,-1.3455987137,0.7685128033,-0.8093029647
 O,0,1.7987294252,-0.5451289218,-1.5263886468
 H,0,2.0622847771,-0.0375279634,1.008627441
 H,0,0.2250851391,1.1470288727,2.2821459734
 H,0,-2.1671466868,0.3581112876,1.1683381934
 H,0,-1.5868173459,2.0065781624,0.9571884692
 H,0,-2.370200454,0.7491677574,-1.1973611828
 H,0,-0.8493597695,1.6292670263,-1.2768437645
 H,0,-1.0792651321,-1.3940511261,-0.7800518596
 H,0,-0.6188916935,-0.6444038825,-2.3275977013
 O,0,0.1446854723,-0.8451219017,1.5659740956
```

## Cyclohexenone oxide (8) – chair conformation –6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -383.897712197

 Zero-point correction=                           0.131609 (Hartree/Particle)
 Thermal correction to Energy=                    0.138331
 Thermal correction to Enthalpy=                  0.139275
 Thermal correction to Gibbs Free Energy=         0.100605
 Sum of electronic and zero-point Energies=           -383.766104
 Sum of electronic and thermal Energies=              -383.759381
 Sum of electronic and thermal Enthalpies=            -383.758437
 Sum of electronic and thermal Free Energies=         -383.797107

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   86.804             25.838             81.389

 C,0,-0.604254733,-0.5124540763,-1.2467129726
 C,0,0.8295304894,-0.4442959389,-0.7772441398
 C,0,1.0286973296,-0.1256481226,0.6762904737
 C,0,-0.0679148766,0.5696173091,1.4060045465
 C,0,-1.3676149191,0.955420296,0.7202435591
 C,0,-1.3467879734,0.7712654489,-0.8085559888
 O,0,1.7973496559,-0.5753562859,-1.5191061524
 H,0,2.064813779,-0.030327565,1.0047722164
 H,0,0.2280113788,1.1572174853,2.2780368932
 H,0,-2.1645592609,0.3472934762,1.1684771992
 H,0,-1.5939229634,1.9999548903,0.9630826614
 H,0,-2.3707049963,0.7490682948,-1.196907272
 H,0,-0.8530687459,1.6347936693,-1.2728579869
 H,0,-1.0837525029,-1.3924786828,-0.7968668764
 H,0,-0.6116903529,-0.6305885604,-2.3338468077
 O,0,0.1535040249,-0.8413587195,1.5773360363
```

## Cyclohexenone oxide (8) – boat conformation –6-31G* Gas Phase

E(RB+HF-LYP) = -383.860029883

| | |
|---|---|
| Zero-point correction= | 0.132884 (Hartree/Particle) |
| Thermal correction to Energy= | 0.139573 |
| Thermal correction to Enthalpy= | 0.140517 |
| Thermal correction to Gibbs Free Energy= | 0.101774 |
| Sum of electronic and zero-point Energies= | -383.727146 |
| Sum of electronic and thermal Energies= | -383.720457 |
| Sum of electronic and thermal Enthalpies= | -383.719513 |
| Sum of electronic and thermal Free Energies= | -383.758256 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 87.583 | 25.620 | 81.542 |

C,0,-1.4833690685,0.3221382798,0.8038813089
C,0,-0.259695231,-0.3185222486,1.4758800677
C,0,0.8847031554,-0.6976104798,0.5400877398
C,0,0.870826677,-0.1292903567,-0.8554481054
C,0,-0.1009545952,0.9314129573,-1.2069001179
C,0,-1.0849851611,1.4390855181,-0.1726511181
O,0,1.8270728247,-1.3708715985,0.9131983311
O,0,-0.3034726436,-0.4118542793,-1.648476059
H,0,1.8159440156,-0.2232868526,-1.3889810088
H,0,0.1849049831,1.624287811,-2.0005274141
H,0,-0.6275763767,2.2835240714,0.3629424393
H,0,-1.974794331,1.8327555997,-0.6801089763
H,0,-2.1546742724,0.7231168379,1.571444832
H,0,-2.0432621271,-0.4412661228,0.2547920891
H,0,0.1831314813,0.3861995672,2.1969122352
H,0,-0.5316294812,-1.20680591,2.0566489771

## Cyclohexenone oxide (8) – boat conformation –6-31+G** Gas Phase

E(RB+HF-LYP) = -383.887129778

| | |
|---|---|
| Zero-point correction= | 0.132097 (Hartree/Particle) |
| Thermal correction to Energy= | 0.138810 |
| Thermal correction to Enthalpy= | 0.139755 |
| Thermal correction to Gibbs Free Energy= | 0.100985 |
| Sum of electronic and zero-point Energies= | -383.755033 |
| Sum of electronic and thermal Energies= | -383.748319 |
| Sum of electronic and thermal Enthalpies= | -383.747375 |
| Sum of electronic and thermal Free Energies= | -383.786145 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 87.105 | 25.801 | 81.598 |

C,0,-1.4850057972,0.3245772284,0.8080395052
C,0,-0.2607084998,-0.3209293628,1.4756925492
C,0,0.8809512263,-0.6969683127,0.5401227762
C,0,0.8743554793,-0.1276261469,-0.8551294536
C,0,-0.099173911,0.9334751363,-1.2055079177
C,0,-1.0883234348,1.4369765523,-0.1747267095
O,0,1.82479462,-1.3729685117,0.9138472162
O,0,-0.2974828007,-0.4115115281,-1.6531680234
H,0,1.8207835177,-0.2197310207,-1.3850689454
H,0,0.186450749,1.6265437304,-1.9979224614
H,0,-0.6343801135,2.2854492137,0.3567380397
H,0,-1.9775327352,1.824498903,-0.6866527901
H,0,-2.1474053781,0.7322969868,1.5789901807

```
H,0,-2.0541693586,-0.4380409892,0.2679382324
H,0,0.1874854159,0.3789936871,2.1972439291
H,0,-0.5322970294,-1.211200761,2.0523557733
```

## Cyclohexenone oxide (8) – boat conformation –6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -383.869229545

 Zero-point correction=                           0.132280 (Hartree/Particle)
 Thermal correction to Energy=                    0.138979
 Thermal correction to Enthalpy=                  0.139923
 Thermal correction to Gibbs Free Energy=         0.101186
 Sum of electronic and zero-point Energies=           -383.736949
 Sum of electronic and thermal Energies=              -383.730251
 Sum of electronic and thermal Enthalpies=            -383.729307
 Sum of electronic and thermal Free Energies=         -383.768044

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  87.210             25.712            81.528

 C,0,-1.4825465328,0.3250441549,0.8084706789
 C,0,-0.2548496168,-0.3107406701,1.4774173746
 C,0,0.8753427018,-0.7015837234,0.5381398672
 C,0,0.87950102,-0.115222218,-0.8485216422
 C,0,-0.0957982666,0.941223126,-1.2004727253
 C,0,-1.0895376032,1.4388651886,-0.173101611
 O,0,1.8038089371,-1.4086049041,0.9003609064
 O,0,-0.2890441282,-0.4068620576,-1.6532581015
 H,0,1.8306196713,-0.1981389172,-1.3773196846
 H,0,0.1957092207,1.6374652158,-1.9906743251
 H,0,-0.6385231082,2.2884003904,0.3598197758
 H,0,-1.979739013,1.8240645829,-0.6865878347
 H,0,-2.1470675951,0.7292947897,1.5799829266
 H,0,-2.0474262539,-0.4431866698,0.2699468827
 H,0,0.1988349463,0.4084673053,2.1790124651
 H,0,-0.5231965543,-1.1881461518,2.0774057007
```

## Cyclohexenone oxide (8) – boat conformation –6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -383.898528125

 Zero-point correction=                           0.131371 (Hartree/Particle)
 Thermal correction to Energy=                    0.138090
 Thermal correction to Enthalpy=                  0.139034
 Thermal correction to Gibbs Free Energy=         0.100301
 Sum of electronic and zero-point Energies=           -383.767157
 Sum of electronic and thermal Energies=              -383.760438
 Sum of electronic and thermal Enthalpies=            -383.759494
 Sum of electronic and thermal Free Energies=         -383.798227

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  86.653             25.902            81.520

 C,0,-1.4834852256,0.3286576597,0.8147870477
 C,0,-0.2536652101,-0.3096713837,1.4784879536
 C,0,0.8680898055,-0.7035512948,0.5374365537
 C,0,0.8858138122,-0.1082658123,-0.8453285009
 C,0,-0.0916325126,0.9474184311,-1.1959085928
 C,0,-1.0949860449,1.4367125077,-0.175264601
 O,0,1.7915634874,-1.4267494812,0.894962537
 O,0,-0.2766260071,-0.4032191749,-1.6606642133
```

```
H,0,1.8407808334,-0.1854982168,-1.3677560521
H,0,0.2014248288,1.6458464226,-1.9831540045
H,0,-0.6514593186,2.2931969968,0.3523773344
H,0,-1.984965337,1.8113228103,-0.6958646341
H,0,-2.1369977292,0.7407559794,1.5908696805
H,0,-2.0586223091,-0.4403457164,0.2887500821
H,0,0.2100961478,0.4106171886,2.1723405112
H,0,-0.520564706,-1.1839468612,2.0827913308
```

## DBU Model (9) – 6-31G* Gas Phase

```
E(RB+HF-LYP) = -345.358944743

 Zero-point correction=                           0.180313 (Hartree/Particle)
 Thermal correction to Energy=                    0.188577
 Thermal correction to Enthalpy=                  0.189521
 Thermal correction to Gibbs Free Energy=         0.147807
 Sum of electronic and zero-point Energies=           -345.178632
 Sum of electronic and thermal Energies=              -345.170368
 Sum of electronic and thermal Enthalpies=            -345.169424
 Sum of electronic and thermal Free Energies=         -345.211137

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 118.334             30.794             87.793

 N,0,-0.4424517558,-0.6671718896,0.3131946191
 C,0,0.7165659404,-0.6936312107,1.2020009473
 C,0,1.9521020171,-0.1841579595,0.4654126107
 C,0,1.639717136,1.1841554197,-0.1472664573
 N,0,0.3877131467,1.222936492,-0.8943173882
 C,0,-0.5309160846,0.364418871,-0.6234046311
 C,0,-1.8085374495,0.4493320224,-1.4312506773
 C,0,-1.6201368695,-1.3408826835,0.8322718498
 H,0,2.4479287991,1.4899082248,-0.8237948322
 H,0,1.6028165527,1.9503463563,0.6431813864
 H,0,-1.3311718993,-2.3316499894,1.2021413065
 H,0,-2.0914416062,-0.7956824726,1.6679556611
 H,0,-2.3679020681,-1.4837127868,0.0515181285
 H,0,0.5308947731,-0.0833283748,2.1034427616
 H,0,2.2125422524,-0.8934388349,-0.3299603626
 H,0,2.8052483639,-0.1303862532,1.1521222102
 H,0,0.8617975766,-1.7272698338,1.5416318027
 H,0,-2.0232582509,-0.4907017836,-1.9541621792
 H,0,-2.6775540913,0.6870445599,-0.8055285603
 H,0,-1.6794982774,1.2431122153,-2.1672697913
```

## DBU Model (9) – 6-31+G** Gas Phase

```
E(RB+HF-LYP) = -345.386270400

 Zero-point correction=                           0.179010 (Hartree/Particle)
 Thermal correction to Energy=                    0.187330
 Thermal correction to Enthalpy=                  0.188274
 Thermal correction to Gibbs Free Energy=         0.146446
 Sum of electronic and zero-point Energies=           -345.207260
 Sum of electronic and thermal Energies=              -345.198940
 Sum of electronic and thermal Enthalpies=            -345.197996
 Sum of electronic and thermal Free Energies=         -345.239824

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 117.551             31.054             88.035
```

```
N,0,-0.4413329394,-0.6710578998,0.3080831445
C,0,0.7186126556,-0.6967467463,1.1986810856
C,0,1.9538547608,-0.1849283024,0.4639847216
C,0,1.642281668,1.1857938114,-0.1430393445
N,0,0.3877997417,1.2257202113,-0.8888982944
C,0,-0.5334673274,0.3642718441,-0.624117201
C,0,-1.8105529586,0.4493117006,-1.4314359616
C,0,-1.6228174421,-1.3396314591,0.8326484002
H,0,2.4468964304,1.4940719742,-0.8210698888
H,0,1.6043051469,1.9495503598,0.6488053433
H,0,-1.332784154,-2.3227375654,1.2184088629
H,0,-2.0952786082,-0.7789800064,1.6567072158
H,0,-2.3669423134,-1.4965889207,0.0521228358
H,0,0.528874041,-0.0846569976,2.0979666585
H,0,2.2170523023,-0.8916763423,-0.3324398479
H,0,2.8055350166,-0.130295042,1.1518044021
H,0,0.8637928877,-1.7295988556,1.5378698301
H,0,-2.0227144991,-0.4897225748,-1.9555695819
H,0,-2.67773988,0.6850617748,-0.8037861214
H,0,-1.6837321234,1.2445109256,-2.1654438608
```

## DBU Model (9) – 6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -345.364976362

 Zero-point correction=                           0.180034 (Hartree/Particle)
 Thermal correction to Energy=                    0.188329
 Thermal correction to Enthalpy=                  0.189274
 Thermal correction to Gibbs Free Energy=         0.147438
 Sum of electronic and zero-point Energies=           -345.184942
 Sum of electronic and thermal Energies=              -345.176647
 Sum of electronic and thermal Enthalpies=            -345.175703
 Sum of electronic and thermal Free Energies=         -345.217539

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 118.179             30.839            88.051

 N,0,-0.4488270413,-0.6455927148,0.3237632957
 C,0,0.7185481026,-0.6919958482,1.2048717047
 C,0,1.9527257492,-0.1884106007,0.4637696135
 C,0,1.6431421294,1.1809127099,-0.1444683592
 N,0,0.395625988,1.2183946914,-0.9092641242
 C,0,-0.5312101866,0.3641675807,-0.6242633699
 C,0,-1.8113315641,0.4432827732,-1.4296975982
 C,0,-1.6235724725,-1.3394091449,0.8309064693
 H,0,2.459496034,1.4939024026,-0.8088668778
 H,0,1.594685861,1.9400689834,0.6527079453
 H,0,-1.3219948846,-2.3272601029,1.1967838789
 H,0,-2.1020497622,-0.8020308671,1.6658021569
 H,0,-2.3655974348,-1.4878286266,0.0459788885
 H,0,0.5419686719,-0.0883688245,2.1113011054
 H,0,2.2102320014,-0.8976676551,-0.3333135245
 H,0,2.8073679539,-0.1357546682,1.1484865383
 H,0,0.8553967723,-1.7302836403,1.5323693648
 H,0,-2.030926683,-0.5020118079,-1.9403367249
 H,0,-2.6761635169,0.6883421407,-0.8015111496
 H,0,-1.6898181878,1.2279940102,-2.1776065618
```

## DBU Model (9) – 6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -345.393699812
```

```
 Zero-point correction=                           0.178755 (Hartree/Particle)
 Thermal correction to Energy=                    0.187104
 Thermal correction to Enthalpy=                  0.188048
 Thermal correction to Gibbs Free Energy=         0.146084
 Sum of electronic and zero-point Energies=           -345.214945
 Sum of electronic and thermal Energies=              -345.206596
 Sum of electronic and thermal Enthalpies=            -345.205652
 Sum of electronic and thermal Free Energies=         -345.247616

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 117.409             31.080            88.321

 N,0,-0.4497629139,-0.6436122481,0.3219127112
 C,0,0.719857511,-0.6921150291,1.203481563
 C,0,1.954082416,-0.1899201448,0.4625885179
 C,0,1.6479474434,1.1816429909,-0.1408739993
 N,0,0.398133485,1.2195956769,-0.9063185814
 C,0,-0.5351134622,0.3646995908,-0.6247594771
 C,0,-1.814120679,0.4418990924,-1.4302962211
 C,0,-1.6257460872,-1.3404791301,0.8297578806
 H,0,2.4614120361,1.4957475005,-0.8061334339
 H,0,1.5975551558,1.9380531209,0.6578610845
 H,0,-1.3213161516,-2.3257007021,1.1971289564
 H,0,-2.1016836338,-0.7988587239,1.6625025811
 H,0,-2.3675417271,-1.4925178426,0.0464932528
 H,0,0.5411639899,-0.0858640617,2.1074633975
 H,0,2.2130241027,-0.8982166053,-0.3347409035
 H,0,2.8073876232,-0.136870455,1.1483197214
 H,0,0.8541770143,-1.7299150018,1.5307053819
 H,0,-2.0333945683,-0.5051915305,-1.9359502592
 H,0,-2.6760666608,0.6902114762,-0.800801183
 H,0,-1.6947540294,1.2228746027,-2.1813970897
```

## Dbu model complex with HOOtBu 6-31G* Gas Phase

```
E(RB+HF-LYP) = -654.181398974

 Zero-point correction=                           0.322020 (Hartree/Particle)
 Thermal correction to Energy=                    0.339778
 Thermal correction to Enthalpy=                  0.340722
 Thermal correction to Gibbs Free Energy=         0.274558
 Sum of electronic and zero-point Energies=           -653.859379
 Sum of electronic and thermal Energies=              -653.841621
 Sum of electronic and thermal Enthalpies=            -653.840677
 Sum of electronic and thermal Free Energies=         -653.906841

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 213.214             64.015           139.255

 C,0,-3.5027746004,1.2722240777,0.889972451
 C,0,-2.3994189,2.324753604,0.934000631
 C,0,-1.4083667747,2.053185247,-0.1979249749
 N,0,-0.9501773191,0.6668823699,-0.2333709861
 C,0,-1.6972426838,-0.2692743072,0.2545645372
 N,0,-2.9218704255,-0.0698914588,0.867909991
 C,0,-1.1726620309,-1.6859776496,0.1831842384
 C,0,-3.8682443572,-1.146950417,1.1094492914
 O,0,1.3778904737,0.2644213503,-1.7392212725
 O,0,1.935529294,-0.9322989605,-1.1269194239
 C,0,3.1435129707,-0.5874370415,-0.4116506928
```

C,0,3.5860116417,-1.9426028065,0.1532826042
C,0,4.1835124769,-0.0308607464,-1.3916690196
C,0,2.8395317573,0.4102229134,0.7120188924
H,0,3.7415220174,0.6199027646,1.298465989
H,0,2.4708449454,1.3504204727,0.293950454
H,0,2.0737102356,0.0080830059,1.3843220274
H,0,5.1229281263,0.1968221214,-0.8741532142
H,0,4.3893758685,-0.7611086364,-2.1816139637
H,0,3.8094997342,0.8836666745,-1.858684925
H,0,4.5311683058,-1.8366484879,0.6967314107
H,0,2.8341342832,-2.3415132533,0.842803458
H,0,3.7306993286,-2.6657227274,-0.6560297513
H,0,0.5568822279,0.3794799234,-1.1797578789
H,0,-0.5263623924,2.6969404622,-0.0999544918
H,0,-1.864287558,2.3034346517,-1.1681838727
H,0,-4.4504929318,-0.920066631,2.0101809482
H,0,-4.5753446986,-1.2740919221,0.2739351253
H,0,-3.3553166698,-2.093943257,1.2719603668
H,0,-4.1462328894,1.4264270881,0.0076197646
H,0,-1.8817918493,2.2666999623,1.8992164731
H,0,-2.8331783149,3.3276303583,0.8507047082
H,0,-4.1489373361,1.3464424271,1.7736348582
H,0,-1.1595399143,-2.1569483637,1.1732070397
H,0,-1.7904969885,-2.3104398594,-0.4733687722
H,0,-0.154964456,-1.6650795124,-0.2090009664

## Dbu model complex with HOOtBu 6-31+G** Gas Phase

E(RB+HF-LYP) = -654.237108355

| | |
|---|---|
| Zero-point correction= | 0.319533 (Hartree/Particle) |
| Thermal correction to Energy= | 0.337504 |
| Thermal correction to Enthalpy= | 0.338448 |
| Thermal correction to Gibbs Free Energy= | 0.270655 |
| Sum of electronic and zero-point Energies= | -653.917576 |
| Sum of electronic and thermal Energies= | -653.899604 |
| Sum of electronic and thermal Enthalpies= | -653.898660 |
| Sum of electronic and thermal Free Energies= | -653.966453 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 211.787 | 64.380 | 142.682 |

C,0,-3.324463523,0.7616961321,1.6224688223
C,0,-2.1938428749,0.2871502151,2.5303070437
C,0,-0.8653350282,0.4147514032,1.7849630824
N,0,-0.9032637345,-0.1870076321,0.4522987112
C,0,-2.0295112628,-0.3023513703,-0.1739448882
N,0,-3.2624404359,0.071990377,0.3318795529
C,0,-2.0009862651,-0.9330372497,-1.5480128189
C,0,-4.4402999051,0.2333193385,-0.5090806541
O,0,1.5184749843,-1.2865559511,-0.2515011101
O,0,2.4355213764,-0.2861434892,0.2857942853
C,0,3.3313031356,0.1553985301,-0.7597855775
C,0,4.2292043082,1.1527920549,-0.0170807062
C,0,4.1457360586,-1.0324724816,-1.2886365126
C,0,2.5507519504,0.8475759582,-1.8843486071
H,0,3.2377624531,1.238710836,-2.6430138074
H,0,1.8694308709,0.1419795821,-2.3661973436
H,0,1.9632223228,1.6808010391,-1.4846214828
H,0,4.8691153109,-0.6977510062,-2.040670088
H,0,4.6908345796,-1.5132428196,-0.4700649972
H,0,3.4858052947,-1.774587326,-1.7443102886

```
H,0,4.9800557798,1.5602569031,-0.7018728398
H,0,3.6385435225,1.9824544103,0.384024142
H,0,4.7458279167,0.6611737719,0.8128538178
H,0,0.6373014059,-0.8602315228,-0.0315232495
H,0,-0.0560408098,-0.0653201549,2.3446425136
H,0,-0.582760407,1.4729223752,1.684937578
H,0,-5.3360464847,0.0607056524,0.0963544955
H,0,-4.5101542689,1.2456626331,-0.9378417266
H,0,-4.4474947677,-0.4884457807,-1.3247693357
H,0,-3.2664345505,1.8530145857,1.47485853
H,0,-2.3650225452,-0.7604511179,2.8054815827
H,0,-2.185002833,0.8742655658,3.4550581626
H,0,-4.3018215284,0.5485848929,2.0710913503
H,0,-2.6443159316,-1.8182729887,-1.5976768002
H,0,-2.3331754202,-0.2321098499,-2.3217558004
H,0,-0.9770111645,-1.2323385545,-1.7696727656
```

## Dbu model complex with HOOtBu 6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -654.189415415

 Zero-point correction=                           0.320935 (Hartree/Particle)
 Thermal correction to Energy=                    0.337944
 Thermal correction to Enthalpy=                  0.338889
 Thermal correction to Gibbs Free Energy=         0.274644
 Sum of electronic and zero-point Energies=           -653.868481
 Sum of electronic and thermal Energies=              -653.851471
 Sum of electronic and thermal Enthalpies=            -653.850527
 Sum of electronic and thermal Free Energies=         -653.914771

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 212.063             62.153            135.214

 C,0,3.4236333543,1.0122284472,0.5296635944
 C,0,2.6680301725,1.9996320876,-0.3545850047
 C,0,1.1732078182,1.687880046,-0.2895070686
 N,0,0.8781779659,0.276652807,-0.5343840074
 C,0,1.7758362288,-0.6215129338,-0.2711534047
 N,0,3.0448118745,-0.3629472465,0.1926459001
 C,0,1.4026083075,-2.065364973,-0.5271390774
 C,0,3.9167035778,-1.3977493311,0.7319855758
 O,0,-1.6313900196,-0.2988373999,-1.4729924112
 O,0,-2.4344472565,0.6634175261,-0.7302226218
 C,0,-3.1615368145,-0.0035613829,0.3298522773
 C,0,-3.9420327987,1.1561672065,0.9608914556
 C,0,-4.1122662015,-1.0520508543,-0.259100094
 C,0,-2.1942973488,-0.6285412821,1.3411434292
 H,0,-2.7465012449,-1.0581782029,2.184936441
 H,0,-1.6085411231,-1.423408087,0.8724166459
 H,0,-1.5024006618,0.1278706111,1.7266047437
 H,0,-4.7031461897,-1.5271658937,0.5325125494
 H,0,-4.8010516568,-0.5850892159,-0.9720388176
 H,0,-3.5448706874,-1.8265429666,-0.7820361996
 H,0,-4.5616925228,0.7890072679,1.7860059715
 H,0,-3.2572585212,1.9155712398,1.353580992
 H,0,-4.5968743402,1.6287944055,0.2209204749
 H,0,-0.7102281871,-0.0879776718,-1.1150585994
 H,0,0.6215432991,2.2813185836,-1.0283153024
 H,0,0.7701887362,1.9698224522,0.6951591991
 H,0,4.958972577,-1.1041331486,0.5676906261
 H,0,3.7704187694,-1.5404857898,1.8137633475
 H,0,3.7564850977,-2.352482004,0.2312445731
```

```
H,0,3.2208133482,1.2122890701,1.5941741966
H,0,3.0205863021,1.9044161814,-1.3893260474
H,0,2.8721662692,3.0254658958,-0.0275792133
H,0,4.506255478,1.1085582973,0.3835036819
H,0,2.0799735314,-2.5355053618,-1.2495065169
H,0,1.4335332869,-2.6603615158,0.3929216057
H,0,0.3880799914,-2.0971262603,-0.9259974341
```

## Dbu model complex with HOOtBu 6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -654.247510760

 Zero-point correction=                           0.318764 (Hartree/Particle)
 Thermal correction to Energy=                    0.336621
 Thermal correction to Enthalpy=                  0.337565
 Thermal correction to Gibbs Free Energy=         0.270910
 Sum of electronic and zero-point Energies=           -653.928747
 Sum of electronic and thermal Energies=              -653.910890
 Sum of electronic and thermal Enthalpies=            -653.909946
 Sum of electronic and thermal Free Energies=         -653.976601

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 211.233             64.268            140.287

 N,0,3.025753471,-0.3611033532,0.3257832003
 C,0,3.5233209625,1.0175924102,0.455963292
 C,0,2.7047177998,1.9790762696,-0.3993250914
 C,0,1.2181970457,1.6895832361,-0.1929331533
 N,0,0.8929074854,0.2900803939,-0.4676207538
 C,0,1.7852330067,-0.6184573895,-0.195923335
 C,0,1.4185173279,-2.0602407871,-0.4652941182
 C,0,4.003957734,-1.3944448606,0.6458790243
 O,0,-1.5840460104,-0.1150856891,-1.4343931908
 O,0,-2.4024279345,0.7534958416,-0.5971451985
 C,0,-3.2340880421,-0.0391997932,0.2941065411
 C,0,-2.3665382464,-0.8706191973,1.245353042
 C,0,-4.0074087411,1.0421032197,1.0586563515
 C,0,-4.1830944077,-0.9245928772,-0.5213613505
 H,0,-2.9986834445,-1.397043144,1.9688804542
 H,0,-1.7869314985,-1.6134939762,0.6917979552
 H,0,-1.6715319226,-0.2264950582,1.793322871
 H,0,-4.8454587386,-1.4884120174,0.1446043225
 H,0,-4.8006540274,-0.312583818,-1.1871718284
 H,0,-3.615939098,-1.6345823915,-1.1288527477
 H,0,-4.6984603066,0.5727345069,1.7660237785
 H,0,-3.3233113817,1.6870440315,1.6192770409
 H,0,-4.5884771128,1.6637696235,0.3699578771
 H,0,-0.6546971069,0.0200371471,-1.0354019456
 H,0,0.602942917,2.3168736983,-0.8467771331
 H,0,0.9294880561,1.9354386025,0.8412221792
 H,0,4.7459069148,-1.5128876835,-0.1570458339
 H,0,4.5349775821,-1.1096757904,1.5607571894
 H,0,3.5263384438,-2.3560136288,0.8263996437
 H,0,3.4952262247,1.3147377071,1.5145194798
 H,0,2.9580646151,1.842520184,-1.4582338775
 H,0,2.9492188072,3.012423264,-0.1303183972
 H,0,4.5751461519,1.0275219462,0.1435738924
 H,0,2.1426445306,-2.5455019448,-1.1281839843
 H,0,1.3723971496,-2.6422552651,0.4621109276
 H,0,0.4360714742,-2.0890778825,-0.9360190908
```

## Ts 1 from axial attack with DBU model, orientation A (10) – 6-31G* - Gas Phase

E(RB+HF-LYP) = -962.824032082

| | |
|---|---|
| Zero-point correction= | 0.452643 (Hartree/Particle) |
| Thermal correction to Energy= | 0.476337 |
| Thermal correction to Enthalpy= | 0.477281 |
| Thermal correction to Gibbs Free Energy= | 0.399425 |
| Sum of electronic and zero-point Energies= | -962.371390 |
| Sum of electronic and thermal Energies= | -962.347695 |
| Sum of electronic and thermal Enthalpies= | -962.346751 |
| Sum of electronic and thermal Free Energies= | -962.424607 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 298.906 | 89.385 | 163.862 |

C,0,-1.4629132232,2.4728145391,0.8560201038
C,0,-0.1961960162,2.2595488381,1.6911625679
C,0,1.0580927611,2.7709771263,0.9701820124
C,0,1.1634130339,2.3122849699,-0.4931864917
C,0,-0.0499894486,2.1277344789,-1.2064038299
C,0,-1.2968166282,1.9763832407,-0.5617491825
O,0,2.3090097033,2.1730758071,-0.9915796256
O,0,-1.4350298739,0.1772618508,-0.4242454119
O,0,-2.3574642084,-0.4194265415,0.5572764899
C,0,-3.451433967,-1.0813106787,-0.1117877171
C,0,-4.2568224011,-0.0813998389,-0.9499058593
C,0,-2.921004792,-2.2276166493,-0.9832076809
C,0,-4.2884425508,-1.6178558557,1.0567265595
H,0,0.0188407183,1.9522085751,-2.2778479135
H,0,-2.18757031,2.0983259469,-1.1758112785
H,0,-1.7008904926,3.5466503885,0.8028019306
H,0,-2.3183097887,1.9755054957,1.3251252042
H,0,-0.3021610777,2.7422121568,2.6720726605
H,0,-0.0949430089,1.184798366,1.8818677933
H,0,1.0620436156,3.8718900889,0.964444933
H,0,1.9746045915,2.4649254293,1.489351663
H,0,-3.7421327384,-2.7606607291,-1.4764949011
H,0,-2.2521230795,-1.8310950249,-1.7518486499
H,0,-2.3634699809,-2.9471286934,-0.3719538264
H,0,-5.1237177365,-0.5692090399,-1.4110624211
H,0,-4.6182025538,0.7405846083,-0.3221768142
H,0,-3.6311773757,0.335167449,-1.7434189386
H,0,-5.1659723819,-2.157560235,0.6835982966
H,0,-3.6974688727,-2.3046871803,1.6725055582
H,0,-4.631600177,-0.7950406279,1.6926366944
H,0,-0.0046136263,-0.6327829355,-0.5639748955
N,0,0.9952083098,-0.9859450311,-0.6142258788
C,0,1.7174075868,-0.733768598,-1.8679166275
C,0,3.1171903567,-1.3327912292,-1.7951916389
H,0,1.1277645548,-1.173354566,-2.6785096053
H,0,1.7887766332,0.3505182529,-2.009200717
C,0,1.5725665389,-1.2703807158,0.5330639641
N,0,2.9097189865,-1.357042485,0.6479024158
C,0,3.589523248,-1.6040093125,1.9136207647
C,0,3.7534969029,-0.9024206096,-0.4756883902
H,0,4.4429086389,-2.2668472472,1.7383264112
H,0,3.9615837396,-0.6676076655,2.3496916202
H,0,2.9251316196,-2.0858628889,2.6294183161
H,0,3.8351269888,0.1918131669,-0.4377337949
C,0,0.6748487157,-1.5298257983,1.7143064994
H,0,3.0893692739,-2.4279075488,-1.8554055663
H,0,3.7178963792,-0.9646979619,-2.6323568935

```
H,0,4.7443616451,-1.3462693898,-0.3432677762
H,0,0.7723408682,-2.5718927906,2.0412410293
H,0,0.9367077738,-0.8844873624,2.5578728782
H,0,-0.3672405827,-1.3440677964,1.4424913024
```

## Ts 1 from axial attack with DBU model, orientation A (10) – 6-31+G** - Gas Phase

E(RB+HF-LYP) = -962.900689997

```
 Zero-point correction=                           0.448927 (Hartree/Particle)
 Thermal correction to Energy=                    0.473034
 Thermal correction to Enthalpy=                  0.473978
 Thermal correction to Gibbs Free Energy=         0.393922
 Sum of electronic and zero-point Energies=           -962.451763
 Sum of electronic and thermal Energies=              -962.427656
 Sum of electronic and thermal Enthalpies=            -962.426712
 Sum of electronic and thermal Free Energies=         -962.506767

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 296.833             90.274           168.492
```

```
C,0,-1.5374614185,2.5082830006,0.8697517688
C,0,-0.2634731615,2.3533851593,1.7070895065
C,0,0.9730082099,2.8912241497,0.97325309
C,0,1.0879171489,2.4248353405,-0.4852036433
C,0,-0.1145117683,2.1587984715,-1.1891193163
C,0,-1.3599310585,1.976121805,-0.5344218056
O,0,2.2394972333,2.3441140345,-0.9921550876
O,0,-1.4143885993,0.2060986549,-0.3662111584
O,0,-2.3685706112,-0.4225801869,0.5728102078
C,0,-3.4249255219,-1.1105093193,-0.1375786552
C,0,-4.2190431113,-0.1335699603,-1.0132933506
C,0,-2.8426305103,-2.2553508785,-0.9780393775
C,0,-4.296739567,-1.6553139526,1.0019889165
H,0,-0.0428319691,1.9680453627,-2.2571336651
H,0,-2.2512628711,2.0652793176,-1.1529875528
H,0,-1.8035390392,3.572595704,0.7829898175
H,0,-2.379989689,2.0038867912,1.3541559749
H,0,-0.3840090692,2.8558858749,2.675681584
H,0,-0.1269104684,1.287513335,1.9236777977
H,0,0.9472249596,3.9909510748,0.95049641
H,0,1.8994269866,2.6178387796,1.491462446
H,0,-3.6401845354,-2.809195953,-1.4857691541
H,0,-2.1619057254,-1.8588880776,-1.7358867428
H,0,-2.2906970059,-2.9556915592,-0.3413558078
H,0,-5.0667508375,-0.6432415477,-1.4847833974
H,0,-4.6060450721,0.6936448298,-0.4096203576
H,0,-3.5827037625,0.2758337481,-1.8016091713
H,0,-5.1420137467,-2.219669118,0.5938924345
H,0,-3.716924211,-2.3217692298,1.6487213955
H,0,-4.6884712499,-0.8360351771,1.6127125356
H,0,0.0421249211,-0.5513633567,-0.4879270544
N,0,1.0349312304,-0.9160069218,-0.561581113
C,0,1.7376739838,-0.6696403163,-1.8270443717
C,0,3.0655968786,-1.4179947367,-1.8355171641
H,0,1.080831708,-1.0030107392,-2.635252684
H,0,1.9022740486,0.4112190151,-1.921752702
C,0,1.6259256772,-1.2727272563,0.5572311264
N,0,2.9560036614,-1.4784623678,0.6225039481
C,0,3.6590361282,-1.7588677602,1.8711147737
C,0,3.8053211598,-1.1264135559,-0.5325992983
H,0,4.4486628449,-2.4911086914,1.6790197102
```

```
H,0,4.1197097511,-0.8478725944,2.2742171422
H,0,2.986061472,-2.1735118,2.6189192738
H,0,4.0692030571,-0.0625343056,-0.4726431123
C,0,0.7541615932,-1.4711237679,1.7682271053
H,0,2.9099277742,-2.4988533668,-1.9382875981
H,0,3.6716338314,-1.084637226,-2.6827007651
H,0,4.7215419358,-1.7188866071,-0.4570392855
H,0,0.7999152532,-2.5124453954,2.1045436307
H,0,1.0790348615,-0.8318403943,2.5939093135
H,0,-0.2817305511,-1.2287322208,1.5233022172
```

## Ts 1 from axial attack with DBU model, orientation A (10) – 6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.843277653

 Zero-point correction=                           0.450769 (Hartree/Particle)
 Thermal correction to Energy=                    0.474956
 Thermal correction to Enthalpy=                  0.475900
 Thermal correction to Gibbs Free Energy=         0.395556
 Sum of electronic and zero-point Energies=           -962.392509
 Sum of electronic and thermal Energies=              -962.368322
 Sum of electronic and thermal Enthalpies=            -962.367378
 Sum of electronic and thermal Free Energies=         -962.447722

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 298.039             89.885           169.098

    1          6             0       -1.930779    2.084752    1.237219
    2          6             0       -0.548327    2.178429    1.890486
    3          6             0        0.308142    3.264999    1.230129
    4          6             0        0.333647    3.186130   -0.303105
    5          6             0       -0.793518    2.601913   -0.951520
    6          6             0       -1.824046    1.961152   -0.260835
    7          8             0        1.304989    3.695716   -0.911129
    8          8             0       -1.390728    0.060578   -0.434560
    9          8             0       -2.070568   -0.880062    0.454478
   10          6             0       -2.952250   -1.740336   -0.300983
   11          6             0       -4.022478   -0.911007   -1.020558
   12          6             0       -2.141061   -2.577354   -1.298897
   13          6             0       -3.582007   -2.626185    0.780851
   14          1             0       -0.804217    2.628563   -2.040688
   15          1             0       -2.764734    1.803300   -0.781987
   16          1             0       -2.515378    2.991711    1.464629
   17          1             0       -2.491663    1.231773    1.632011
   18          1             0       -0.644058    2.365220    2.968156
   19          1             0       -0.050436    1.207937    1.777291
   20          1             0       -0.082096    4.261008    1.495490
   21          1             0        1.344431    3.237310    1.588181
   22          1             0       -2.794738   -3.229743   -1.889432
   23          1             0       -1.597959   -1.914527   -1.977703
   24          1             0       -1.414423   -3.207048   -0.772065
   25          1             0       -4.725734   -1.562377   -1.552782
   26          1             0       -4.587561   -0.309213   -0.299692
   27          1             0       -3.552792   -0.239218   -1.743349
   28          1             0       -4.277351   -3.343520    0.330928
   29          1             0       -2.810251   -3.187525    1.319189
   30          1             0       -4.133623   -2.016862    1.505073
   31          1             0        0.160919   -0.274457   -0.348149
   32          7             0        1.215426   -0.462579   -0.416311
   33          6             0        1.920533    0.175609   -1.530531
   34          6             0        3.167059   -0.631390   -1.876096
   35          1             0        1.221204    0.217945   -2.370489
```

| | | | | | |
|---|---|---|---|---|---|
| 36 | 1 | 0 | 2.166556 | 1.210472 | -1.263794 |
| 37 | 6 | 0 | 1.807249 | -1.216427 | 0.486676 |
| 38 | 7 | 0 | 3.129086 | -1.445355 | 0.461003 |
| 39 | 6 | 0 | 3.840139 | -2.223883 | 1.473326 |
| 40 | 6 | 0 | 3.978699 | -0.889985 | -0.610146 |
| 41 | 1 | 0 | 4.184467 | -3.175794 | 1.051454 |
| 42 | 1 | 0 | 4.713402 | -1.654901 | 1.810207 |
| 43 | 1 | 0 | 3.208909 | -2.424157 | 2.336708 |
| 44 | 1 | 0 | 4.449478 | 0.032914 | -0.244748 |
| 45 | 6 | 0 | 0.942774 | -1.819260 | 1.562175 |
| 46 | 1 | 0 | 2.879400 | -1.587260 | -2.330405 |
| 47 | 1 | 0 | 3.783833 | -0.089866 | -2.600158 |
| 48 | 1 | 0 | 4.776093 | -1.615335 | -0.803195 |
| 49 | 1 | 0 | 1.088073 | -2.903164 | 1.614323 |
| 50 | 1 | 0 | 1.196010 | -1.397768 | 2.541759 |
| 51 | 1 | 0 | -0.109532 | -1.612685 | 1.350939 |

## Ts 1 from axial attack with DBU model, orientation A (10) – 6-31+G** - PCM Dichloroethane

E(RB+HF-LYP) = -962.924990533

| | |
|---|---|
| Zero-point correction= | 0.447370 (Hartree/Particle) |
| Thermal correction to Energy= | 0.470821 |
| Thermal correction to Enthalpy= | 0.471765 |
| Thermal correction to Gibbs Free Energy= | 0.393708 |
| Sum of electronic and zero-point Energies= | -962.477620 |
| Sum of electronic and thermal Energies= | -962.454169 |
| Sum of electronic and thermal Enthalpies= | -962.453225 |
| Sum of electronic and thermal Free Energies= | -962.531282 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 295.445 | 88.485 | 164.285 |

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.196604 | 1.589361 | 1.442786 |
| 2 | 6 | 0 | -0.843478 | 2.157675 | 1.882118 |
| 3 | 6 | 0 | -0.516227 | 3.457348 | 1.136337 |
| 4 | 6 | 0 | -0.733717 | 3.379641 | -0.376712 |
| 5 | 6 | 0 | -1.643262 | 2.407452 | -0.876904 |
| 6 | 6 | 0 | -2.286117 | 1.474689 | -0.056139 |
| 7 | 8 | 0 | -0.152554 | 4.230613 | -1.106479 |
| 8 | 8 | 0 | -1.306285 | -0.215609 | -0.352986 |
| 9 | 8 | 0 | -1.748319 | -1.335862 | 0.474307 |
| 10 | 6 | 0 | -2.394729 | -2.356342 | -0.328097 |
| 11 | 6 | 0 | -3.623314 | -1.784943 | -1.046118 |
| 12 | 6 | 0 | -1.398309 | -2.950789 | -1.332431 |
| 13 | 6 | 0 | -2.809956 | -3.400019 | 0.716789 |
| 14 | 1 | 0 | -1.832341 | 2.406458 | -1.949529 |
| 15 | 1 | 0 | -3.182745 | 0.996108 | -0.436604 |
| 16 | 1 | 0 | -3.009409 | 2.254360 | 1.778448 |
| 17 | 1 | 0 | -2.380767 | 0.608946 | 1.892704 |
| 18 | 1 | 0 | -0.832722 | 2.328477 | 2.965865 |
| 19 | 1 | 0 | -0.068374 | 1.412492 | 1.667997 |
| 20 | 1 | 0 | -1.156309 | 4.274699 | 1.504300 |
| 21 | 1 | 0 | 0.517984 | 3.774050 | 1.315480 |
| 22 | 1 | 0 | -1.871314 | -3.744320 | -1.921593 |
| 23 | 1 | 0 | -1.043639 | -2.173823 | -2.014507 |
| 24 | 1 | 0 | -0.535642 | -3.378375 | -0.810099 |
| 25 | 1 | 0 | -4.142073 | -2.574337 | -1.601394 |
| 26 | 1 | 0 | -4.324960 | -1.354530 | -0.323713 |
| 27 | 1 | 0 | -3.322617 | -1.006041 | -1.751321 |
| 28 | 1 | 0 | -3.309043 | -4.244000 | 0.229015 |
| 29 | 1 | 0 | -1.935569 | -3.781964 | 1.253944 |

| | | | | | |
|---|---|---|---|---|---|
| 30 | 1 | 0 | -3.501192 | -2.964158 | 1.445484 |
| 31 | 1 | 0 | 0.262622 | -0.229771 | -0.286772 |
| 32 | 7 | 0 | 1.335784 | -0.206811 | -0.368401 |
| 33 | 6 | 0 | 1.893917 | 0.554340 | -1.487806 |
| 34 | 6 | 0 | 3.225068 | -0.057695 | -1.910321 |
| 35 | 1 | 0 | 1.160755 | 0.532130 | -2.298192 |
| 36 | 1 | 0 | 2.022435 | 1.602584 | -1.189418 |
| 37 | 6 | 0 | 2.083764 | -0.851711 | 0.505897 |
| 38 | 7 | 0 | 3.423358 | -0.853636 | 0.426947 |
| 39 | 6 | 0 | 4.292858 | -1.494057 | 1.415052 |
| 40 | 6 | 0 | 4.130706 | -0.195718 | -0.690994 |
| 41 | 1 | 0 | 4.736921 | -2.406991 | 1.000778 |
| 42 | 1 | 0 | 5.098329 | -0.800862 | 1.676866 |
| 43 | 1 | 0 | 3.749038 | -1.742005 | 2.323654 |
| 44 | 1 | 0 | 4.489809 | 0.784944 | -0.350688 |
| 45 | 6 | 0 | 1.380582 | -1.591757 | 1.610894 |
| 46 | 1 | 0 | 3.054898 | -1.042246 | -2.361602 |
| 47 | 1 | 0 | 3.715107 | 0.572808 | -2.658494 |
| 48 | 1 | 0 | 5.007345 | -0.807664 | -0.927468 |
| 49 | 1 | 0 | 1.724240 | -2.629062 | 1.664294 |
| 50 | 1 | 0 | 1.581267 | -1.118518 | 2.578243 |
| 51 | 1 | 0 | 0.304149 | -1.584253 | 1.429658 |

### Intermediate from axial attack with DBU model, orientation A (11) – 6-31G* Gas Phase

E(RB+HF-LYP) = -962.827702437

Zero-point correction= 0.454296 (Hartree/Particle)
Thermal correction to Energy= 0.478235
Thermal correction to Enthalpy= 0.479179
Thermal correction to Gibbs Free Energy= 0.400711
Sum of electronic and zero-point Energies= -962.373406
Sum of electronic and thermal Energies= -962.349467
Sum of electronic and thermal Enthalpies= -962.348523
Sum of electronic and thermal Free Energies= -962.426991

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 300.097 | 90.765 | 165.151 |

C,0,-1.4206363323,2.4546982925,1.1473376434
C,0,-0.1227263744,2.2183812991,1.9253824503
C,0,1.1125726508,2.5952318564,1.0956916452
C,0,1.0884391421,2.1112076017,-0.3659298622
C,0,-0.154798348,1.8637645068,-0.9577603902
C,0,-1.4080938875,1.7377020934,-0.2006262174
O,0,2.2102109366,2.015469041,-0.9575486919
O,0,-1.5068216326,0.2449635562,0.0050508937
O,0,-2.7881115725,-0.1440113165,0.6985761463
C,0,-3.5850726499,-0.9746341532,-0.1645078802
C,0,-3.947991866,-0.249521605,-1.4661423143
C,0,-2.860933017,-2.2983535173,-0.4529145707
C,0,-4.8364489885,-1.2209406912,0.6916294782
H,0,-0.1830635543,1.6515774448,-2.025058952
H,0,-2.3014071251,2.0000476588,-0.77979941
H,0,-1.5459406389,3.5281172861,0.946789862
H,0,-2.2894605061,2.1281180453,1.7298582057
H,0,-0.1389389331,2.7798415542,2.8695637422
H,0,-0.0761509575,1.1570907642,2.1998421344
H,0,1.2185758808,3.6903628688,1.0637479573
H,0,2.034998381,2.2230397333,1.5614921136
H,0,-3.5002327971,-2.9769681387,-1.0295768432
H,0,-1.9477137972,-2.1236432626,-1.0298718369
H,0,-2.5903663896,-2.7948942868,0.4857544245

```
H,0,-4.6034898593,-0.8730781984,-2.0855138157
H,0,-4.4695262413,0.6887369911,-1.2497992241
H,0,-3.0469794491,-0.0197946526,-2.0417141522
H,0,-5.5413965696,-1.8683727542,0.1581239326
H,0,-4.567505383,-1.7044535562,1.6365278764
H,0,-5.3368705181,-0.2744688218,0.9194335905
H,0,0.1173214904,-0.6754868366,-0.6459951309
N,0,1.0794474142,-1.0288274897,-0.7485720637
C,0,1.7377642992,-0.7202387207,-2.0269589645
C,0,3.1613303641,-1.262797555,-2.0148250854
H,0,1.1358042342,-1.165644741,-2.8248939178
H,0,1.7668662481,0.3742588883,-2.1211518919
C,0,1.7205066168,-1.255065291,0.3851881955
N,0,3.0587904854,-1.3031641073,0.4343695162
C,0,3.7918466902,-1.5056718541,1.679593428
C,0,3.8345234094,-0.8071519404,-0.7225192335
H,0,4.7190997136,-2.0412879715,1.4575620898
H,0,4.0469016064,-0.5470964855,2.149896682
H,0,3.2137291549,-2.1050501705,2.3825356437
H,0,3.8522137681,0.2900504709,-0.6770592616
C,0,0.8870974484,-1.4952476306,1.6139519691
H,0,3.1793261397,-2.357792817,-2.0823381562
H,0,3.7083479379,-0.8637997893,-2.8744143176
H,0,4.8487183701,-1.2058178015,-0.6336605895
H,0,0.9354025543,-2.5505448485,1.9075775135
H,0,1.2393514289,-0.8894102556,2.4526729355
H,0,-0.1517762823,-1.2292415319,1.4107180951
```

### Intermediate from axial attack with DBU model, orientation A (11) – 6-31+G** Gas Phase

```
E(RB+HF-LYP) = -962.903855215

 Zero-point correction=                           0.450992 (Hartree/Particle)
 Thermal correction to Energy=                    0.475214
 Thermal correction to Enthalpy=                  0.476159
 Thermal correction to Gibbs Free Energy=         0.396692
 Sum of electronic and zero-point Energies=           -962.452864
 Sum of electronic and thermal Energies=              -962.428641
 Sum of electronic and thermal Enthalpies=            -962.427697
 Sum of electronic and thermal Free Energies=         -962.507163

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 298.202             91.600           167.251

 C,0,-1.4582449036,2.4567701651,1.144188616
 C,0,-0.1940555279,2.2001517827,1.9701795662
 C,0,1.0820338396,2.5489416419,1.189051888
 C,0,1.1011869844,2.0860728707,-0.2775048721
 C,0,-0.1215522588,1.8719131649,-0.9216642196
 C,0,-1.4019423315,1.7487319552,-0.2073481077
 O,0,2.2464978037,1.9688847742,-0.8286752888
 O,0,-1.5177639768,0.2487289513,-0.0158225888
 O,0,-2.8130152534,-0.1351844247,0.649374237
 C,0,-3.6137132952,-0.9474717739,-0.2356858915
 C,0,-3.9725746036,-0.1887535338,-1.5197511431
 C,0,-2.8934927969,-2.2659298481,-0.5560136309
 C,0,-4.8671876108,-1.2108806222,0.6121226402
 H,0,-0.1142986061,1.669901427,-1.9904669454
 H,0,-2.2705164409,2.0187483474,-0.8181681186
 H,0,-1.5638202321,3.5316553992,0.9426622822
 H,0,-2.3513699517,2.1374992125,1.6920873943
 H,0,-0.2344460978,2.7678415345,2.9092148801
 H,0,-0.180235288,1.1403635406,2.2513714247
```

```
H,0,1.221991022,3.639769506,1.1677902038
H,0,1.9748678972,2.1459617216,1.6845039638
H,0,-3.5417655423,-2.9270607029,-1.1418092837
H,0,-1.9863111865,-2.08216237,-1.1383126245
H,0,-2.6185671884,-2.7842575093,0.3687194077
H,0,-4.6263990737,-0.7989368738,-2.1528874247
H,0,-4.4950566946,0.7432102733,-1.2826583898
H,0,-3.0718427512,0.053089214,-2.0899907715
H,0,-5.5701900427,-1.8409227469,0.0567939959
H,0,-4.603131523,-1.7216383154,1.5432504403
H,0,-5.3662423267,-0.2701458154,0.8627228287
H,0,0.1040109096,-0.7648035386,-0.5399136296
N,0,1.0718404662,-1.0845375857,-0.6760402151
C,0,1.6573224871,-0.8201778821,-1.997717022
C,0,3.0814747063,-1.3589469955,-2.045158221
H,0,1.0164674269,-1.2961096324,-2.7454168751
H,0,1.6655281432,0.2661754485,-2.1400321581
C,0,1.779269095,-1.244871127,0.4308939211
N,0,3.1175501111,-1.2765296596,0.4098883346
C,0,3.919380343,-1.3656249532,1.6282903143
C,0,3.8323925701,-0.856335814,-0.8153237949
H,0,4.8415052073,-1.9062638936,1.4011666468
H,0,4.1803871281,-0.3661507489,1.9975810404
H,0,3.3908417595,-1.9103319204,2.4090053867
H,0,3.8779609781,0.2407610996,-0.8213609679
C,0,1.017858089,-1.4301475019,1.7139493699
H,0,3.0932699774,-2.4554773143,-2.0731879216
H,0,3.5771514743,-0.9944788104,-2.9493681208
H,0,4.8405489828,-1.275592098,-0.7651121293
H,0,1.1344824126,-2.45522988,2.0820590016
H,0,1.3762830327,-0.7442235576,2.4847598485
H,0,-0.0415147526,-1.2338038609,1.5439924266
```

### Intermediate from axial attack with DBU model, orientation A (11) – 6-31G* – PCM Dichloroethane

```
E(RB+HF-LYP) =  -962.849221182

Zero-point correction=                           0.453209 (Hartree/Particle)
 Thermal correction to Energy=                    0.477490
 Thermal correction to Enthalpy=                  0.478434
 Thermal correction to Gibbs Free Energy=         0.397738
 Sum of electronic and zero-point Energies=           -962.396013
 Sum of electronic and thermal Energies=              -962.371731
 Sum of electronic and thermal Enthalpies=            -962.370787
 Sum of electronic and thermal Free Energies=         -962.451483

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 299.630             90.957            169.840

 C,0,-1.7487249329,2.277775,1.1812809146
 C,0,-0.3723269329,2.284246,1.8506309146
 C,0,0.6539310671,3.036556,0.9964679146
 C,0,0.6357970671,2.67255,-0.5000670854
 C,0,-0.5338649329,2.126398,-1.0325430854
 C,0,-1.6852469329,1.682136,-0.2240540854
 O,0,1.6880570671,2.945929,-1.1658130854
 O,0,-1.4821769329,0.195797,-0.1503290854
 O,0,-2.5643729329,-0.495811,0.6225569146
 C,0,-3.2893679329,-1.397773,-0.2440600854
 C,0,-3.9747729329,-0.638692,-1.3858430854
 C,0,-2.3548009329,-2.486558,-0.7876250854
 C,0,-4.3275089329,-2.000043,0.7138559146
```

H,0,-0.5601479329,1.925133,-2.1037610854
H,0,-2.6513519329,1.806819,-0.7303190854
H,0,-2.1253569329,3.307155,1.0912269146
H,0,-2.4760109329,1.718654,1.7803149146
H,0,-0.4371329329,2.722677,2.8558949146
H,0,-0.0453319329,1.245229,1.9853169146
H,0,0.4775420671,4.121743,1.0740659146
H,0,1.6745030671,2.872278,1.3657899146
H,0,-2.9148479329,-3.211071,-1.3896870854
H,0,-1.5780649329,-2.046698,-1.4199050854
H,0,-1.8725599329,-3.025284,0.0358009146
H,0,-4.5803519329,-1.323474,-1.9908120854
H,0,-4.6317919329,0.142498,-0.9885310854
H,0,-3.2318459329,-0.171189,-2.0381970854
H,0,-4.9470929329,-2.732008,0.1841599146
H,0,-3.8338219329,-2.505638,1.5505689146
H,0,-4.9809339329,-1.219172,1.1166759146
H,0,0.2439190671,-0.378083,-0.4094470854
N,0,1.2268910671,-0.667037,-0.5231220854
C,0,1.8896850671,-0.252399,-1.7671870854
C,0,3.2346140671,-0.960515,-1.8850690854
H,0,1.2291610671,-0.537232,-2.5928470854
H,0,1.9774990671,0.843321,-1.7690530854
C,0,1.8326740671,-1.188247,0.5285689146
N,0,3.1571660671,-1.371327,0.5487569146
C,0,3.8851750671,-1.932226,1.6856429146
C,0,3.9904410671,-0.87011,-0.5622730854
H,0,4.5099390671,-2.763056,1.3413149146
H,0,4.5324910671,-1.166722,2.1297429146
H,0,3.2043520671,-2.302473,2.4494439146
H,0,4.2812950671,0.166466,-0.3446700854
C,0,0.9710440671,-1.578795,1.7004449146
H,0,3.0897590671,-2.015683,-2.1468280854
H,0,3.8306260671,-0.499128,-2.6786480854
H,0,4.9000000671,-1.477316,-0.5886190854
H,0,1.0279550671,-2.658963,1.8746889146
H,0,1.2959760671,-1.069579,2.6132339146
H,o,-0.0693139329,-1.313794,1.5032999146

## Intermediate from axial attack with DBU model, orientation A (11) – 6-31+G** - PCM Dichloroethane

E(RB+HF-LYP) = -962.932821155

| | |
|---|---|
| Zero-point correction= | 0.450061 (Hartree/Particle) |
| Thermal correction to Energy= | 0.474516 |
| Thermal correction to Enthalpy= | 0.475460 |
| Thermal correction to Gibbs Free Energy= | 0.394258 |
| Sum of electronic and zero-point Energies= | -962.482760 |
| Sum of electronic and thermal Energies= | -962.458305 |
| Sum of electronic and thermal Enthalpies= | -962.457361 |
| Sum of electronic and thermal Free Energies= | -962.538563 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 297.763 | 91.577 | 170.904 |

C,0,-1.7285224066,2.2514444949,1.2362915408
C,0,-0.3060877187,2.334185592,1.7964241962
C,0,0.5993325053,3.170632243,0.8837861176
C,0,0.4621671227,2.8639884112,-0.6135980609
C,0,-0.6736870996,2.2005676627,-1.0646743775
C,0,-1.7407826471,1.6778156158,-0.1807554687
O,0,1.4097341533,3.2924638835,-1.3727976158

```
O,0,-1.4777461051,0.2020372387,-0.149067645
O,0,-2.5373797149,-0.5215252184,0.6099304879
C,0,-3.2319523715,-1.4487411299,-0.2662917077
C,0,-3.9254190641,-0.7083300973,-1.4153587427
C,0,-2.260541874,-2.5112302213,-0.7967425273
C,0,-4.2612402529,-2.0767641016,0.6832105216
H,0,-0.7710389425,2.0192318785,-2.1349727487
H,0,-2.7424148922,1.771282707,-0.6178873949
H,0,-2.170839739,3.2569256264,1.1928090922
H,0,-2.372671772,1.6437689051,1.8810358849
H,0,-0.3187493389,2.7516646355,2.8116322041
H,0,0.0980392037,1.3177613467,1.8833598423
H,0,0.3775699662,4.2411639212,1.0160525757
H,0,1.6554212243,3.047560026,1.1559296897
H,0,-2.7987801915,-3.255806507,-1.3931424239
H,0,-1.4965021898,-2.0555462484,-1.4323624279
H,0,-1.7673067666,-3.0289367361,0.0326799739
H,0,-4.4943394531,-1.4154041588,-2.029008321
H,0,-4.6179559082,0.0456057831,-1.027811174
H,0,-3.1904008888,-0.214303354,-2.0563712345
H,0,-4.8551865731,-2.8227300743,0.1447526398
H,0,-3.7642750374,-2.5722017397,1.5233335051
H,0,-4.9398343766,-1.3146217662,1.0789729531
H,0,0.2906997399,-0.3582911094,-0.327359847
N,0,1.2803641477,-0.6183850742,-0.4279150846
C,0,1.9694658929,-0.1762066098,-1.6472664216
C,0,3.2446886622,-0.9917893523,-1.8265660999
H,0,1.2813023711,-0.3281939011,-2.4835921043
H,0,2.1619473046,0.9011043089,-1.5781764892
C,0,1.8621813917,-1.2249784923,0.594097683
N,0,3.1738550304,-1.4793212018,0.597088524
C,0,3.879029033,-2.1119888367,1.7135237989
C,0,4.0306558048,-1.0279766316,-0.5196616508
H,0,4.4059693995,-3.0012408855,1.3532680681
H,0,4.6119948667,-1.4114057515,2.1286973859
H,0,3.1922485531,-2.4082580031,2.502550681
H,0,4.4387791039,-0.0387109014,-0.2724831904
C,0,0.9858070405,-1.6218597915,1.7507605146
H,0,2.998463997,-2.0154947978,-2.1328966478
H,0,3.8643786047,-0.5487175253,-2.6117652929
H,0,4.8685877206,-1.7274748351,-0.590048748
H,0,1.0075984194,-2.706707013,1.895360331
H,0,1.3239257592,-1.1475566042,2.6770632735
H,0,-0.0435951878,-1.3169430562,1.5585681596
```

## Ts 2 from axial attack with DBU model, orientation A (12) – 6-31G* - Gas Phase

```
E(RB+HF-LYP) = -962.822771071

 Zero-point correction=                           0.452274 (Hartree/Particle)
 Thermal correction to Energy=                    0.476067
 Thermal correction to Enthalpy=                  0.477011
 Thermal correction to Gibbs Free Energy=         0.398497
 Sum of electronic and zero-point Energies=           -962.370497
 Sum of electronic and thermal Energies=              -962.346704
 Sum of electronic and thermal Enthalpies=            -962.345760
 Sum of electronic and thermal Free Energies=         -962.424274

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  298.736             89.428           165.246

 C,0,-1.8042348647,2.3699884006,1.138601134
```

```
C,0,-0.3839926168,2.4379513141,1.7093511269
C,0,0.5507990684,3.2514924264,0.8043689148
C,0,0.4890272201,2.8713725298,-0.6831441008
C,0,-0.7458124322,2.3516325274,-1.1833257506
C,0,-1.813609273,1.8554570056,-0.2974398267
O,0,1.4873549036,3.0894371541,-1.401406958
O,0,-1.3060027221,0.5219837402,-0.4286528848
O,0,-2.1942635608,-0.7277042016,0.6197156565
C,0,-2.9483633404,-1.5875473961,-0.1960477023
C,0,-4.0363173742,-0.8159476809,-0.9673811679
C,0,-2.0523376633,-2.3604273809,-1.1853832709
C,0,-3.6167735755,-2.5772277932,0.7869288228
H,0,-0.8403789777,2.2070855856,-2.2546094101
H,0,-2.8233447397,1.9036974418,-0.7227299212
H,0,-2.2609330733,3.3703521047,1.1448706768
H,0,-2.434729336,1.7104792295,1.7442940329
H,0,-0.4005229215,2.8625505033,2.7215963068
H,0,0.001030035,1.4155423869,1.8075201008
H,0,0.2891363771,4.3191759604,0.8673201371
H,0,1.596238391,3.1766841936,1.1261453107
H,0,-2.6325570002,-3.0573907212,-1.8033227543
H,0,-1.5406804754,-1.6552979189,-1.8480448076
H,0,-1.2945698523,-2.9397223257,-0.6428567102
H,0,-4.6932913718,-1.4928027836,-1.5284308409
H,0,-4.6509135997,-0.2372738442,-0.2688509295
H,0,-3.5738310209,-0.121409487,-1.675509213
H,0,-4.244342575,-3.3022758436,0.2527574654
H,0,-2.8560426122,-3.1284987923,1.3511168129
H,0,-4.242967386,-2.0328310535,1.5014032794
H,0,0.2276384867,-0.0767626797,-0.3332745609
N,0,1.2082877106,-0.4479843183,-0.3808162472
C,0,1.9967846538,-0.0564030846,-1.5543248889
C,0,3.1661462614,-1.0186914222,-1.721953934
H,0,1.32186257,-0.0878600016,-2.4136315774
H,0,2.3134529515,0.9873715355,-1.4437363322
C,0,1.6629116965,-1.1499823642,0.6331500347
N,0,2.949079077,-1.5489558181,0.6821669575
C,0,3.5427102834,-2.232628502,1.8258247284
C,0,3.8919283033,-1.1827402623,-0.3889414841
H,0,3.9311091758,-3.2121470861,1.5222387773
H,0,4.3749523469,-1.6372164189,2.2204709793
H,0,2.8149452148,-2.3738723441,2.6215683927
H,0,4.4109068336,-0.2558887111,-0.1084058539
C,0,0.6935367639,-1.4983046835,1.7296832044
H,0,2.8075780634,-1.9971019858,-2.063388684
H,0,3.8632195904,-0.6389010906,-2.4747523082
H,0,4.6428803822,-1.9775332802,-0.4487097412
H,0,0.740247809,-2.5680777814,1.957484341
H,0,0.9345548443,-0.945462205,2.6450345173
H,0,-0.3333432729,-1.2537269779,1.4199359952
```

### Ts 2 from axial attack with DBU model, orientation A (12) – 6-31+G** - Gas Phase

```
E(RB+HF-LYP) = -962.899796469

 Zero-point correction=                           0.448861 (Hartree/Particle)
 Thermal correction to Energy=                    0.472906
 Thermal correction to Enthalpy=                  0.473851
 Thermal correction to Gibbs Free Energy=         0.394685
 Sum of electronic and zero-point Energies=           -962.450936
 Sum of electronic and thermal Energies=              -962.426890
 Sum of electronic and thermal Enthalpies=            -962.425946
 Sum of electronic and thermal Free Energies=         -962.505111
```

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 296.753 | 90.250 | 166.617 |

```
C,0,-1.8219827801,2.3823585275,1.1462088355
C,0,-0.4156148268,2.4411258503,1.7518379648
C,0,0.5554356974,3.2309034465,0.8627129178
C,0,0.5151794587,2.8506501478,-0.621612318
C,0,-0.7105713871,2.3392113272,-1.1500931434
C,0,-1.8017717058,1.8545671761,-0.2849642409
O,0,1.5315802475,3.0614109454,-1.324670067
O,0,-1.2986139381,0.5102917624,-0.393956698
O,0,-2.2189012045,-0.7479856594,0.614420005
C,0,-2.9888493337,-1.5840769457,-0.2188377536
C,0,-4.0574918617,-0.784168955,-0.9886287205
C,0,-2.1013114923,-2.3649753096,-1.2103288916
C,0,-3.6822130683,-2.5727895219,0.7485617675
H,0,-0.7844200871,2.1942786156,-2.2227607118
H,0,-2.7990936572,1.9060790641,-0.7364103457
H,0,-2.2673869635,3.3872117146,1.1263834775
H,0,-2.4749814032,1.739527889,1.7454569875
H,0,-0.4535587394,2.8825543322,2.7556215971
H,0,-0.0479560805,1.4159291889,1.8761823727
H,0,0.3164101837,4.3040024772,0.9111439803
H,0,1.5914916942,3.1352604448,1.2065002073
H,0,-2.6943918386,-3.0478822972,-1.8307260026
H,0,-1.5776544551,-1.6667644039,-1.8703243217
H,0,-1.3560039244,-2.9584616106,-0.6677959596
H,0,-4.7159313508,-1.4464973481,-1.5637728681
H,0,-4.671665326,-0.2075511399,-0.2889878523
H,0,-3.5793812377,-0.0886016749,-1.6843716455
H,0,-4.3145406859,-3.2785315298,0.1954065035
H,0,-2.9359047259,-3.1429064119,1.3116873595
H,0,-4.3072617777,-2.0272093908,1.4620314967
H,0,0.2230765291,-0.1228763956,-0.3694814517
N,0,1.2043917438,-0.4910396697,-0.4232255109
C,0,1.973806336,-0.136033782,-1.6215586093
C,0,3.1701871636,-1.0710249585,-1.7551124294
H,0,1.2972771389,-0.2265693112,-2.4751168868
H,0,2.2674246682,0.9186540382,-1.5591708398
C,0,1.684762426,-1.1390647452,0.6157976327
N,0,2.9785688206,-1.5143441198,0.6668379083
C,0,3.5962498696,-2.138078906,1.8338663627
C,0,3.9063210791,-1.15403764,-0.4206971312
H,0,4.0620114257,-3.0872081152,1.5468070695
H,0,4.3718813432,-1.4792757002,2.2423053772
H,0,2.8633961928,-2.3308705297,2.6130693723
H,0,4.3877450513,-0.1964933515,-0.1799171636
C,0,0.7355242184,-1.4560918284,1.7382087182
H,0,2.8407046148,-2.0736376473,-2.0521315875
H,0,3.850476152,-0.7020248989,-2.52766326
H,0,4.6866295079,-1.9206922282,-0.4517060626
H,0,0.7650740752,-2.5243860436,1.9735224742
H,0,1.0076372518,-0.9009510248,2.6421618275
H,0,-0.2903071248,-1.1969998708,1.4482583879
```

## Ts 2 from axial attack with DBU model, orientation A (12) – 6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.843032970

 Zero-point correction=                           0.451265 (Hartree/Particle)
 Thermal correction to Energy=                    0.475487
```

```
Thermal correction to Enthalpy=                  0.476431
Thermal correction to Gibbs Free Energy=         0.395373
Sum of electronic and zero-point Energies=           -962.391768
Sum of electronic and thermal Energies=              -962.367546
Sum of electronic and thermal Enthalpies=            -962.366602
Sum of electronic and thermal Free Energies=         -962.447660

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  298.373             89.913            170.601

C,0,-2.287932946,1.5537454503,1.5906728803
C,0,-0.8974947579,2.0912444435,1.9465919829
C,0,-0.50643307,3.2851330347,1.0648385358
C,0,-0.7731215932,3.1075300184,-0.4350697994
C,0,-1.7944834285,2.192213975,-0.8318389411
C,0,-2.4066979846,1.2271658215,0.1058826463
O,0,-0.1539008576,3.8342335051,-1.2459352112
O,0,-1.4705831786,0.2745803894,-0.3621627465
O,0,-1.6927366278,-1.4018379147,0.5478164015
C,0,-2.1648355868,-2.3618536822,-0.3579673103
C,0,-3.5500500419,-1.9712981275,-0.9135096779
C,0,-1.179866986,-2.5767242595,-1.5266737334
C,0,-2.2928062424,-3.6728421648,0.4549449948
H,0,-2.0570603292,2.142280787,-1.8848031198
H,0,-3.4297805753,0.9240151179,-0.1510580791
H,0,-3.0579011607,2.2990125823,1.8397243563
H,0,-2.5087829849,0.6443767366,2.1603420942
H,0,-0.8613431993,2.378899615,3.0051540558
H,0,-0.1639678312,1.2871774089,1.8186168069
H,0,-1.0786257124,4.1748411859,1.3735903598
H,0,0.5505480288,3.5491895804,1.1922137754
H,0,-1.5337396059,-3.3471095637,-2.2242043614
H,0,-1.0542449255,-1.6404329195,-2.0797175736
H,0,-0.198727535,-2.8871340622,-1.1472341441
H,0,-3.972490244,-2.75944173,-1.5502859904
H,0,-4.2455164235,-1.7850656379,-0.0868110167
H,0,-3.4696650284,-1.0554927165,-1.5077151987
H,0,-2.6780294824,-4.4916157751,-0.1668768472
H,0,-1.3167360532,-3.9725851359,0.8531703156
H,0,-2.9758643016,-3.5277879408,1.2994532739
H,0,0.2453714166,-0.0550444125,-0.1400182137
N,0,1.2716765013,-0.0556100629,-0.2760975734
C,0,1.7836662241,0.758279171,-1.3821809419
C,0,3.1131872857,0.1815756683,-1.8541639638
H,0,1.0287259886,0.7419736334,-2.1719054144
H,0,1.888742714,1.79981205,-1.0561021909
C,0,2.0299013564,-0.7727179928,0.5356691549
N,0,3.361779523,-0.7777395891,0.4153094701
C,0,4.2524776107,-1.4932445719,1.3291241458
C,0,4.0391223812,-0.0241420872,-0.6592534024
H,0,4.6849874462,-2.3704371011,0.8336066747
H,0,5.06492432,-0.8215770505,1.6252776005
H,0,3.726197616,-1.810280605,2.2272388978
H,0,4.3819770172,0.9362008376,-0.2512631787
C,0,1.3347895408,-1.5775440245,1.5976049076
H,0,2.9445202543,-0.7766333042,-2.3599242077
H,0,3.5878328893,0.8589768756,-2.5706722332
H,0,4.9248828556,-0.5979481496,-0.9505999897
H,0,1.709936885,-2.6054899258,1.6103009485
H,0,1.5146290519,-1.1398647197,2.5869178032
H,0,0.2562414817,-1.5942999683,1.3933251
```

## Ts 2 from axial attack with DBU model, orientation A (12) – 6-31+G** - PCM Dichloroethane

E(RB+HF-LYP) = -962.926859787

| | |
|---|---|
| Zero-point correction= | 0.447998 (Hartree/Particle) |
| Thermal correction to Energy= | 0.471364 |
| Thermal correction to Enthalpy= | 0.472309 |
| Thermal correction to Gibbs Free Energy= | 0.394614 |
| Sum of electronic and zero-point Energies= | -962.478862 |
| Sum of electronic and thermal Energies= | -962.455495 |
| Sum of electronic and thermal Enthalpies= | -962.454551 |
| Sum of electronic and thermal Free Energies= | -962.532246 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 295.786 | 88.451 | 163.522 |

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.914808 | -0.851066 | -1.831361 |
| 2 | 6 | 0 | -1.205791 | -2.102165 | -1.301821 |
| 3 | 6 | 0 | -2.172461 | -3.009988 | -0.530102 |
| 4 | 6 | 0 | -3.096183 | -2.284679 | 0.451876 |
| 5 | 6 | 0 | -3.315865 | -0.902658 | 0.287172 |
| 6 | 6 | 0 | -2.587240 | -0.072403 | -0.701145 |
| 7 | 8 | 0 | -3.697958 | -2.990243 | 1.323002 |
| 8 | 8 | 0 | -1.662145 | 0.420350 | 0.275339 |
| 9 | 8 | 0 | -0.600596 | 1.633380 | -0.424276 |
| 10 | 6 | 0 | -0.848899 | 2.899332 | 0.192083 |
| 11 | 6 | 0 | -2.287545 | 3.361080 | -0.087351 |
| 12 | 6 | 0 | -0.587522 | 2.837489 | 1.706676 |
| 13 | 6 | 0 | 0.150949 | 3.862337 | -0.481079 |
| 14 | 1 | 0 | -4.007582 | -0.406146 | 0.963933 |
| 15 | 1 | 0 | -3.181701 | 0.760111 | -1.101108 |
| 16 | 1 | 0 | -2.689812 | -1.132957 | -2.558851 |
| 17 | 1 | 0 | -1.209793 | -0.189681 | -2.347594 |
| 18 | 1 | 0 | -0.744456 | -2.659106 | -2.127361 |
| 19 | 1 | 0 | -0.394431 | -1.787702 | -0.636070 |
| 20 | 1 | 0 | -2.828513 | -3.544901 | -1.234501 |
| 21 | 1 | 0 | -1.630878 | -3.785189 | 0.025564 |
| 22 | 1 | 0 | -0.772366 | 3.810525 | 2.175604 |
| 23 | 1 | 0 | -1.243473 | 2.096222 | 2.170913 |
| 24 | 1 | 0 | 0.453498 | 2.559718 | 1.907881 |
| 25 | 1 | 0 | -2.455918 | 4.367707 | 0.312124 |
| 26 | 1 | 0 | -2.478303 | 3.380899 | -1.165517 |
| 27 | 1 | 0 | -3.003606 | 2.680856 | 0.381380 |
| 28 | 1 | 0 | 0.029644 | 4.874989 | -0.078831 |
| 29 | 1 | 0 | 1.182922 | 3.545052 | -0.297493 |
| 30 | 1 | 0 | -0.017034 | 3.897345 | -1.562302 |
| 31 | 1 | 0 | 0.691683 | 0.662319 | 0.067320 |
| 32 | 7 | 0 | 1.497985 | 0.050138 | 0.338733 |
| 33 | 6 | 0 | 1.475155 | -0.582713 | 1.659175 |
| 34 | 6 | 0 | 2.905706 | -0.782539 | 2.147817 |
| 35 | 1 | 0 | 0.902869 | 0.063017 | 2.328202 |
| 36 | 1 | 0 | 0.943615 | -1.540081 | 1.594505 |
| 37 | 6 | 0 | 2.488356 | -0.099340 | -0.524543 |
| 38 | 7 | 0 | 3.558963 | -0.849448 | -0.242887 |
| 39 | 6 | 0 | 4.658397 | -1.078931 | -1.183236 |
| 40 | 6 | 0 | 3.717225 | -1.501478 | 1.075203 |
| 41 | 1 | 0 | 5.545740 | -0.514264 | -0.875411 |
| 42 | 1 | 0 | 4.902598 | -2.145555 | -1.183160 |
| 43 | 1 | 0 | 4.384306 | -0.790912 | -2.195569 |
| 44 | 1 | 0 | 3.413401 | -2.552703 | 0.982982 |
| 45 | 6 | 0 | 2.362661 | 0.603024 | -1.848817 |
| 46 | 1 | 0 | 3.362028 | 0.189292 | 2.370679 |
| 47 | 1 | 0 | 2.913956 | -1.374768 | 3.067649 |

| | | | | | |
|---|---|---|---|---|---|
| 48 | 1 | 0 | 4.783746 | -1.482954 | 1.320668 |
| 49 | 1 | 0 | 3.216745 | 1.264180 | -2.023220 |
| 50 | 1 | 0 | 2.319915 | -0.121902 | -2.668121 |
| 51 | 1 | 0 | 1.445346 | 1.192051 | -1.861023 |

## Ts 1 from axial attack with DBU model, orientation B – 6-31G* - Gas Phase

E(RB+HF-LYP) = -962.823755913

Zero-point correction= 0.452744 (Hartree/Particle)
Thermal correction to Energy= 0.476284
Thermal correction to Enthalpy= 0.477228
Thermal correction to Gibbs Free Energy= 0.399923
Sum of electronic and zero-point Energies= -962.371012
Sum of electronic and thermal Energies= -962.347472
Sum of electronic and thermal Enthalpies= -962.346528
Sum of electronic and thermal Free Energies= -962.423833

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 298.872 | 89.230 | 162.701 |

C,0,-1.2350469784,2.4225336598,0.9535541259
C,0,0.0343260457,2.1033952631,1.7492164827
C,0,1.2991704223,2.5681560694,1.0149309189
C,0,1.3469636233,2.1557922271,-0.4661334813
C,0,0.1092105197,2.0502135863,-1.1482259083
C,0,-1.134602872,1.9574935224,-0.4816774422
O,0,2.4756453271,1.9905262608,-0.9981388014
O,0,-1.4259160182,0.1839751023,-0.4019463337
O,0,-2.4543674129,-0.2967103373,0.5345546901
C,0,-3.5744664325,-0.8530618264,-0.1837910918
C,0,-4.2230684805,0.2008762198,-1.0890036361
C,0,-3.1248554164,-2.075261327,-0.9958842346
C,0,-4.5254055897,-1.2644108466,0.948200782
H,0,0.1413978847,1.9129269865,-2.2262480693
H,0,-2.023967518,2.173864425,-1.0715597498
H,0,-1.3999940165,3.5110252818,0.9345612144
H,0,-2.1118871927,1.9710866751,1.4287246137
H,0,-0.0199554757,2.5537066484,2.7494667528
H,0,0.0745816543,1.0172270864,1.8987521865
H,0,1.3634736285,3.6667371555,1.0462213416
H,0,2.2107495573,2.1986675594,1.5016788636
H,0,-3.9735674871,-2.5412174629,-1.5100670352
H,0,-2.3870628674,-1.775535983,-1.7452199874
H,0,-2.6679835907,-2.8237769602,-0.3380362468
H,0,-5.1160837199,-0.2043919176,-1.5794393255
H,0,-4.5202235426,1.0772987642,-0.5026776487
H,0,-3.519738208,0.5214278116,-1.8619472687
H,0,-5.430521491,-1.7277917638,0.5401003325
H,0,-4.0398073883,-1.9838764191,1.6163010724
H,0,-4.8193672767,-0.3908564918,1.5394582178
H,0,-0.1643856493,-0.8254250259,-0.2174972522
N,0,0.7237334473,-1.3472910854,0.0533098507
C,0,0.8218397645,-1.7721837944,1.4477603755
C,0,2.1363057511,-1.2824899987,2.0498377465
H,0,-0.0487864969,-1.3680175481,1.9690410997
H,0,0.7584526082,-2.8677052044,1.4959668364
C,0,1.7841034895,-1.1544911675,-0.7132422238
N,0,3.0307164782,-1.3693270107,-0.2699807244
C,0,4.1888401923,-0.9616583581,-1.0760456003
C,0,3.2978526654,-1.6895101957,1.1459964178
H,0,4.285513571,0.1299938066,-1.0550791255

```
H,0,5.081658821,-1.432580136,-0.6597088111
H,0,4.081597759,-1.2957040665,-2.1089514309
H,0,3.5047549932,-2.7649500428,1.2303490602
C,0,1.5618374654,-0.7173229488,-2.1300193533
H,0,2.1098181173,-0.1924326648,2.1439863677
H,0,2.2868059353,-1.7037640713,3.0488816607
H,0,4.206166308,-1.1551324043,1.4386346539
H,0,2.028561694,0.2652912465,-2.2753174694
H,0,1.9944762056,-1.4493166316,-2.8213576141
H,0,0.4932535204,-0.631200695,-2.3209208291
```

## Ts 1 from axial attack with DBU model, orientation B – 6-31+G** - Gas Phase

```
E(RB+HF-LYP) = -962.900565519

 Zero-point correction=                           0.449017 (Hartree/Particle)
 Thermal correction to Energy=                    0.472991
 Thermal correction to Enthalpy=                  0.473936
 Thermal correction to Gibbs Free Energy=         0.395050
 Sum of electronic and zero-point Energies=           -962.451548
 Sum of electronic and thermal Energies=              -962.427574
 Sum of electronic and thermal Enthalpies=            -962.426630
 Sum of electronic and thermal Free Energies=         -962.505515

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 296.807             90.216            166.028

 C,0,-1.2821683242,2.4586358971,1.0046404393
 C,0,-0.0255535369,2.1515352691,1.8262298902
 C,0,1.2533372487,2.6002155145,1.1049068617
 C,0,1.3237373468,2.1719955113,-0.3689097871
 C,0,0.0998825183,2.0645583954,-1.0742168644
 C,0,-1.1586700919,1.9765505126,-0.423333971
 O,0,2.4632811664,1.9896282859,-0.8807577027
 O,0,-1.4186798123,0.2182236543,-0.3373623056
 O,0,-2.5063657303,-0.2845626934,0.5236506515
 C,0,-3.5821988637,-0.8412703966,-0.2672679799
 C,0,-4.2030866121,0.2272576726,-1.1760925359
 C,0,-3.0777182552,-2.0365655703,-1.0871729437
 C,0,-4.5827883372,-1.2955151578,0.8044568939
 H,0,0.1485483996,1.9159863111,-2.1494013046
 H,0,-2.0357505632,2.1907499411,-1.0315991666
 H,0,-1.4479625491,3.5458927729,0.9665294601
 H,0,-2.1672064926,2.0132434242,1.4702481778
 H,0,-0.0945117221,2.6236081242,2.8148497613
 H,0,0.0114294528,1.0693487918,2.0004699912
 H,0,1.3235270781,3.6981538535,1.1165694517
 H,0,2.1537499064,2.2345155477,1.6123900945
 H,0,-3.9010211156,-2.502847771,-1.6397524461
 H,0,-2.3212507726,-1.7098752484,-1.8054038998
 H,0,-2.6334870216,-2.7912475278,-0.4291620269
 H,0,-5.0691313044,-0.1793268621,-1.7104400442
 H,0,-4.5354641935,1.0865766562,-0.5847972889
 H,0,-3.4751838731,0.5711984112,-1.9151313076
 H,0,-5.4593368377,-1.7531858754,0.3336970373
 H,0,-4.1250725583,-2.0316849689,1.4729418002
 H,0,-4.9170902384,-0.4444213141,1.405755524
 H,0,-0.1399398818,-0.7744922029,-0.1368332921
 N,0,0.7510559734,-1.2993871062,0.1118918967
 C,0,0.9096782107,-1.7024472831,1.5079533966
 C,0,2.2599823538,-1.2210075828,2.0327129835
 H,0,0.0757334359,-1.2750806512,2.0681707729
```

```
H,0,0.8324275942,-2.7956022616,1.5798267436
C,0,1.7795557853,-1.1812990971,-0.7120069417
N,0,3.0339359986,-1.4500860108,-0.3205791457
C,0,4.177182884,-1.2084878605,-1.2080970777
C,0,3.3698225619,-1.6922239895,1.0974978187
H,0,4.4338016067,-0.1429715211,-1.2138577482
H,0,5.0244771596,-1.7928209071,-0.8433171787
H,0,3.9583032781,-1.5310596753,-2.2254095104
H,0,3.5733488805,-2.7630670467,1.2305463598
C,0,1.5136570346,-0.7638713741,-2.1265876072
H,0,2.2608288624,-0.1281911352,2.0829419519
H,0,2.4443524541,-1.6056942988,3.040248207
H,0,4.29547561,-1.1493476981,1.3101989031
H,0,2.0255132823,0.1852784632,-2.3198833167
H,0,1.8676652097,-1.5317446761,-2.8220356339
H,0,0.4444865814,-0.6202555765,-2.2700699268
```

## Ts 1 from axial attack with DBU model, orientation B – 6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.841832029

 Zero-point correction=                           0.450623 (Hartree/Particle)
 Thermal correction to Energy=                    0.474920
 Thermal correction to Enthalpy=                  0.475864
 Thermal correction to Gibbs Free Energy=         0.394191
 Sum of electronic and zero-point Energies=           -962.391209
 Sum of electronic and thermal Energies=              -962.366912
 Sum of electronic and thermal Enthalpies=            -962.365968
 Sum of electronic and thermal Free Energies=         -962.447641

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 298.017             89.877            171.895

    1          6             0       -1.651611    2.180524    1.296383
    2          6             0       -0.233811    2.169250    1.876477
    3          6             0        0.674278    3.175063    1.158877
    4          6             0        0.611155    3.084845   -0.372729
    5          6             0       -0.596124    2.600279   -0.952715
    6          6             0       -1.635904    2.041550   -0.204556
    7          8             0        1.589685    3.503119   -1.036850
    8          8             0       -1.379345    0.125426   -0.393911
    9          8             0       -2.190952   -0.734726    0.468925
   10          6             0       -3.140666   -1.485049   -0.316895
   11          6             0       -4.080506   -0.541944   -1.078166
   12          6             0       -2.401061   -2.421134   -1.282284
   13          6             0       -3.907942   -2.283819    0.744116
   14          1             0       -0.664044    2.624025   -2.039910
   15          1             0       -2.614819    1.967407   -0.670849
   16          1             0       -2.150450    3.132000    1.545093
   17          1             0       -2.258440    1.377861    1.727473
   18          1             0       -0.258306    2.373350    2.954964
   19          1             0        0.179347    1.160905    1.752092
   20          1             0        0.385220    4.202353    1.434054
   21          1             0        1.722037    3.060924    1.462600
   22          1             0       -3.107119   -3.013247   -1.876241
   23          1             0       -1.776670   -1.834908   -1.961772
   24          1             0       -1.755616   -3.111374   -0.726402
   25          1             0       -4.842388   -1.108999   -1.625993
   26          1             0       -4.588554    0.133958   -0.380975
   27          1             0       -3.512337    0.058677   -1.793324
   28          1             0       -4.661205   -2.923776    0.271464
   29          1             0       -3.223770   -2.919986    1.316307
```

| | | | | | |
|---|---|---|---|---|---|
| 30 | 1 | 0 | -4.415786 | -1.608791 | 1.441653 |
| 31 | 1 | 0 | 0.016149 | -0.534442 | -0.117051 |
| 32 | 7 | 0 | 0.940221 | -1.033020 | 0.115980 |
| 33 | 6 | 0 | 0.989689 | -1.833480 | 1.339517 |
| 34 | 6 | 0 | 2.394652 | -1.786199 | 1.930525 |
| 35 | 1 | 0 | 0.240768 | -1.430942 | 2.025577 |
| 36 | 1 | 0 | 0.699685 | -2.866626 | 1.106146 |
| 37 | 6 | 0 | 1.987304 | -0.806772 | -0.652112 |
| 38 | 7 | 0 | 3.199600 | -1.301560 | -0.359982 |
| 39 | 6 | 0 | 4.378848 | -1.121080 | -1.204405 |
| 40 | 6 | 0 | 3.414336 | -2.123901 | 0.846167 |
| 41 | 1 | 0 | 5.170889 | -0.630265 | -0.628078 |
| 42 | 1 | 0 | 4.745789 | -2.097366 | -1.542751 |
| 43 | 1 | 0 | 4.153742 | -0.509776 | -2.075374 |
| 44 | 1 | 0 | 3.358371 | -3.184927 | 0.566635 |
| 45 | 6 | 0 | 1.765480 | 0.038142 | -1.877704 |
| 46 | 1 | 0 | 2.598141 | -0.785186 | 2.328961 |
| 47 | 1 | 0 | 2.489262 | -2.499569 | 2.755236 |
| 48 | 1 | 0 | 4.432007 | -1.927572 | 1.198758 |
| 49 | 1 | 0 | 2.269997 | 1.006591 | -1.787395 |
| 50 | 1 | 0 | 2.127081 | -0.470928 | -2.776092 |
| 51 | 1 | 0 | 0.698461 | 0.234492 | -1.985082 |

## Ts 1 from axial attack with DBU model, orientation B – 6-31+G** - PCM Dichloroethane

E(RB+HF-LYP) = -962.924560565

| | |
|---|---|
| Zero-point correction= | 0.447056 (Hartree/Particle) |
| Thermal correction to Energy= | 0.470654 |
| Thermal correction to Enthalpy= | 0.471598 |
| Thermal correction to Gibbs Free Energy= | 0.392933 |
| Sum of electronic and zero-point Energies= | -962.477505 |
| Sum of electronic and thermal Energies= | -962.453907 |
| Sum of electronic and thermal Enthalpies= | -962.452962 |
| Sum of electronic and thermal Free Energies= | -962.531628 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 295.340 | 88.625 | 165.566 |

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.027501 | 1.705476 | 1.484703 |
| 2 | 6 | 0 | -0.648821 | 2.298507 | 1.793033 |
| 3 | 6 | 0 | -0.381843 | 3.551824 | 0.950066 |
| 4 | 6 | 0 | -0.704786 | 3.383481 | -0.536172 |
| 5 | 6 | 0 | -1.636073 | 2.377138 | -0.912325 |
| 6 | 6 | 0 | -2.221282 | 1.497745 | 0.005138 |
| 7 | 8 | 0 | -0.186512 | 4.195142 | -1.352873 |
| 8 | 8 | 0 | -1.286661 | -0.222501 | -0.252303 |
| 9 | 8 | 0 | -1.838954 | -1.312785 | 0.549192 |
| 10 | 6 | 0 | -2.472997 | -2.307066 | -0.293104 |
| 11 | 6 | 0 | -3.638380 | -1.692261 | -1.078532 |
| 12 | 6 | 0 | -1.444407 | -2.936936 | -1.242466 |
| 13 | 6 | 0 | -2.981958 | -3.338384 | 0.722039 |
| 14 | 1 | 0 | -1.896444 | 2.309003 | -1.967740 |
| 15 | 1 | 0 | -3.143863 | 1.002445 | -0.279580 |
| 16 | 1 | 0 | -2.816169 | 2.392191 | 1.834210 |
| 17 | 1 | 0 | -2.179619 | 0.756376 | 2.007902 |
| 18 | 1 | 0 | -0.561963 | 2.532992 | 2.861293 |
| 19 | 1 | 0 | 0.113645 | 1.543144 | 1.568217 |
| 20 | 1 | 0 | -0.999176 | 4.388445 | 1.313371 |
| 21 | 1 | 0 | 0.660575 | 3.880194 | 1.036752 |
| 22 | 1 | 0 | -1.907961 | -3.729472 | -1.840437 |
| 23 | 1 | 0 | -1.042065 | -2.179914 | -1.920386 |

| | | | | | |
|---|---|---|---|---|---|
| 24 | 1 | 0 | -0.615907 | -3.372912 | -0.673972 |
| 25 | 1 | 0 | -4.141177 | -2.458413 | -1.679431 |
| 26 | 1 | 0 | -4.374138 | -1.253788 | -0.395734 |
| 27 | 1 | 0 | -3.272842 | -0.910961 | -1.749824 |
| 28 | 1 | 0 | -3.485508 | -4.161162 | 0.203609 |
| 29 | 1 | 0 | -2.150875 | -3.752612 | 1.302116 |
| 30 | 1 | 0 | -3.694455 | -2.879375 | 1.415155 |
| 31 | 1 | 0 | 0.215773 | -0.470688 | 0.049059 |
| 32 | 7 | 0 | 1.245799 | -0.709125 | 0.264896 |
| 33 | 6 | 0 | 1.562527 | -1.328209 | 1.552338 |
| 34 | 6 | 0 | 2.971159 | -0.929845 | 1.980906 |
| 35 | 1 | 0 | 0.809713 | -1.000061 | 2.273008 |
| 36 | 1 | 0 | 1.477433 | -2.419180 | 1.461515 |
| 37 | 6 | 0 | 2.163305 | -0.419532 | -0.637388 |
| 38 | 7 | 0 | 3.465684 | -0.668420 | -0.432594 |
| 39 | 6 | 0 | 4.508150 | -0.415001 | -1.428295 |
| 40 | 6 | 0 | 3.949707 | -1.223152 | 0.848076 |
| 41 | 1 | 0 | 5.122891 | 0.441234 | -1.127561 |
| 42 | 1 | 0 | 5.149600 | -1.299141 | -1.500524 |
| 43 | 1 | 0 | 4.082956 | -0.220569 | -2.410156 |
| 44 | 1 | 0 | 4.104063 | -2.303992 | 0.727222 |
| 45 | 6 | 0 | 1.694587 | 0.204004 | -1.923754 |
| 46 | 1 | 0 | 2.997497 | 0.138114 | 2.227396 |
| 47 | 1 | 0 | 3.271016 | -1.485583 | 2.874545 |
| 48 | 1 | 0 | 4.924388 | -0.768599 | 1.052819 |
| 49 | 1 | 0 | 2.205837 | 1.153222 | -2.108458 |
| 50 | 1 | 0 | 1.893521 | -0.461968 | -2.769938 |
| 51 | 1 | 0 | 0.621567 | 0.388260 | -1.868265 |

## Intermediate from axial attack with DBU model, orientation B – 6-31G* Gas Phase

E(RB+HF-LYP) = -962.826959810

| | |
|---|---|
| Zero-point correction= | 0.454082 (Hartree/Particle) |
| Thermal correction to Energy= | 0.477971 |
| Thermal correction to Enthalpy= | 0.478915 |
| Thermal correction to Gibbs Free Energy= | 0.400278 |
| Sum of electronic and zero-point Energies= | -962.372878 |
| Sum of electronic and thermal Energies= | -962.348989 |
| Sum of electronic and thermal Enthalpies= | -962.348044 |
| Sum of electronic and thermal Free Energies= | -962.426682 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 299.932 | 90.708 | 165.507 |

C,0,-1.2067163348,2.431667423,1.1759262679
C,0,0.1051717461,2.1348452451,1.9078141346
C,0,1.3194110069,2.4973336256,1.0432149439
C,0,1.2394586156,2.0116624067,-0.4153035152
C,0,-0.0252489134,1.7852805507,-0.9632974225
C,0,-1.268460059,1.7317257703,-0.1796618544
O,0,2.3452101904,1.9012684967,-1.0404310551
O,0,-1.4831496916,0.2494140858,0.0139533037
O,0,-2.7738958304,-0.0278955009,0.7281728434
C,0,-3.656581105,-0.7891131164,-0.1155230659
C,0,-3.9913425533,-0.0339738898,-1.4075630559
C,0,-3.0511061386,-2.1671593573,-0.4220168528
C,0,-4.901703815,-0.9345382964,0.7721123587
H,0,-0.0944969375,1.5819980488,-2.0296873881
H,0,-2.1520716112,2.0668195181,-0.7364209399
H,0,-1.2919897453,3.5122817285,0.9931213409
H,0,-2.0700657648,2.1350353364,1.7815988568

H,0,0.1375478415,2.6725726007,2.8653225607
H,0,0.1282128116,1.0647424501,2.1550176397
H,0,1.4361025919,3.5913934839,1.0095644743
H,0,2.2534218561,2.117337644,1.4789320108
H,0,-3.7672560933,-2.7970153004,-0.9625275333
H,0,-2.1546256655,-2.069849649,-1.0419725692
H,0,-2.7780309667,-2.6767148263,0.50880688
H,0,-4.7060709901,-0.6032641266,-2.0135584295
H,0,-4.4341951992,0.9409599187,-1.1785268304
H,0,-3.0879118387,0.1275186719,-2.002210467
H,0,-5.6740047055,-1.5127928129,0.2527102528
H,0,-4.6514323522,-1.4489269151,1.7057550999
H,0,-5.3115699641,0.0495516431,1.020434016
H,0,-0.0192906747,-0.9449555272,-0.5083194642
N,0,0.8422030746,-1.4244315088,-0.2173850928
C,0,0.8787909071,-1.7923298652,1.2000944001
C,0,2.1715984222,-1.2891401506,1.8329599357
H,0,-0.0039835847,-1.345666465,1.6621216356
H,0,0.7980872552,-2.8833248004,1.2893693614
C,0,1.9244192631,-1.1514639598,-0.9404394659
N,0,3.1548638815,-1.316549686,-0.4463474227
C,0,4.311117073,-0.7536180498,-1.1617608352
C,0,3.359712071,-1.6965528327,0.9660467986
H,0,4.251635778,0.3407346424,-1.1236574648
H,0,5.2219932531,-1.1118370367,-0.6796490079
H,0,4.3267785761,-1.0849197928,-2.2013812913
H,0,3.5340283478,-2.779609651,1.0179706449
C,0,1.7346210618,-0.6607636165,-2.3398749572
H,0,2.1389945663,-0.1988504911,1.9154472764
H,0,2.2922399906,-1.7036423242,2.8387365751
H,0,4.2681620751,-1.1979502715,1.3119431995
H,0,2.0185734999,0.4082170465,-2.3394219942
H,0,2.3571607716,-1.2276533942,-3.0384162392
H,0,0.6904233531,-0.7607889584,-2.6349022198

### Intermediate from axial attack with DBU model, orientation B – 6-31+G** Gas Phase

E(RB+HF-LYP) = -962.904888505

| | |
|---|---|
| Zero-point correction= | 0.450385 (Hartree/Particle) |
| Thermal correction to Energy= | 0.474665 |
| Thermal correction to Enthalpy= | 0.475609 |
| Thermal correction to Gibbs Free Energy= | 0.395391 |
| Sum of electronic and zero-point Energies= | -962.454503 |
| Sum of electronic and thermal Energies= | -962.430224 |
| Sum of electronic and thermal Enthalpies= | -962.429280 |
| Sum of electronic and thermal Free Energies= | -962.509498 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 297.857 | 91.476 | 168.833 |

C,0,-1.465333962,2.5287081345,1.2127140984
C,0,-0.2531954839,2.2338754834,2.1013200111
C,0,1.0561269527,2.4671232819,1.3366413103
C,0,1.0935265512,1.8581256007,-0.0717309016
C,0,-0.1209466131,1.5568596676,-0.70298902
C,0,-1.4530625209,1.6665130378,-0.0517887737
O,0,2.2422038391,1.6628471966,-0.5913398712
O,0,-1.7961013778,0.2625087707,0.2784477647
O,0,-3.2014723363,0.2123964737,0.7658194772
C,0,-3.9408896104,-0.7556238036,-0.0088785677
C,0,-3.9992612691,-0.3495150231,-1.4875338072

```
C,0,-3.327892952,-2.1532973433,0.1616505359
C,0,-5.3338373954,-0.6905426399,0.6331133831
H,0,-0.1031446541,1.3383099832,-1.7698754925
H,0,-2.2328765263,2.0060700659,-0.7454679896
H,0,-1.448739574,3.5822856211,0.9000091604
H,0,-2.4020662317,2.3635704138,1.7549594663
H,0,-0.2831605,2.8548522176,3.0059630155
H,0,-0.3102471075,1.189601868,2.4357788055
H,0,1.2273527412,3.5468026275,1.2102133589
H,0,1.9230115026,2.0944439299,1.8960891513
H,0,-3.9358833823,-2.9059380915,-0.3528290424
H,0,-2.3180921272,-2.1823916389,-0.2555695752
H,0,-3.2741725078,-2.4159385705,1.223166194
H,0,-4.6027666053,-1.0653332523,-2.0568169527
H,0,-4.4483963205,0.6428142619,-1.5959803399
H,0,-2.9949340381,-0.3263022565,-1.9182661473
H,0,-6.0083840877,-1.3970844335,0.1379578186
H,0,-5.2809721538,-0.9465887158,1.6956997385
H,0,-5.754899792,0.3151912849,0.5398943507
H,0,0.4794206757,-0.4617039758,-0.820288744
N,0,1.2117664249,-1.1679685427,-0.6072036041
C,0,1.1486683168,-1.6913952308,0.7606199465
C,0,2.4018689988,-1.2802618628,1.52913807
H,0,0.2384077384,-1.289991843,1.2109642812
H,0,1.0585668346,-2.784468965,0.7179904972
C,0,2.3723500861,-0.9608262156,-1.2275183685
N,0,3.5302687182,-1.3583835555,-0.6836987715
C,0,4.8090566902,-1.1822360847,-1.3707047436
C,0,3.6362613099,-1.7142937366,0.7469036799
H,0,5.227762998,-0.1904701404,-1.1618175486
H,0,5.5026637265,-1.9469348184,-1.0114864728
H,0,4.6979733533,-1.3053157235,-2.4469201955
H,0,3.7984656464,-2.7978574755,0.823858118
C,0,2.3396673299,-0.4207444288,-2.6264740878
H,0,2.4103826857,-0.1942334083,1.651893565
H,0,2.4179426757,-1.741581586,2.5212294349
H,0,4.5284829088,-1.2153192246,1.1391247253
H,0,3.0104316557,0.4328693729,-2.7225094955
H,0,2.6161812896,-1.2077633771,-3.3393197367
H,0,1.3317636021,-0.0839620119,-2.8616428741
```

## Intermediate from axial attack with DBU model, orientation B – 6-31G* – PCM Dichloroethane

```
E(RB+HF-LYP) = -962.848186241

 Zero-point correction=                           0.452581 (Hartree/Particle)
 Thermal correction to Energy=                    0.476230
 Thermal correction to Enthalpy=                  0.477174
 Thermal correction to Gibbs Free Energy=         0.393389
 Sum of electronic and zero-point Energies=           -962.395605
 Sum of electronic and thermal Energies=              -962.371956
 Sum of electronic and thermal Enthalpies=            -962.371012
 Sum of electronic and thermal Free Energies=         -962.454798

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 298.839             88.961           176.342

 C,0,-1.5330261807,2.6225550746,0.568744156
 C,0,-0.1526766138,2.666603433,1.2291589434
 C,0,0.9272858089,3.0855628333,0.2246995255
 C,0,0.8484698801,2.3742417054,-1.1378544077
 C,0,-0.3626091488,1.7988954132,-1.5159586656
```

```
C,0,-1.5460025521,1.6873584873,-0.6408969193
O,0,1.9051708086,2.4008003745,-1.856207202
O,0,-1.5127491339,0.2607458612,-0.1926985085
O,0,-2.7243057822,-0.073752388,0.6148172858
C,0,-3.4614606428,-1.1315324358,-0.0376772711
C,0,-3.9237298657,-0.708312372,-1.436706199
C,0,-2.6150195335,-2.4105463017,-0.0971715466
C,0,-4.6604713847,-1.3170457198,0.902740239
H,0,-0.4251267028,1.3494605377,-2.5069640259
H,0,-2.4975085601,1.7857413989,-1.1802364355
H,0,-1.8095464768,3.6282386801,0.2195358085
H,0,-2.3031209993,2.3058694768,1.2812403497
H,0,-0.1625364807,3.343687272,2.0941513154
H,0,0.0805807439,1.6669782477,1.6193946221
H,0,0.8617936371,4.1696125131,0.0372542239
H,0,1.9329812853,2.9140580606,0.6306775704
H,0,-3.2004980279,-3.2450638394,-0.499757965
H,0,-1.7413022002,-2.2659446518,-0.7389872612
H,0,-2.2700753309,-2.6844207286,0.9063305309
H,0,-4.5312873634,-1.4976429319,-1.8943906911
H,0,-4.5281727728,0.2035491964,-1.3835774341
H,0,-3.0625109023,-0.5195169586,-2.0837005758
H,0,-5.314856888,-2.1111065212,0.5268881528
H,0,-4.3253642843,-1.5923147376,1.908493343
H,0,-5.2426950373,-0.3920848894,0.9727669559
H,0,0.1775945384,-0.5477245296,-0.0237979222
N,0,1.0191972965,-0.9981517209,0.3611709348
C,0,1.0135786091,-1.2986171156,1.7928498166
C,0,2.3952658723,-1.002985904,2.3651279825
H,0,0.2353715502,-0.6863450958,2.2542616198
H,0,0.7464134404,-2.3528075083,1.9443473627
C,0,2.0917726467,-1.1114259029,-0.4119399513
N,0,3.2591810643,-1.5233001179,0.0913126797
C,0,4.4408509437,-1.7439121497,-0.7525773867
C,0,3.4513692986,-1.7354361623,1.54432933
H,0,4.8777816177,-0.7952827937,-1.08307371
H,0,5.1805885306,-2.2843894358,-0.1599264428
H,0,4.1971986791,-2.3547911895,-1.6241432481
H,0,3.429953763,-2.8148014023,1.7435476613
C,0,1.9537714649,-0.7382335745,-1.85513663
H,0,2.5826560693,0.0766905137,2.3389554326
H,0,2.4582955634,-1.3295357674,3.4077880795
H,0,4.4506766736,-1.3678605227,1.7975559353
H,0,2.1880369212,0.3353705784,-1.9866931703
H,0,2.5999168651,-1.338039816,-2.4972139783
H,0,0.91697487,-0.8747869162,-2.1657901012
```

### Intermediate from axial attack with DBU model, orientation B – 6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.931089719

 Zero-point correction=                           0.449743 (Hartree/Particle)
 Thermal correction to Energy=                    0.473420
 Thermal correction to Enthalpy=                  0.474365
 Thermal correction to Gibbs Free Energy=         0.394307
 Sum of electronic and zero-point Energies=           -962.481347
 Sum of electronic and thermal Energies=              -962.457669
 Sum of electronic and thermal Enthalpies=            -962.456725
 Sum of electronic and thermal Free Energies=         -962.536783

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 297.076             89.538            168.496
```

```
C,0,-1.741169548,2.2290685591,1.250781529
C,0,-0.3280909787,2.2753478861,1.8392151158
C,0,0.6278562758,3.0631328082,0.9334341713
C,0,0.5140927528,2.7319056343,-0.5603410619
C,0,-0.6487852163,2.1329626651,-1.0295749561
C,0,-1.7441823064,1.6449526065,-0.161744119
O,0,1.5094179811,3.0769204893,-1.3049766911
O,0,-1.5209488781,0.1614895177,-0.1175954231
O,0,-2.6327238517,-0.5200652983,0.605185073
C,0,-3.3076604954,-1.4447690586,-0.2878162667
C,0,-3.9182111454,-0.7103435863,-1.4870967509
C,0,-2.3405522813,-2.5460223661,-0.7419452467
C,0,-4.4047862342,-2.022515475,0.6166346912
H,0,-0.7302887866,1.9397949571,-2.0988712748
H,0,-2.7358134957,1.7597685249,-0.6158672303
H,0,-2.1525842956,3.246795331,1.1902201181
H,0,-2.4151961785,1.6463577792,1.8880139124
H,0,-0.3484546573,2.711521664,2.8464562356
H,0,0.0399507872,1.2478820573,1.9533446816
H,0,0.4393057811,4.1429282234,1.0403873333
H,0,1.6717842472,2.9091306664,1.2343252533
H,0,-2.8694907253,-3.2965155533,-1.3392675507
H,0,-1.5380178131,-2.127967474,-1.3555575181
H,0,-1.8962205179,-3.0457672651,0.1251428725
H,0,-4.4657616162,-1.4159768238,-2.121497683
H,0,-4.6166118922,0.0633205504,-1.1521653746
H,0,-3.1377422516,-0.2413831461,-2.091765724
H,0,-4.995217383,-2.7575089257,0.0597254652
H,0,-3.968027274,-2.5198117639,1.4885909863
H,0,-5.0762996867,-1.2316219896,0.9649534276
H,0,0.2195666583,-0.5342456268,-0.0144913211
N,0,1.1301095981,-0.9562930468,0.2123338489
C,0,1.28103157,-1.5713895248,1.5337410231
C,0,2.7004161334,-1.3333251401,2.0375637266
H,0,0.5354125747,-1.1267969233,2.1967667141
H,0,1.0678632633,-2.6458212807,1.4614969094
C,0,2.1306860139,-0.7927466536,-0.643905482
N,0,3.369864175,-1.1931198143,-0.3480253829
C,0,4.4669183093,-1.0840167522,-1.3223814823
C,0,3.7032331163,-1.7693815689,0.9746973456
H,0,4.6891051693,-0.0380317687,-1.5538855917
H,0,5.3537691199,-1.5399710742,-0.8823715397
H,0,4.2326831608,-1.6200362319,-2.2457237614
H,0,3.7336318371,-2.8630979111,0.8826777026
C,0,1.8344464098,-0.125758832,-1.952239398
H,0,2.8404987028,-0.271131587,2.267926576
H,0,2.8781132166,-1.9007994432,2.9558633668
H,0,4.7075096784,-1.4259783056,1.2375593099
H,0,2.0523280374,0.9524100043,-1.8828258702
H,0,2.4143129054,-0.5621901869,-2.7662351989
H,0,0.7726587583,-0.218731329,-2.178125193
```

## Ts 2 from axial attack with DBU model, orientation B – 6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) =  -962.844439077

Zero-point correction=                           0.451581 (Hartree/Particle)
 Thermal correction to Energy=                    0.475623
 Thermal correction to Enthalpy=                  0.476567
 Thermal correction to Gibbs Free Energy=         0.396212
 Sum of electronic and zero-point Energies=           -962.392858
 Sum of electronic and thermal Energies=              -962.368816
```

```
 Sum of electronic and thermal Enthalpies=           -962.367872
 Sum of electronic and thermal Free Energies=        -962.448227

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 298.458             89.686            169.122

C,0,2.039487441,-0.6931479636,1.8521617771
 C,0,1.201896507,-1.94504621,1.5750614153
 C,0,2.0140720171,-2.9998926408,0.814451181
 C,0,2.8388319764,-2.4623709214,-0.3678612317
 C,0,3.1408974777,-1.0870942321,-0.3970565066
 C,0,2.6049627494,-0.1009531126,0.561847614
 O,0,3.276045842,-3.3043924532,-1.2010202205
 O,0,1.5713593505,0.4109171655,-0.3092109076
 O,0,0.7392966785,1.6946194494,0.4019375419
 C,0,0.9753842086,2.8901839747,-0.3489318163
 C,0,2.4647922293,3.2614427388,-0.3116927732
 C,0,0.4930721351,2.7387836269,-1.800062276
 C,0,0.1452721878,3.9587890169,0.3873563563
 H,0,3.7598061847,-0.7208193207,-1.2138944859
 H,0,3.2999243876,0.7190261508,0.791402272
 H,0,2.8835636929,-0.9442840386,2.511468584
 H,0,1.4440213776,0.0723908265,2.3638090018
 H,0,0.8157773665,-2.3631568791,2.5146460656
 H,0,0.3274935486,-1.6557211532,0.9798144996
 H,0,2.724124737,-3.4883882929,1.5010723293
 H,0,1.3681471784,-3.8022434553,0.4348551483
 H,0,0.6530384248,3.6650693856,-2.3644044907
 H,0,1.0403342109,1.9312652143,-2.2941849905
 H,0,-0.5779744417,2.505554005,-1.8316463622
 H,0,2.6387436638,4.2246419277,-0.8058036767
 H,0,2.8124999159,3.3375852231,0.7244431707
 H,0,3.0594058994,2.4994861157,-0.8231847302
 H,0,0.2738855061,4.937680659,-0.0898196152
 H,0,-0.9217185565,3.7093751171,0.3672835204
 H,0,0.4624210954,4.0387554605,1.4325177949
 H,0,-0.7632824565,0.8425335605,0.1980727706
 N,0,-1.7256896676,0.4448422454,0.2488932003
 C,0,-2.5973518805,0.9758340544,1.2987598422
 C,0,-3.6030507496,-0.0956311077,1.7054293112
 H,0,-1.9592505497,1.2732236474,2.1352339673
 H,0,-3.1116480636,1.8735229071,0.9302896706
 C,0,-2.1039501423,-0.4810327472,-0.6181889434
 N,0,-3.3363738999,-0.9966763264,-0.5889307651
 C,0,-3.8255651534,-1.9655281613,-1.5721371786
 C,0,-4.3076040341,-0.6298019354,0.4628426987
 H,0,-3.8249942007,-2.9777642664,-1.1507731363
 H,0,-4.8519127703,-1.6966768214,-1.8398529338
 H,0,-3.2220857143,-1.9501530817,-2.4778101095
 H,0,-5.0054101187,0.1108329189,0.0500997149
 C,0,-1.1017125102,-0.9338766173,-1.6427076094
 H,0,-3.0851109416,-0.9127679973,2.2212141552
 H,0,-4.3451797273,0.3187613346,2.3946058029
 H,0,-4.8816167419,-1.5309042851,0.7029514071
 H,0,-1.0806983158,-2.0253488929,-1.7092227153
 H,0,-1.3649799138,-0.5393386889,-2.6314682775
 H,0,-0.1031014286,-0.5823985798,-1.3707338722
```

### Ts 2 from axial attack with DBU model, orientation B – 6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.927256281
```

```
Zero-point correction=                           0.447886 (Hartree/Particle)
Thermal correction to Energy=                    0.471236
Thermal correction to Enthalpy=                  0.472181
Thermal correction to Gibbs Free Energy=         0.394609
Sum of electronic and zero-point Energies=           -962.479371
Sum of electronic and thermal Energies=              -962.456020
Sum of electronic and thermal Enthalpies=            -962.455076
Sum of electronic and thermal Free Energies=         -962.532648

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  295.705             88.382            163.264

C,0,2.0039412257,-0.7283985773,1.8757071373
C,0,1.2446342329,-1.9976574284,1.475662681
C,0,2.1419735833,-2.9710732759,0.6996219235
C,0,3.0158085989,-2.3292418357,-0.3808079178
C,0,3.2701175724,-0.9430334693,-0.3188462293
C,0,2.6216580622,-0.0391173033,0.6601515966
O,0,3.5525708436,-3.0992540231,-1.2379111521
O,0,1.6542506974,0.4020976017,-0.2957269375
O,0,0.6323576524,1.6830018092,0.3840019137
C,0,0.861131191,2.9008287008,-0.3243487875
C,0,2.3164268827,3.3620597378,-0.1448344899
C,0,0.5260685083,2.7475214233,-1.8184961968
C,0,-0.0938716542,3.9206380399,0.3314969904
H,0,3.9285878904,-0.5048632737,-1.0651640981
H,0,3.2534508477,0.804519738,0.9686836107
H,0,2.8154250348,-0.9761766691,2.5753184492
H,0,1.3397129218,-0.0202848533,2.3838409005
H,0,0.8350441401,-2.4929616057,2.3650777707
H,0,0.3900236886,-1.7129626915,0.8520904349
H,0,2.8321303208,-3.4776804145,1.3921414987
H,0,1.5515701205,-3.7659113252,0.2279914988
H,0,0.6848535614,3.6908548811,-2.3535515442
H,0,1.1609866423,1.9801988877,-2.2695093397
H,0,-0.5219178034,2.456278984,-1.9526919901
H,0,2.4763447301,4.3381346254,-0.6172243994
H,0,2.558095898,3.4499092316,0.9196885729
H,0,3.0027464078,2.6430657944,-0.6000366363
H,0,0.0229665005,4.9052416982,-0.1366538401
H,0,-1.1376421957,3.610461838,0.2143394798
H,0,0.1228005546,4.0168130801,1.4001944091
H,0,-0.8299632593,0.8571980326,0.2362685533
N,0,-1.7806879564,0.412188964,0.2847405193
C,0,-2.6606959276,0.8332881578,1.3780176602
C,0,-3.6144770399,-0.3040124904,1.7277284444
H,0,-2.0274212728,1.104479132,2.2269681993
H,0,-3.2196381923,1.7283271447,1.07540394
C,0,-2.1329150998,-0.4756229227,-0.6312367565
N,0,-3.3387980677,-1.0546566365,-0.617525758
C,0,-3.7935194798,-1.9940411518,-1.6460681516
C,0,-4.3130163285,-0.7909756914,0.4627599186
H,0,-3.7589403155,-3.0227697291,-1.2696473403
H,0,-4.8275272673,-1.7492364975,-1.9061045941
H,0,-3.1895105621,-1.9196327633,-2.5477022413
H,0,-5.0437457757,-0.0554923808,0.1024010017
C,0,-1.1275517688,-0.8158163403,-1.6950656553
H,0,-3.0563335142,-1.1291649417,2.1866384809
H,0,-4.3627649329,0.0347918863,2.4500107091
H,0,-4.8473151,-1.7273510078,0.6540064415
H,0,-1.0150514793,-1.8989724929,-1.7922129312
H,0,-1.4505224036,-0.4208968715,-2.6650167985
H,0,-0.1577519175,-0.3874802703,-1.4376151236
```

## Ts 1 from equatorial attack with DBU model, orientation A – 6-31G* - Gas Phase

E(RB+HF-LYP) = -962.820709099

| | |
|---|---|
| Zero-point correction= | 0.452570 (Hartree/Particle) |
| Thermal correction to Energy= | 0.476330 |
| Thermal correction to Enthalpy= | 0.477274 |
| Thermal correction to Gibbs Free Energy= | 0.398056 |
| Sum of electronic and zero-point Energies= | -962.368139 |
| Sum of electronic and thermal Energies= | -962.344379 |
| Sum of electronic and thermal Enthalpies= | -962.343435 |
| Sum of electronic and thermal Free Energies= | -962.422653 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 298.902 | 89.330 | 166.729 |

C,0,-1.4373411217,2.3628372674,0.9399629472
C,0,-0.2410353699,3.21439458,1.384217235
C,0,1.0712287712,2.4949883366,1.0630461008
C,0,1.1901356482,2.1345983485,-0.4274928379
C,0,-0.0246296462,2.0311123281,-1.1458312282
C,0,-1.2760441752,1.8571416803,-0.4941155955
O,0,2.3424063332,1.9607236225,-0.9064389352
O,0,-1.4293439545,0.1061393746,-0.4137237844
O,0,-2.383620142,-0.4506970103,0.5631586891
C,0,-3.4954639433,-1.0747517432,-0.1108444594
C,0,-4.254920478,-0.0585328985,-0.9719469541
C,0,-3.0018601157,-2.2559176104,-0.9570720672
C,0,-4.3635264857,-1.5594870396,1.0582289312
H,0,0.0306070178,1.8918025285,-2.222759844
H,0,-2.1567496079,2.0111674506,-1.1147447165
H,0,-2.3646698502,2.9444962563,1.0182405978
H,0,-1.5659459988,1.5061978586,1.611304637
H,0,-0.2576425541,4.1745360874,0.8529265094
H,0,-0.3159324401,3.4401213742,2.4567669532
H,0,1.9493858599,3.0960633017,1.3267029282
H,0,1.131743769,1.5726278828,1.6628459733
H,0,-3.8400191428,-2.7745118316,-1.4370552745
H,0,-2.321680305,-1.9000003812,-1.7356428607
H,0,-2.4649717106,-2.9766307817,-0.3293996494
H,0,-5.1436172371,-0.5170242689,-1.4216401268
H,0,-4.5774825989,0.7926082295,-0.3624398667
H,0,-3.6139460857,0.3122041708,-1.776239526
H,0,-5.2552003458,-2.0753731154,0.6850458805
H,0,-3.8024618544,-2.2539127514,1.6928122685
H,0,-4.6845754003,-0.7131224019,1.6743171812
H,0,-0.0813389599,-0.7866799189,-0.1677532991
N,0,0.8296067383,-1.2562935043,0.1102240664
C,0,0.9784220104,-1.5928171598,1.524711753
C,0,2.3572484501,-1.1685361236,2.0230026441
H,0,0.1731827254,-1.0863163344,2.0624347244
H,0,0.8332454293,-2.6734747485,1.6559995973
C,0,1.850809559,-1.1170773404,-0.7160164805
N,0,3.1135922923,-1.3586572447,-0.3329299615
C,0,4.2395305872,-0.9670791049,-1.1888979939
C,0,3.4314871843,-1.6864274421,1.0699100028
H,0,5.1397704812,-1.4686451423,-0.8281014804
H,0,4.0716632265,-1.2768593897,-2.2209421171

```
H,0,4.3710263392,0.1204448086,-1.1550880125
H,0,3.5493658051,-2.7747615449,1.1610897596
C,0,1.5648144754,-0.7074377108,-2.1296554836
H,0,2.4129771898,-0.0764597813,2.0662625527
H,0,2.5396470996,-1.5581477019,3.0294720072
H,0,4.395834301,-1.2290229188,1.306543421
H,0,2.0001726544,0.2872080899,-2.2898630865
H,0,1.9882210077,-1.4325340042,-2.8326126064
H,0,0.4883279776,-0.6427238807,-2.2807480978
```

## Ts 1 from equatorial attack with DBU model, orientation A – 6-31+G** - Gas Phase

```
E(RB+HF-LYP) = -962.898243086

 Zero-point correction=                           0.448904 (Hartree/Particle)
 Thermal correction to Energy=                    0.473024
 Thermal correction to Enthalpy=                  0.473968
 Thermal correction to Gibbs Free Energy=         0.394255
 Sum of electronic and zero-point Energies=           -962.449339
 Sum of electronic and thermal Energies=              -962.425219
 Sum of electronic and thermal Enthalpies=            -962.424275
 Sum of electronic and thermal Free Energies=         -962.503988

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 296.827             90.264            167.770

 C,0,-1.4758490062,2.389675029,1.0221446007
 C,0,-0.2839536887,3.256657393,1.450907499
 C,0,1.0378370924,2.5698633039,1.0942808824
 C,0,1.1294721529,2.2040712554,-0.3949058314
 C,0,-0.0944891334,2.0745652612,-1.093275224
 C,0,-1.3338910205,1.8858503151,-0.4146503237
 O,0,2.2760119313,2.042656935,-0.8987415671
 O,0,-1.4263695276,0.145025733,-0.3315244681
 O,0,-2.4312617572,-0.4583157369,0.572771268
 C,0,-3.4824483749,-1.1084431341,-0.1787641895
 C,0,-4.2263853921,-0.1019159717,-1.0653080201
 C,0,-2.9046123923,-2.2589888553,-1.0143032725
 C,0,-4.4015017889,-1.6431953426,0.9283660307
 H,0,-0.055794441,1.9321558324,-2.1699587546
 H,0,-2.2272891188,2.0239341005,-1.0201367719
 H,0,-2.4094140588,2.9572776059,1.1170495257
 H,0,-1.5802704122,1.5292697732,1.6931667172
 H,0,-0.3293863857,4.2243158712,0.9359674444
 H,0,-0.339213487,3.4643308235,2.5277973086
 H,0,1.9042637762,3.1984984852,1.3284019308
 H,0,1.1470523998,1.6520045244,1.6927968413
 H,0,-3.7022309297,-2.7957928839,-1.5397615265
 H,0,-2.2016839393,-1.8722206616,-1.7567108467
 H,0,-2.3763846624,-2.9701888578,-0.3700546986
 H,0,-5.0719457585,-0.5855643371,-1.5671880628
 H,0,-4.6114077734,0.7271131775,-0.4629719831
 H,0,-3.5589295508,0.3018458102,-1.8307169509
 H,0,-5.2502496663,-2.1774714905,0.4884541778
 H,0,-3.8587437988,-2.3338031803,1.5815416915
 H,0,-4.7874716687,-0.8212157395,1.5390326748
 H,0,-0.0491757598,-0.6902997058,-0.0785233973
 N,0,0.8673119862,-1.1619613999,0.177965068
 C,0,1.0715234746,-1.4808205525,1.5901500931
 C,0,2.4859514247,-1.0920246443,2.0116161199
 H,0,0.3123522145,-0.9397503842,2.1592972419
 H,0,0.898819799,-2.5536432772,1.7482618674
```

```
C,0,1.8515192078,-1.1220744308,-0.7026061433
N,0,3.1128865134,-1.4362481432,-0.3660228282
C,0,4.2284520495,-1.2791120263,-1.3026459757
C,0,3.4949491815,-1.6911973013,1.0366984752
H,0,5.0153110938,-1.9848030198,-1.0253818753
H,0,3.9201182453,-1.5001421634,-2.3227457612
H,0,4.6210045969,-0.2565156166,-1.2627260905
H,0,3.5943503272,-2.7752040975,1.1835084183
C,0,1.5227830944,-0.7377518204,-2.1136946504
H,0,2.5830214898,-0.0022534026,2.0109993731
H,0,2.6976813823,-1.4497858144,3.0236493873
H,0,4.4809065831,-1.2442318399,1.193762172
H,0,2.0194560506,0.2117926606,-2.3431134742
H,0,1.8423036666,-1.5166148535,-2.8125414142
H,0,0.4483738322,-0.5914568559,-2.2088531276
```

## Ts 1 from equatorial attack with DBU model, orientation A – 6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.838772209

 Zero-point correction=                           0.450679 (Hartree/Particle)
 Thermal correction to Energy=                    0.475045
 Thermal correction to Enthalpy=                  0.475989
 Thermal correction to Gibbs Free Energy=         0.394101
 Sum of electronic and zero-point Energies=           -962.388093
 Sum of electronic and thermal Energies=              -962.363727
 Sum of electronic and thermal Enthalpies=            -962.362783
 Sum of electronic and thermal Free Energies=         -962.444671

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 298.095             89.958            172.348

C,0,-1.7839749634,2.1510149268,1.1817669634
C,0,-0.7188189634,3.1315279268,1.6949509634
C,0,0.6472910366,2.8467889268,1.0615289634
C,0,0.5839340366,2.8854589268,-0.4709660366
C,0,-0.6481889634,2.4939849268,-1.0623510366
C,0,-1.6966559634,1.9278439268,-0.3205380366
O,0,1.5990060366,3.2511979268,-1.1135130366
O,0,-1.3795449634,0.0592049268,-0.4681560366
O,0,-2.1195529634,-0.8070540732,0.4530669634
C,0,-3.0761099634,-1.6131440732,-0.2673380366
C,0,-4.0842419634,-0.7275470732,-1.0095630366
C,0,-2.3454149634,-2.5496810732,-1.2387950366
C,0,-3.7636219634,-2.4067060732,0.8508799634
H,0,-0.7080029634,2.5158519268,-2.1499990366
H,0,-2.6548159634,1.8289109268,-0.8228270366
H,0,-2.7854609634,2.5284599268,1.4292469634
H,0,-1.6989569634,1.1831439268,1.6880889634
H,0,-1.0155489634,4.1577369268,1.4381439634
H,0,-0.6603539634,3.0853919268,2.7905629634
H,0,1.4063010366,3.5680239268,1.3873159634
H,0,1.0025970366,1.8514229268,1.3717239634
H,0,-3.0549969634,-3.1784610732,-1.7893670366
H,0,-1.7681079634,-1.9608700732,-1.9566440366
H,0,-1.6562869634,-3.2049080732,-0.6931400366
H,0,-4.8561839634,-1.3386960732,-1.4919130366
H,0,-4.5747279634,-0.0406360732,-0.3107350366
H,0,-3.5761419634,-0.1388380732,-1.7778060366
H,0,-4.5085289634,-3.0927220732,0.4325619634
H,0,-3.0293689634,-2.9951160732,1.4120069634
```

```
H,0,-4.2692529634,-1.7301830732,1.5485469634
H,0,0.0577630366,-0.5230850732,-0.1252630366
N,0,0.9918270366,-0.9535840732,0.1682389634
C,0,1.0527160366,-1.6253820732,1.4660879634
C,0,2.4597530366,-1.5088380732,2.0419319634
H,0,0.3050320366,-1.1602690732,2.1128389634
H,0,0.7677790366,-2.6783780732,1.3403359634
C,0,2.0340060366,-0.7853840732,-0.6219760366
N,0,3.2547910366,-1.2263580732,-0.2845570366
C,0,4.4322110366,-1.0991000732,-1.1413130366
C,0,3.4791620366,-1.9363170732,0.9892969634
H,0,4.8004100366,-2.0934360732,-1.4208520366
H,0,4.2051880366,-0.5396270732,-2.0458980366
H,0,5.2238020366,-0.5732090732,-0.5962840366
H,0,3.4295130366,-3.0185100732,0.8063989634
C,0,1.7957850366,-0.0642120732,-1.9207200366
H,0,2.6557710366,-0.4732640732,2.3442729634
H,0,2.5641320366,-2.1407060732,2.9295409634
H,0,4.4962200366,-1.7023010732,1.3194749634
H,0,2.2561070366,0.9302159268,-1.9018480366
H,0,2.1906820366,-0.6327010732,-2.7675070366
H,0,0.7228640366,0.0777169268,-2.0552350366
```

## Ts 1 from equatorial attack with DBU model, orientation A – 6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.921368923

 Zero-point correction=                           0.447221 (Hartree/Particle)
 Thermal correction to Energy=                    0.470874
 Thermal correction to Enthalpy=                  0.471819
 Thermal correction to Gibbs Free Energy=         0.392549
 Sum of electronic and zero-point Energies=           -962.474148
 Sum of electronic and thermal Energies=              -962.450494
 Sum of electronic and thermal Enthalpies=            -962.449550
 Sum of electronic and thermal Free Energies=         -962.528820

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 295.478             88.645            166.837

C,0,-1.9634489146,1.9762200061,1.2606550183
C,0,-1.0430899146,3.1450370061,1.6465300183
C,0,0.2676170854,3.1128600061,0.8499200183
C,0,0.0121730854,3.1037220061,-0.6577559817
C,0,-1.1591369146,2.4379180061,-1.1063609817
C,0,-1.9990329146,1.7230890061,-0.2372889817
O,0,0.8347810854,3.6828860061,-1.4217259817
O,0,-1.3461939146,-0.0860459939,-0.3819049817
O,0,-1.9667909146,-1.0578009939,0.5214930183
C,0,-2.7634099146,-2.0168249939,-0.2150059817
C,0,-3.9033549146,-1.3148289939,-0.9635759817
C,0,-1.8767439146,-2.8131469939,-1.1819539817
C,0,-3.3150459146,-2.9237149939,0.8923630183
H,0,-1.3433509146,2.4076600061,-2.1793739817
H,0,-2.9606989146,1.4109570061,-0.6312859817
H,0,-2.9844629146,2.1746320061,1.6113680183
H,0,-1.6510609146,1.0544180061,1.7634500183
H,0,-1.5529089146,4.0954210061,1.4392740183
H,0,-0.8405909146,3.1239770061,2.7248600183
H,0,0.9039270854,3.9733890061,1.0848480183
H,0,0.8422040854,2.2100960061,1.1068990183
H,0,-2.4634259146,-3.5789389939,-1.7016949817
H,0,-1.4368789146,-2.1461599939,-1.9277829817
```

H,0,-1.0668399146,-3.3092529939,-0.6362309817
H,0,-4.5405699146,-2.0501129939,-1.4677269817
H,0,-4.5235349146,-0.7417769939,-0.2660279817
H,0,-3.5011209146,-0.6328079939,-1.7170329817
H,0,-3.9410269146,-3.7104349939,0.4580100183
H,0,-2.4979399146,-3.3984199939,1.4454410183
H,0,-3.9231689146,-2.3475589939,1.5973030183
H,0,0.1493050854,-0.4284749939,-0.0081459817
N,0,1.1327180854,-0.7386539939,0.2857890183
C,0,1.3292960854,-1.1892499939,1.6641230183
C,0,2.7625100854,-0.9008449939,2.0991470183
H,0,0.6013400854,-0.6691129939,2.2911040183
H,0,1.1105210854,-2.2630419939,1.7292830183
C,0,2.1057980854,-0.6901759939,-0.6039449817
N,0,3.3624830854,-1.0459069939,-0.2998329817
C,0,4.4605340854,-1.0639239939,-1.2672879817
C,0,3.7308920854,-1.4691709939,1.0665650183
H,0,4.9548530854,-2.0403249939,-1.2281779817
H,0,4.1018270854,-0.9006249939,-2.2805789817
H,0,5.1939290854,-0.2884359939,-1.0192149817
H,0,3.7488050854,-2.5669059939,1.1018410183
C,0,1.7512480854,-0.2190789939,-1.9878919817
H,0,2.9137720854,0.1809750061,2.1941070183
H,0,2.9640400854,-1.3523469939,3.0752860183
H,0,4.7489260854,-1.1134369939,1.2547730183
H,0,2.3545750854,0.6471310061,-2.2741299817
H,0,1.9183670854,-1.0145389939,-2.7213009817
H,0,0.6995770854,0.0663570061,-2.0131479817

## Intermediate from equatorial attack with DBU model, orientation A – 6-31G* Gas Phase

E(RB+HF-LYP) = -962.825708289

| | |
|---|---|
| Zero-point correction= | 0.453871 (Hartree/Particle) |
| Thermal correction to Energy= | 0.477904 |
| Thermal correction to Enthalpy= | 0.478848 |
| Thermal correction to Gibbs Free Energy= | 0.398726 |
| Sum of electronic and zero-point Energies= | -962.371837 |
| Sum of electronic and thermal Energies= | -962.347804 |
| Sum of electronic and thermal Enthalpies= | -962.346860 |
| Sum of electronic and thermal Free Energies= | -962.426982 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 299.889 | 90.570 | 168.631 |

C,0,-1.4220643096,2.1441709402,1.3335880124
C,0,-0.3697461018,3.2555331106,1.3158561508
C,0,1.0139196314,2.6498840978,1.061729202
C,0,1.0538782675,1.7543175527,-0.1873530132
C,0,-0.1599133543,1.2781884036,-0.693376995
C,0,-1.4788241786,1.4018755997,-0.0126218122
O,0,2.2027225366,1.4945544546,-0.6752129633
O,0,-1.8848877839,0.0077383161,0.1982968029
O,0,-3.2699985267,0.0082574878,0.727184125
C,0,-4.0740312333,-0.8754888825,-0.0761751283
C,0,-4.1541209905,-0.3804012237,-1.5259442725
C,0,-3.5217153897,-2.3062289788,-0.0043301092
C,0,-5.442153295,-0.7829102366,0.6129417072
H,0,-0.1774084392,0.9010923619,-1.7157914412
H,0,-2.2508026982,1.8463286992,-0.6586856925
H,0,-2.4151950132,2.5286331875,1.589433647
H,0,-1.1594862298,1.4118913654,2.1088381372

```
H,0,-0.6038677845,3.9784997024,0.521889557
H,0,-0.3844585871,3.8116156821,2.2628149047
H,0,1.7798623799,3.4220831407,0.9209502228
H,0,1.3283262088,2.0680499566,1.9435736374
H,0,-4.1714654844,-3.0023253036,-0.5479023368
H,0,-2.5215499658,-2.3519592351,-0.4435655759
H,0,-3.456626364,-2.6342256329,1.0387833944
H,0,-4.8058754797,-1.0296584068,-2.122435561
H,0,-4.5564175023,0.6377720323,-1.5605304284
H,0,-3.1601859302,-0.376428602,-1.9812006747
H,0,-6.1673619445,-1.4263194566,0.1026172603
H,0,-5.3690106544,-1.1015145263,1.6578867058
H,0,-5.8153058987,0.2462784048,0.5915167255
H,0,0.5268091766,-0.6724698633,-0.5555494509
N,0,1.3373999775,-1.2802563058,-0.3120382324
C,0,1.4186891716,-1.5647250305,1.1243988359
C,0,2.6693073591,-0.9181033144,1.7147442457
H,0,0.5012228751,-1.1747429,1.5714077819
H,0,1.4349477318,-2.652396359,1.2729808066
C,0,2.4293828594,-1.0114258665,-1.0315986973
N,0,3.6580898131,-1.2240051032,-0.5372500102
C,0,4.8550447839,-0.944653254,-1.3263154631
C,0,3.887172325,-1.364425467,0.914230463
H,0,5.6815261555,-1.5375611393,-0.924869541
H,0,4.713157707,-1.2267118972,-2.3695045187
H,0,5.1140443108,0.120090318,-1.2720710227
H,0,4.1490028133,-2.4098274154,1.1286572364
C,0,2.2493444192,-0.7094723664,-2.4918126853
H,0,2.5819661921,0.1690314945,1.6439972479
H,0,2.7959812356,-1.1973915844,2.7655524389
H,0,4.7540394246,-0.7463167944,1.170231354
H,0,2.8068528776,0.1840668059,-2.7696978884
H,0,2.5760968338,-1.5663656055,-3.0958394465
H,0,1.1950439245,-0.5306011384,-2.6983761441
```

## Intermediate from equatorial attack with DBU model, orientation A – 6-31+G** Gas Phase

```
E(RB+HF-LYP) = -962.902046132

 Zero-point correction=                           0.450332 (Hartree/Particle)
 Thermal correction to Energy=                    0.474633
 Thermal correction to Enthalpy=                  0.475577
 Thermal correction to Gibbs Free Energy=         0.394600
 Sum of electronic and zero-point Energies=           -962.451714
 Sum of electronic and thermal Energies=              -962.427413
 Sum of electronic and thermal Enthalpies=            -962.426469
 Sum of electronic and thermal Free Energies=         -962.507446

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 297.837             91.368            170.430

 C,0,-1.4449507487,2.0771116129,1.389955846
 C,0,-0.4367169242,3.229536107,1.3613849562
 C,0,0.965826933,2.6893676137,1.0608041852
 C,0,1.0110694686,1.7833994073,-0.1787000739
 C,0,-0.1876417851,1.2287664729,-0.6441453513
 C,0,-1.5115085087,1.3652214134,0.0308028188
 O,0,2.1553725047,1.5773598887,-0.7078896404
 O,0,-1.9599235484,-0.0225775104,0.2047498737
 O,0,-3.3559259616,0.005710642,0.7020431072
 C,0,-4.1689693603,-0.8541659025,-0.1262520043
 C,0,-4.2093339047,-0.3420985396,-1.5721390126
```

```
C,0,-3.6531839611,-2.2986082196,-0.0578099821
C,0,-5.5474461071,-0.7344770919,0.5377323009
H,0,-0.2059154977,0.8490328879,-1.6650917098
H,0,-2.2678621743,1.8428647725,-0.6106793685
H,0,-2.4432321696,2.4196581764,1.6801843553
H,0,-1.1315060243,1.3401744473,2.1415666649
H,0,-0.7233002039,3.954737937,0.5870889262
H,0,-0.4475329938,3.7696818804,2.3169954519
H,0,1.6857072529,3.4969582503,0.8851284256
H,0,1.3416474843,2.1294369507,1.9319622483
H,0,-4.3130801103,-2.9692824864,-0.6196354934
H,0,-2.6480187336,-2.3671798948,-0.4811357272
H,0,-3.6154790802,-2.6382038949,0.9822699709
H,0,-4.8676966813,-0.9704741797,-2.1823669499
H,0,-4.5852579554,0.6854670512,-1.6049475131
H,0,-3.2094055136,-0.3611907635,-2.0128786222
H,0,-6.2737335714,-1.3572203648,0.0048984174
H,0,-5.5037349658,-1.0653704498,1.5798806405
H,0,-5.8979244555,0.3020682535,0.5176857086
H,0,0.614775531,-0.6757611784,-0.4652131056
N,0,1.4409165146,-1.2685106908,-0.2326914593
C,0,1.5856245298,-1.5439864736,1.1995084975
C,0,2.844906568,-0.865125309,1.7326792102
H,0,0.6819605129,-1.1760098532,1.6895843917
H,0,1.6336070753,-2.6302042466,1.3499422326
C,0,2.5021315725,-1.0493763274,-1.0088438769
N,0,3.7486684508,-1.2285588325,-0.5505494771
C,0,4.9211550555,-1.0393413843,-1.4035014608
C,0,4.0400984955,-1.3059238754,0.8961075845
H,0,5.7355003512,-1.6556737939,-1.0136492233
H,0,4.7190195734,-1.353916292,-2.426144436
H,0,5.2345615377,0.0115853942,-1.4041823973
H,0,4.3408439249,-2.3347788806,1.1358896746
C,0,2.2668509307,-0.7703162944,-2.463746335
H,0,2.7303859326,0.2193621126,1.6549665345
H,0,3.0154086507,-1.1270711707,2.7813197751
H,0,4.8982971892,-0.653910967,1.0888986718
H,0,2.8100514801,0.1224033028,-2.7737414711
H,0,2.5754939703,-1.6332720735,-3.0667877492
H,0,1.2056674265,-0.5982676833,-2.6333723074
```

## Intermediate from equatorial attack with DBU model, orientation A – 6-31G* – PCM Dichloroethane

```
E(RB+HF-LYP) = -962.845008985

 Zero-point correction=                           0.452764 (Hartree/Particle)
 Thermal correction to Energy=                    0.475396
 Thermal correction to Enthalpy=                  0.476341
 Thermal correction to Gibbs Free Energy=         0.400257
 Sum of electronic and zero-point Energies=           -962.392245
 Sum of electronic and thermal Energies=              -962.369613
 Sum of electronic and thermal Enthalpies=            -962.368668
 Sum of electronic and thermal Free Energies=         -962.444752

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 298.316             86.774            160.132

 C,0,-1.1266346035,2.3617806557,0.5063772934
 C,0,-0.2373528575,3.5513699218,0.1334251454
 C,0,1.0608111749,3.0467938706,-0.5032604839
 C,0,0.8145482975,2.1006947994,-1.6914215663
```

```
C,0,-0.4350370743,1.494755378,-1.7828331593
C,0,-1.4567372888,1.4842572394,-0.7156809108
O,0,1.7684967562,1.9629064634,-2.5310031659
O,0,-1.5095278907,0.0477555534,-0.3072805097
O,0,-2.5575274055,-0.1450852688,0.7401928836
C,0,-3.4885550971,-1.1580655069,0.299962966
C,0,-4.2109982466,-0.7224388442,-0.9801195114
C,0,-2.7654195834,-2.4972544415,0.1043551297
C,0,-4.4635083441,-1.2328771457,1.4834462793
H,0,-0.6500331769,0.9043715998,-2.6738825635
H,0,-2.4751133578,1.690595723,-1.075750786
H,0,-2.050895245,2.6886937887,0.9960229043
H,0,-0.591503629,1.7425447761,1.2385731551
H,0,-0.7644263683,4.2016765747,-0.578687863
H,0,-0.0308802256,4.1602783924,1.0246358464
H,0,1.6802674087,3.8760185696,-0.8692109956
H,0,1.6692249532,2.5255642819,0.254691938
H,0,-3.480750576,-3.2898682044,-0.1432169298
H,0,-2.03760936,-2.4272617938,-0.7091284825
H,0,-2.2379179729,-2.7832772011,1.0213400816
H,0,-4.9629296434,-1.4661654427,-1.2685951001
H,0,-4.7164954167,0.2372476353,-0.8273775234
H,0,-3.5004876588,-0.614515773,-1.804406744
H,0,-5.2353264891,-1.9850543296,1.287034597
H,0,-3.9364328021,-1.5097158861,2.40260782
H,0,-4.953907495,-0.2665982025,1.6415238492
H,0,0.0785962637,-0.669208753,0.2144305533
N,0,0.9816959418,-0.967423538,0.6185590125
C,0,1.0902038976,-0.9619892084,2.078027359
C,0,2.4946116258,-0.5193604959,2.4724986762
H,0,0.3243220264,-0.2848177919,2.4642615493
H,0,0.8751025398,-1.9669604608,2.4648190468
C,0,2.0026307617,-1.1904609413,-0.1984211258
N,0,3.2235737597,-1.4443409188,0.283453564
C,0,4.3821422106,-1.7161284786,-0.5727931847
C,0,3.5208633756,-1.3690734557,1.7313160162
H,0,5.0761421688,-2.3485966333,-0.0139284674
H,0,4.0932802091,-2.2486487223,-1.4779557353
H,0,4.8932780273,-0.786098086,-0.8481514963
H,0,3.555095245,-2.3907144549,2.1317111955
C,0,1.7426805863,-1.1261028659,-1.6733044592
H,0,2.6337774158,0.5385802458,2.2209751362
H,0,2.6434917357,-0.6295166311,3.5511190241
H,0,4.5205552535,-0.9356029002,1.8356435069
H,0,2.0751732138,-0.154069548,-2.0759904772
H,0,2.2423895907,-1.9377102811,-2.2066503325
H,0,0.6701007651,-1.1888361625,-1.8552651897
```

## Intermediate from equatorial attack with DBU model, orientation A – 6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.929006771

 Zero-point correction=                           0.449391 (Hartree/Particle)
 Thermal correction to Energy=                    0.473296
 Thermal correction to Enthalpy=                  0.474240
 Thermal correction to Gibbs Free Energy=         0.393564
 Sum of electronic and zero-point Energies=           -962.479616
 Sum of electronic and thermal Energies=              -962.455711
 Sum of electronic and thermal Enthalpies=            -962.454767
 Sum of electronic and thermal Free Energies=         -962.535442

                    E (Thermal)             CV                S
```

| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 296.997 | 89.680 | 169.795 |

```
C,0,-1.4364469239,1.6134040963,1.5762306563
C,0,-1.0758284227,3.0820052328,1.8163868289
C,0,0.0866411024,3.4973419075,0.9064580835
C,0,-0.1654175588,3.1736269043,-0.5723319167
C,0,-1.1077999791,2.2004590688,-0.8795620378
C,0,-1.8119511968,1.3478994911,0.1091375941
O,0,0.4894399283,3.8649957811,-1.4389757858
O,0,-1.4152810269,-0.0441937434,-0.2679792077
O,0,-2.1947360602,-1.0245342729,0.5370788722
C,0,-2.9412123608,-1.9000087536,-0.3509905791
C,0,-3.9494759942,-1.1026236151,-1.186650682
C,0,-1.981075679,-2.6952843887,-1.2444430505
C,0,-3.6586937364,-2.8250878809,0.6412722646
H,0,-1.3610779856,2.0468248115,-1.9288968617
H,0,-2.9025905875,1.3480820545,-0.0193192284
H,0,-2.2487173401,1.2907057501,2.2364124307
H,0,-0.5653070433,0.9930804737,1.8241934162
H,0,-1.9472590425,3.71823675,1.6076096337
H,0,-0.8185864625,3.2362720114,2.8729232906
H,0,0.2795676423,4.5748559436,0.9778118077
H,0,1.0136898488,2.9972537591,1.2285161698
H,0,-2.538311011,-3.4109768286,-1.8585186887
H,0,-1.4317507758,-2.0272982588,-1.9130039556
H,0,-1.262967723,-3.2529456031,-0.6340202346
H,0,-4.5452020588,-1.781980718,-1.8057226509
H,0,-4.6299337743,-0.5412220456,-0.5386069675
H,0,-3.4343875657,-0.4008821698,-1.8477104962
H,0,-4.2661063957,-3.5529100128,0.0932778938
H,0,-2.9370440115,-3.371022588,1.2570589686
H,0,-4.3177368096,-2.2508891129,1.2998646208
H,0,0.2826547845,-0.6156918063,0.0019176404
N,0,1.2429279436,-0.9309787926,0.2167117833
C,0,1.4412849905,-1.719709888,1.4368607015
C,0,2.853101417,-1.4852815857,1.9618802216
H,0,0.6832260283,-1.4091103383,2.1596347124
H,0,1.2778197603,-2.7821716782,1.2143090513
C,0,2.2226355541,-0.5787857101,-0.6052038884
N,0,3.4856338921,-0.9429671001,-0.3714843532
C,0,4.6001465386,-0.6320198143,-1.2707511094
C,0,3.8570325641,-1.7103653423,0.8368825577
H,0,5.1552963942,-1.5531138593,-1.4745951331
H,0,4.2493296788,-0.2250759688,-2.2158842398
H,0,5.2740535166,0.089267571,-0.7963121574
H,0,3.9229356727,-2.7731842962,0.5683021012
C,0,1.8604828895,0.2419331764,-1.8086507714
H,0,2.9423397638,-0.461287884,2.3434523895
H,0,3.0697492173,-2.1715340164,2.7858782078
H,0,4.8555251748,-1.3789748777,1.137728827
H,0,2.4471295697,1.1638773304,-1.8405040089
H,0,2.0499086728,-0.3209354511,-2.728499553
H,0,0.8078980552,0.5252127974,-1.7640292623
```

## Ts 2 from equatorial attack with DBU model, orientation A – 6-31G* - Gas Phase

```
E(RB+HF-LYP) = -962.817227828

 Zero-point correction=                           0.451567 (Hartree/Particle)
 Thermal correction to Energy=                    0.475682
 Thermal correction to Enthalpy=                  0.476626
 Thermal correction to Gibbs Free Energy=         0.396366
```

```
Sum of electronic and zero-point Energies=           -962.365661
Sum of electronic and thermal Energies=              -962.341546
Sum of electronic and thermal Enthalpies=            -962.340602
Sum of electronic and thermal Free Energies=         -962.420862

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  298.495             89.834            168.922

C,0,-1.8952414633,2.1669400939,1.1998947083
C,0,-0.8106549999,3.1771710791,1.5983296256
C,0,0.551392101,2.7939056888,1.0102083156
C,0,0.5094444451,2.6972555335,-0.5225907402
C,0,-0.7451990484,2.3489948311,-1.1010635851
C,0,-1.8265021753,1.7644465246,-0.2881039186
O,0,1.5515080986,2.9368227083,-1.1736243883
O,0,-1.3108685129,0.4296713668,-0.4987897508
O,0,-2.066289533,-0.8690764561,0.5161293092
C,0,-2.8866279322,-1.7006592434,-0.2676903618
C,0,-4.0567133253,-0.9158007951,-0.88855809
C,0,-2.0782263304,-2.4087689185,-1.3725506139
C,0,-3.4344527696,-2.7451339373,0.7320149567
H,0,-0.8319757044,2.3376224221,-2.1828364596
H,0,-2.8137638715,1.8247843057,-0.7588742873
H,0,-2.8860254776,2.585943558,1.4151708735
H,0,-1.8167434985,1.2472551114,1.7895261953
H,0,-1.0825556356,4.1720133072,1.2211420961
H,0,-0.7560084484,3.2617747815,2.6920995922
H,0,1.3306651552,3.5196354732,1.2685277822
H,0,0.8751088647,1.8244303228,1.4226344705
H,0,-2.6987881451,-3.1084459917,-1.9464011322
H,0,-1.6653160291,-1.6677099134,-2.064289371
H,0,-1.2463710217,-2.9718696412,-0.9315425063
H,0,-4.7525922376,-1.5784759035,-1.418637708
H,0,-4.6111232351,-0.3866156242,-0.105617772
H,0,-3.6779459693,-0.176966152,-1.601661616
H,0,-4.0948901309,-3.4628525806,0.2288652438
H,0,-2.6099925127,-3.2988700846,1.1949519574
H,0,-4.0005088733,-2.2473690409,1.5262242121
H,0,0.0586294556,-0.3540328851,-0.0702635879
N,0,0.9549155608,-0.8251340275,0.2047634285
C,0,0.991214518,-1.4342129652,1.5321649779
C,0,2.3988986134,-1.3224527051,2.106003263
H,0,0.2461407908,-0.9228207578,2.1440388376
H,0,0.6733748,-2.4810785461,1.4514694294
C,0,1.9964514616,-0.6955225235,-0.5907124744
N,0,3.217795314,-1.1243456072,-0.2190594181
C,0,4.3757414988,-1.049314055,-1.1081030739
C,0,3.4142389143,-1.8063473854,1.0713240804
H,0,4.50805763,-1.9772533146,-1.6797743329
H,0,4.280126928,-0.2120054499,-1.7979081163
H,0,5.2705106817,-0.8860594633,-0.5015867152
H,0,3.3358869425,-2.8930239393,0.9252985119
C,0,1.7799801628,-0.048738598,-1.9269479328
H,0,2.612579345,-0.2794869806,2.3661620053
H,0,2.4924631294,-1.9200504632,3.0179559135
H,0,4.434208495,-1.5934793238,1.4049918691
H,0,2.1363694754,0.9916672754,-1.911024793
H,0,2.2749065836,-0.6107717628,-2.7230266817
H,0,0.7093339441,0.0005520061,-2.1269781647
```

## Ts 2 from equatorial attack with DBU model, orientation A – 6-31+G** - Gas Phase

E(RB+HF-LYP) = -962.895307237

| | |
|---|---|
| Zero-point correction= | 0.448226 (Hartree/Particle) |
| Thermal correction to Energy= | 0.472643 |
| Thermal correction to Enthalpy= | 0.473587 |
| Thermal correction to Gibbs Free Energy= | 0.392450 |
| Sum of electronic and zero-point Energies= | -962.447082 |
| Sum of electronic and thermal Energies= | -962.422664 |
| Sum of electronic and thermal Enthalpies= | -962.421720 |
| Sum of electronic and thermal Free Energies= | -962.502858 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 296.588 | 90.580 | 170.768 |

C,0,-1.8254779288,2.1220426276,1.2840550558
C,0,-0.7584424513,3.1672421656,1.6379261983
C,0,0.5939944115,2.8177587155,1.0050604859
C,0,0.5037886119,2.6876329924,-0.5197746636
C,0,-0.7642174627,2.3206449993,-1.0593579359
C,0,-1.823758633,1.7418851345,-0.2109488136
O,0,1.5225222066,2.9254428052,-1.2128505606
O,0,-1.3198399745,0.4102197074,-0.4649448413
O,0,-2.1267876269,-0.9219743841,0.5062436494
C,0,-2.9420721607,-1.717704708,-0.3243563102
C,0,-4.0857653233,-0.8951053658,-0.9478876864
C,0,-2.1178839351,-2.4023965514,-1.4336975628
C,0,-3.5324057825,-2.7892211478,0.6223754878
H,0,-0.8881872389,2.3115593704,-2.1370260855
H,0,-2.8262820468,1.8172058879,-0.6445647641
H,0,-2.8184147203,2.493397602,1.562842493
H,0,-1.6726227028,1.1998865544,1.8552375658
H,0,-1.0711657884,4.1527507998,1.2692328009
H,0,-0.6650481386,3.2557648858,2.7281753765
H,0,1.3563359265,3.5740554566,1.2204996041
H,0,0.9664648347,1.8676790004,1.4186858536
H,0,-2.7400298862,-3.0683041298,-2.0437575816
H,0,-1.6759156175,-1.6469481907,-2.0903382952
H,0,-1.3093514642,-2.996471026,-0.9921266881
H,0,-4.7711618942,-1.5325466086,-1.5195059992
H,0,-4.6568343724,-0.3890768414,-0.1623735791
H,0,-3.6794621593,-0.1372404629,-1.623983991
H,0,-4.192007174,-3.4708698647,0.0709815304
H,0,-2.7304819785,-3.3769909875,1.0809983974
H,0,-4.1098418433,-2.3127384416,1.420491088
H,0,0.0649261232,-0.3574939599,-0.054915081
N,0,0.9731031126,-0.8044958911,0.2277180523
C,0,1.040520794,-1.3481269918,1.583257268
C,0,2.4566641653,-1.199443309,2.1285000771
H,0,0.3044879239,-0.8130949972,2.1860885165
H,0,0.7293755911,-2.3994698671,1.5603753932
C,0,2.0019445142,-0.7061064691,-0.5896345588
N,0,3.2314417583,-1.1128292429,-0.2186567051
C,0,4.3864634529,-1.0743690529,-1.1145950196
C,0,3.4574224697,-1.726175084,1.1017793893
H,0,4.6199283689,-2.0754758737,-1.4986132519
H,0,4.208935209,-0.402678217,-1.9508765977
H,0,5.2529429432,-0.7022914932,-0.5607858522
H,0,3.3862558207,-2.8190109661,1.0097277328
C,0,1.760582301,-0.1259789465,-1.952536941
H,0,2.6681637671,-0.1449044305,2.3372832626
H,0,2.5665344245,-1.7528265125,3.0655949716

```
H,0,4.4813546873,-1.4882493817,1.4040970295
H,0,2.1860473818,0.8829175299,-2.0214745698
H,0,2.1802322978,-0.7683969812,-2.7307100724
H,0,0.6877085287,-0.0238409966,-2.1112614383
```

## Ts 2 from equatorial attack with DBU model, orientation A – 6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.839963975

 Zero-point correction=                           0.451435 (Hartree/Particle)
 Thermal correction to Energy=                    0.475547
 Thermal correction to Enthalpy=                  0.476491
 Thermal correction to Gibbs Free Energy=         0.395510
 Sum of electronic and zero-point Energies=           -962.388529
 Sum of electronic and thermal Energies=              -962.364417
 Sum of electronic and thermal Enthalpies=            -962.363473
 Sum of electronic and thermal Free Energies=         -962.444454

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 298.410             89.687           170.439

 C,0,1.8041705643,-0.7206185053,1.7980343713
 C,0,2.1634678475,-2.2023518419,1.9539588278
 C,0,1.9723700102,-2.9445778442,0.6263654629
 C,0,2.8314174841,-2.3360677244,-0.4938889717
 C,0,3.132867207,-0.9637235994,-0.3859895525
 C,0,2.5024839857,-0.0507430325,0.5903757344
 O,0,3.2698708985,-3.098717361,-1.3980905648
 O,0,1.5535925656,0.5089894681,-0.3433123403
 O,0,0.6476494729,1.7412864529,0.3773459034
 C,0,0.8740061571,2.9579204725,-0.339665201
 C,0,2.3485413931,3.372353504,-0.2283114002
 C,0,0.4588582347,2.8180291154,-1.8127588892
 C,0,-0.0203918882,3.9874837018,0.3766766941
 H,0,3.7876594526,-0.5243494896,-1.1358833232
 H,0,3.167009952,0.7593895118,0.9211199084
 H,0,2.0398744147,-0.1709488969,2.7177825409
 H,0,0.7217809108,-0.6281526075,1.6497366731
 H,0,3.2118630217,-2.2999435605,2.2685303972
 H,0,1.5534929082,-2.6539423858,2.7487486929
 H,0,2.2452254766,-4.00368079,0.7103908811
 H,0,0.9101424628,-2.9170561397,0.3350925713
 H,0,0.606614825,3.7605904794,-2.3531256312
 H,0,1.0547187909,2.0405027572,-2.2984045473
 H,0,-0.6005241894,2.5456966218,-1.8927180692
 H,0,2.5199253,4.3430962551,-0.7084228145
 H,0,2.6422540376,3.4513005921,0.8242939576
 H,0,2.9875712939,2.628686657,-0.7122476461
 H,0,0.1009486057,4.9786372136,-0.0764697971
 H,0,-1.0777216718,3.7085757198,0.3025485839
 H,0,0.2461681091,4.0567395766,1.4366880081
 H,0,-0.8281133105,0.8627856619,0.1676722027
 N,0,-1.7740489855,0.4259899229,0.2258368017
 C,0,-2.6888127026,0.9775572028,1.2276136229
 C,0,-3.6543680969,-0.1123949332,1.6798776252
 H,0,-2.0805884688,1.3507953947,2.0559094712
 H,0,-3.2345193435,1.82819734,0.7978791629
 C,0,-2.0952738933,-0.5634417744,-0.5928205532
 N,0,-3.3036325492,-1.1325178229,-0.5526541355
 C,0,-3.7348634838,-2.1732600112,-1.4879970254
 C,0,-4.3101880061,-0.7491004526,0.4590487347
 H,0,-3.7282229266,-3.1554219542,-1.0007842103
```

```
H,0,-4.7562124727,-1.9475448794,-1.8100801344
H,0,-3.0976318608,-2.2027654677,-2.3696872522
H,0,-5.0314525772,-0.065702579,-0.0084325675
C,0,-1.0543876977,-1.0244039515,-1.5739103554
H,0,-3.1115988173,-0.8739453193,2.2521911089
H,0,-4.4275104521,0.3079773775,2.3302445098
H,0,-4.8489695821,-1.6595524695,0.7417919034
H,0,-0.9780039462,-2.1154316837,-1.5773501944
H,0,-1.3192000237,-0.7014312027,-2.5879147519
H,0,-0.0794953635,-0.6058368694,-1.3085770324
```

## Ts 2 from equatorial attack with DBU model, orientation A – 6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.923161942

 Zero-point correction=                           0.448142 (Hartree/Particle)
 Thermal correction to Energy=                    0.471463
 Thermal correction to Enthalpy=                  0.472407
 Thermal correction to Gibbs Free Energy=         0.395039
 Sum of electronic and zero-point Energies=           -962.475019
 Sum of electronic and thermal Energies=              -962.451699
 Sum of electronic and thermal Enthalpies=            -962.450755
 Sum of electronic and thermal Free Energies=         -962.528123

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 295.847             88.356            162.833

 C,0,1.9750592429,-0.7414562077,1.8710084104
 C,0,2.0074427781,-2.2766127118,1.9158186915
 C,0,1.6804438312,-2.8870475805,0.5457839951
 C,0,2.6695579863,-2.414212843,-0.5212823355
 C,0,3.1755783345,-1.1063248201,-0.3843365515
 C,0,2.6229361571,-0.1466702975,0.6004873228
 O,0,3.022202259,-3.2267956445,-1.4324093106
 O,0,1.6541028846,0.3663808991,-0.3340145108
 O,0,0.723196085,1.6590112391,0.3576921014
 C,0,0.9954068469,2.8741550089,-0.3464491858
 C,0,2.4731426168,3.2653094644,-0.193139282
 C,0,0.6216182456,2.7482144207,-1.8331208477
 C,0,0.1013804388,3.9256765466,0.3417379166
 H,0,3.8892778162,-0.739175497,-1.1183809299
 H,0,3.3272132661,0.6550820833,0.854446085
 H,0,2.4728446191,-0.3337276744,2.7593066564
 H,0,0.9399148521,-0.3854970926,1.9055181829
 H,0,3.008049361,-2.6157196753,2.2156528603
 H,0,1.3096587832,-2.6442311731,2.6796913037
 H,0,1.7142188193,-3.9819480336,0.5755899953
 H,0,0.661386653,-2.6049490235,0.2433774589
 H,0,0.8072486246,3.6896377937,-2.3627045506
 H,0,1.2140196257,1.9604261212,-2.3059188941
 H,0,-0.4402373919,2.5015789955,-1.9461309466
 H,0,2.6663323633,4.2389044641,-0.6578775883
 H,0,2.7418511453,3.3291096122,0.8665481416
 H,0,3.1160467046,2.522049479,-0.6721295612
 H,0,0.2499037139,4.9086139639,-0.1204531657
 H,0,-0.9574848689,3.6628823013,0.2467672514
 H,0,0.3472563162,4.0022555913,1.4056638903
 H,0,-0.7909597359,0.8871414622,0.2244899388
 N,0,-1.7507361726,0.4737749744,0.2945458831
 C,0,-2.6089693513,0.9618108119,1.3775588676
 C,0,-3.6114359236,-0.1225664009,1.7577165626
 H,0,-1.9636818429,1.2281062625,2.2189383736
```

```
H,0,-3.1291600337,1.8720801636,1.0510615819
C,0,-2.1412667308,-0.4221086509,-0.5994189582
N,0,-3.3680188099,-0.9530957134,-0.5645844388
C,0,-3.8742642239,-1.8891477478,-1.5719827358
C,0,-4.3294848735,-0.613734383,0.505871858
H,0,-3.9318054876,-2.901738758,-1.1568923914
H,0,-4.8789746344,-1.5719794177,-1.8672937549
H,0,-3.2454574528,-1.8988771681,-2.4589907907
H,0,-5.0248418578,0.1447910379,0.1224039531
C,0,-1.1564228847,-0.8203690266,-1.6621501577
H,0,-3.0938858448,-0.9583070011,2.2423254469
H,0,-4.3452491023,0.2697625417,2.4679801894
H,0,-4.9076550544,-1.5178365547,0.721943045
H,0,-1.0951612123,-1.9079481195,-1.7529504983
H,0,-1.4638953376,-0.4172226535,-2.6336293259
H,0,-0.1658326999,-0.4362843053,-1.4128497296
```

## Ts 1 from equatorial attack with DBU model, orientation B (13) – 6-31G* - Gas Phase

```
E(RB+HF-LYP) = -962.822351428

 Zero-point correction=                           0.452736 (Hartree/Particle)
 Thermal correction to Energy=                    0.476433
 Thermal correction to Enthalpy=                  0.477377
 Thermal correction to Gibbs Free Energy=         0.399388
 Sum of electronic and zero-point Energies=           -962.369615
 Sum of electronic and thermal Energies=              -962.345919
 Sum of electronic and thermal Enthalpies=            -962.344975
 Sum of electronic and thermal Free Energies=         -962.422964

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 298.966             89.369            164.142

 C,0,-1.0931994859,2.6175580956,0.5763299367
 C,0,0.1495416323,3.2516783959,1.2157954765
 C,0,1.3526998311,2.3106900573,1.1120731463
 C,0,1.6339257367,1.8817153249,-0.3368523392
 C,0,0.5504161022,1.9567290998,-1.2446136626
 C,0,-0.7976352932,2.0440653178,-0.8085490202
 O,0,2.7955629837,1.492770691,-0.6272204474
 O,0,-1.290000885,0.339546881,-0.7471821452
 O,0,-2.4230535817,-0.0324726631,0.1159883567
 C,0,-3.550308931,-0.4584983955,-0.6800206473
 C,0,-4.0244248365,0.6765554018,-1.5948748066
 C,0,-3.1775823075,-1.7048511137,-1.4930867487
 C,0,-4.6082972935,-0.786116102,0.3816761163
 H,0,0.7549556574,1.7561713783,-2.2941345798
 H,0,-1.5252760722,2.3248055451,-1.5672505642
 H,0,-1.8948996868,3.362922775,0.4967755902
 H,0,-1.4904153712,1.8217732092,1.2162670297
 H,0,0.3900997843,4.1867425302,0.6940106276
 H,0,-0.0577230856,3.5147897032,2.2620946431
 H,0,2.2688954376,2.7708404509,1.5005475571
 H,0,1.174808564,1.412097482,1.7257462339
 H,0,-4.0310565029,-2.0602015884,-2.0821360328
 H,0,-2.3556909828,-1.4712538552,-2.1750727447
 H,0,-2.8589986519,-2.5151476329,-0.8268826516
 H,0,-4.9288080055,0.3825864672,-2.1404889451
 H,0,-4.2526345451,1.5716290877,-1.0060455239
 H,0,-3.2478447932,0.9266552127,-2.3222784228
 H,0,-5.5316977856,-1.1353322229,-0.0935838387
 H,0,-4.2496948204,-1.5717565529,1.055672384
```

```
H,0,-4.8405836804,0.1011425774,0.9799660856
H,0,-0.0309321385,-0.7322626511,-0.5639772122
N,0,0.8730425882,-1.256328243,-0.3996191203
C,0,1.8270057769,-1.2756243984,-1.5157511441
C,0,3.0624395052,-2.0817965882,-1.1321520388
H,0,1.3119687711,-1.7070901731,-2.3797647076
H,0,2.1149215038,-0.2407780266,-1.7321714449
C,0,1.1960668257,-1.4740131747,0.8581986151
N,0,2.4547093982,-1.7709954409,1.2237284817
C,0,2.8597861135,-1.9322657159,2.6151654321
C,0,3.5427094416,-1.6077821492,0.2374656323
H,0,3.6290650568,-2.7084107203,2.6729981687
H,0,3.2771385039,-0.9990426483,3.0155626491
H,0,2.0194002746,-2.23885562,3.2365130575
H,0,3.8172415377,-0.5458690814,0.1936501355
C,0,0.0886532956,-1.4095099521,1.8770004418
H,0,2.8432252508,-3.1563003099,-1.0991588562
H,0,3.8504539706,-1.9220924005,-1.8743242024
H,0,4.3950862622,-2.1963324198,0.5888410537
H,0,-0.0514832752,-2.3896594651,2.3476042775
H,0,0.3230080618,-0.6869852777,2.6647810392
H,0,-0.8476379599,-1.1134838771,1.3979612142
```

## Ts 1 from equatorial attack with DBU model, orientation B (13) – 6-31+G** - Gas Phase

```
E(RB+HF-LYP) = -962.899268353

 Zero-point correction=                           0.449324 (Hartree/Particle)
 Thermal correction to Energy=                    0.473332
 Thermal correction to Enthalpy=                  0.474276
 Thermal correction to Gibbs Free Energy=         0.395293
 Sum of electronic and zero-point Energies=           -962.449944
 Sum of electronic and thermal Energies=              -962.425937
 Sum of electronic and thermal Enthalpies=            -962.424992
 Sum of electronic and thermal Free Energies=         -962.503975

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 297.020             90.209           166.234

 C,0,-1.1158607751,2.6421485486,0.6220762618
 C,0,0.1201551086,3.3089971598,1.2416202586
 C,0,1.3372185963,2.3828645982,1.1543942281
 C,0,1.6143059564,1.9056678152,-0.2783784046
 C,0,0.532037638,1.9492060323,-1.1897435164
 C,0,-0.8203296433,2.0463054165,-0.7536092854
 O,0,2.7795009898,1.5053677357,-0.5555128255
 O,0,-1.2855285904,0.3509017478,-0.660532695
 O,0,-2.4807809168,-0.0202058828,0.123295798
 C,0,-3.5573358923,-0.459291923,-0.7397723916
 C,0,-3.9760663944,0.6589619489,-1.7017372144
 C,0,-3.1400426476,-1.7204696603,-1.5079245588
 C,0,-4.6804292194,-0.7703939273,0.2590233314
 H,0,0.7357108754,1.7325423484,-2.2355348595
 H,0,-1.5445261443,2.3152082535,-1.5194754991
 H,0,-1.9331112202,3.3683134388,0.5359003768
 H,0,-1.4889606835,1.8496813629,1.2806056118
 H,0,0.3450213554,4.2378275369,0.7027995108
 H,0,-0.0864183195,3.5865457386,2.2837669503
 H,0,2.2495460523,2.871046711,1.5149915205
 H,0,1.1817403975,1.5025622931,1.7980122099
 H,0,-3.9663427431,-2.0885230676,-2.1263219794
 H,0,-2.2908696252,-1.5014886285,-2.1603687425
```

```
H,0,-2.8514895708,-2.5153018091,-0.8113983944
H,0,-4.8475211378,0.3506202789,-2.2900531192
H,0,-4.2385573291,1.5647827771,-1.1458689994
H,0,-3.1621817114,0.8946797355,-2.3918965437
H,0,-5.5688313954,-1.1290111939,-0.2715187208
H,0,-4.3657808091,-1.5437729977,0.9670336928
H,0,-4.9524132936,0.126399053,0.8242153288
H,0,-0.0468616877,-0.7459007233,-0.4926207316
N,0,0.8568878283,-1.2753312745,-0.3622687093
C,0,1.7580908057,-1.3191939998,-1.5196280964
C,0,2.9908235623,-2.1530982074,-1.1907792817
H,0,1.1962940233,-1.7412391264,-2.3580126574
H,0,2.0504202587,-0.2907018184,-1.7572155847
C,0,1.2384530817,-1.4782011972,0.8824871104
N,0,2.5065863636,-1.7976563436,1.19226316
C,0,2.977901764,-1.918453932,2.569292375
C,0,3.5518338514,-1.6926557439,0.1521138158
H,0,3.7484480566,-2.6930239794,2.6114259693
H,0,3.4129591421,-0.9737637483,2.9193180678
H,0,2.1698707478,-2.207452603,3.2391773686
H,0,3.8777425432,-0.6464093619,0.0891120576
C,0,0.1848490556,-1.3680880042,1.9520018188
H,0,2.7444019736,-3.2209750468,-1.1461490679
H,0,3.7461417638,-2.0153814727,-1.9697248318
H,0,4.3907483636,-2.3189131047,0.4674579299
H,0,0.0254605988,-2.3413264254,2.4287236495
H,0,0.482961718,-0.6548055551,2.725068837
H,0,-0.7570824905,-1.0356438902,1.5119685717
```

## Ts 1 from equatorial attack with DBU model, orientation B (13) – 6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.840339467

 Zero-point correction=                           0.451312 (Hartree/Particle)
 Thermal correction to Energy=                    0.475419
 Thermal correction to Enthalpy=                  0.476364
 Thermal correction to Gibbs Free Energy=         0.396232
 Sum of electronic and zero-point Energies=           -962.389027
 Sum of electronic and thermal Energies=              -962.364920
 Sum of electronic and thermal Enthalpies=            -962.363976
 Sum of electronic and thermal Free Energies=         -962.444108

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 298.330             89.747            168.652

C,0,-2.201252939,1.9927560183,1.0417629329
C,0,-1.290776939,3.0558640183,1.6751729329
C,0,0.155578061,2.9045840183,1.1913719329
C,0,0.251519061,2.9738450183,-0.3377940671
C,0,-0.860000939,2.4659560183,-1.0627710671
C,0,-1.916697939,1.7834300183,-0.4371730671
O,0,1.285370061,3.4597530183,-0.8621630671
O,0,-1.371731939,-0.0335259817,-0.5272710671
O,0,-1.964214939,-0.9671109817,0.4290399329
C,0,-2.830029939,-1.9079299817,-0.2461490671
C,0,-3.979747939,-1.1722509817,-0.9446480671
C,0,-2.018292939,-2.7404429817,-1.2465330671
C,0,-3.355258939,-2.7783709817,0.9019659329
H,0,-0.804687939,2.4956110183,-2.1504550671
H,0,-2.794725939,1.5831460183,-1.0452700671
H,0,-3.253074939,2.2862750183,1.1630369329
H,0,-2.099394939,1.0315060183,1.5578449329
```

```
H,0,-1.649001939,4.0561010183,1.3951119329
H,0,-1.346601939,2.9964510183,2.7702509329
H,0,0.809476061,3.6796030183,1.6085499329
H,0,0.559202061,1.9349750183,1.5223629329
H,0,-2.656985939,-3.4659839817,-1.7635110671
H,0,-1.560360939,-2.0815229817,-1.9889840671
H,0,-1.221497939,-3.2899079817,-0.7318160671
H,0,-4.674924939,-1.8857569817,-1.4025450671
H,0,-4.536263939,-0.5619119817,-0.2245940671
H,0,-3.589705939,-0.5172419817,-1.7280700671
H,0,-4.036983939,-3.5452599817,0.5177799329
H,0,-2.529152939,-3.2804769817,1.4174459329
H,0,-3.897499939,-2.1676119817,1.6318389329
H,0,0.237688061,-0.2543779817,-0.3939090671
N,0,1.290430061,-0.4072919817,-0.4333380671
C,0,1.990199061,0.1664650183,-1.5868440671
C,0,3.277089061,-0.6113319817,-1.8387350671
H,0,1.307142061,0.1039410183,-2.4390020671
H,0,2.180358061,1.2299400183,-1.3985770671
C,0,1.896288061,-1.0474179817,0.5459719329
N,0,3.226499061,-1.2176169817,0.5605759329
C,0,3.951715061,-1.8630359817,1.6534629329
C,0,4.072809061,-0.7214699817,-0.5418180671
H,0,4.357604061,-2.8272959817,1.3248869329
H,0,4.784087061,-1.2189709817,1.9572689329
H,0,3.309780061,-2.0221879817,2.5174029329
H,0,4.495531061,0.2500820183,-0.2520340671
C,0,1.039347061,-1.5862769817,1.6600479329
H,0,3.041112061,-1.6151209817,-2.2123160671
H,0,3.884828061,-0.1072619817,-2.5967020671
H,0,4.904223061,-1.4249099817,-0.6563500671
H,0,1.246544061,-2.6476349817,1.8299799329
H,0,1.241243061,-1.0496579817,2.5944109329
H,0,-0.016759939,-1.4693369817,1.4047069329
```

## Ts 1 from equatorial attack with DBU model, orientation B (13) – 6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.922154717

 Zero-point correction=                           0.447644 (Hartree/Particle)
 Thermal correction to Energy=                    0.472059
 Thermal correction to Enthalpy=                  0.473004
 Thermal correction to Gibbs Free Energy=         0.391163
 Sum of electronic and zero-point Energies=           -962.474510
 Sum of electronic and thermal Energies=              -962.450095
 Sum of electronic and thermal Enthalpies=            -962.449151
 Sum of electronic and thermal Free Energies=         -962.530991

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 296.222             90.495            172.247

C,0,-1.9585729512,1.9451010183,1.298284939
C,0,-1.0313609512,3.0786140183,1.763329939
C,0,0.3025490488,3.0545730183,1.006544939
C,0,0.0992790488,3.1051580183,-0.508045061
C,0,-1.0789699512,2.5023440183,-1.021103061
C,0,-1.9667359512,1.7741200183,-0.211242061
O,0,0.9731120488,3.6751950183,-1.221676061
O,0,-1.3720669512,-0.0427709817,-0.446951061
O,0,-1.9429959512,-1.0375729817,0.461752939
C,0,-2.8175579512,-1.9527849817,-0.244219061
```

```
C,0,-3.9890519512,-1.1969589817,-0.882864061
C,0,-2.0240299512,-2.7356029817,-1.298692061
C,0,-3.3119659512,-2.8821089817,0.871864939
H,0,-1.2314699512,2.5284320183,-2.099142061
H,0,-2.9287779512,1.5213790183,-0.645191061
H,0,-2.9834379512,2.1364500183,1.641274939
H,0,-1.6647109512,0.9940440183,1.755325939
H,0,-1.5174809512,4.0467890183,1.583141939
H,0,-0.8628469512,3.0061200183,2.845295939
H,0,0.9450380488,3.8947520183,1.293091939
H,0,0.8557340488,2.1341020183,1.247930939
H,0,-2.6692079512,-3.4610499817,-1.806645061
H,0,-1.6116529512,-2.0521609817,-2.045393061
H,0,-1.1966689512,-3.2792729817,-0.829763061
H,0,-4.6826649512,-1.8991659817,-1.358944061
H,0,-4.5387419512,-0.6298399817,-0.124208061
H,0,-3.6250499512,-0.5024129817,-1.644252061
H,0,-3.9871999512,-3.6391919817,0.459239939
H,0,-2.4716249512,-3.3953759817,1.350594939
H,0,-3.8536109512,-2.3149639817,1.635729939
H,0,0.2056720488,-0.3154989817,-0.371822061
N,0,1.2620130488,-0.4663149817,-0.431380061
C,0,1.9282500488,0.0073950183,-1.647863061
C,0,3.1951900488,-0.8071169817,-1.885796061
H,0,1.2185730488,-0.0997399817,-2.472644061
H,0,2.1541730488,1.0760040183,-1.546981061
C,0,1.9066100488,-1.0216129817,0.577334939
N,0,3.2373960488,-1.1876889817,0.560201939
C,0,3.9985390488,-1.7486639817,1.677874939
C,0,4.0441410488,-0.8124829817,-0.619284061
H,0,4.3212590488,-2.7708979817,1.448147939
H,0,4.8858460488,-1.1297679817,1.843076939
H,0,3.4137600488,-1.7554739817,2.594947939
H,0,4.4937550488,0.1731110183,-0.438496061
C,0,1.0938050488,-1.4681089817,1.761933939
H,0,2.9313250488,-1.8356439817,-2.159653061
H,0,3.7734590488,-0.3795549817,-2.710356061
H,0,4.8579340488,-1.5400419817,-0.702546061
H,0,1.3100390488,-2.5118369817,2.008167939
H,0,1.3267260488,-0.8581339817,2.641600939
H,0,0.0308900488,-1.3731179817,1.533348939
```

## Intermediate from equatorial attack with DBU model, orientation B (14) – 6-31G* Gas Phase

```
E(RB+HF-LYP) =  -962.825022182

Zero-point correction=                           0.453871 (Hartree/Particle)
 Thermal correction to Energy=                    0.477936
 Thermal correction to Enthalpy=                  0.478881
 Thermal correction to Gibbs Free Energy=         0.399909
 Sum of electronic and zero-point Energies=           -962.371152
 Sum of electronic and thermal Energies=              -962.347086
 Sum of electronic and thermal Enthalpies=            -962.346142
 Sum of electronic and thermal Free Energies=         -962.425113

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 299.910             90.832            166.209

 C,0,-1.2059963681,2.168275155,1.151531667
 C,0,-0.0886490341,3.2080666982,1.2797434339
 C,0,1.2380712449,2.609460379,0.8049555827
 C,0,1.1492504175,2.0320028822,-0.6186624721
```

```
C,0,-0.1267757636,1.7643219825,-1.1231390086
C,0,-1.3275881902,1.62149463,-0.2860211491
O,0,2.2422744929,1.8645294313,-1.2467907265
O,0,-1.5021277071,0.1198337998,-0.2462620245
O,0,-2.6464801201,-0.2942783614,0.6397852561
C,0,-3.6331619295,-0.9995327803,-0.1377707601
C,0,-4.2284632022,-0.0971975953,-1.2253786733
C,0,-3.0266239721,-2.2723456865,-0.744798579
C,0,-4.6887917216,-1.3499894514,0.921243676
H,0,-0.2197122154,1.5069156505,-2.1766778941
H,0,-2.2462175835,1.9808461681,-0.7660100456
H,0,-2.1676503849,2.5801845547,1.4780643126
H,0,-0.9926501615,1.3293724447,1.8252594642
H,0,-0.3257589394,4.0859220298,0.6648345742
H,0,-0.0174048347,3.5574393213,2.3193775155
H,0,2.0428251417,3.3545236768,0.7968362897
H,0,1.5645869488,1.8215242068,1.5065673172
H,0,-3.7920329048,-2.8586028017,-1.266361042
H,0,-2.2428483318,-2.0174627698,-1.4638947675
H,0,-2.5896391917,-2.8991713862,0.0409248004
H,0,-5.0249508937,-0.6199054818,-1.76799245
H,0,-4.6522907719,0.8091592091,-0.7802964004
H,0,-3.4584072434,0.1963384211,-1.9439583912
H,0,-5.5146643185,-1.9058088561,0.463516465
H,0,-4.2519136598,-1.9672017666,1.713260002
H,0,-5.0926967943,-0.4398473582,1.3761713377
H,0,0.0666832944,-0.8307458598,-0.5142851295
N,0,1.0471864305,-1.1534635881,-0.5617063192
C,0,1.7142567137,-1.009140237,-1.8635508557
C,0,3.1468770285,-1.5189641009,-1.7618995169
H,0,1.1298582448,-1.5723383001,-2.5975963387
H,0,1.7272801623,0.061276339,-2.1117963763
C,0,1.676065161,-1.2125467793,0.5974256085
N,0,3.0148814555,-1.218324158,0.66986791
C,0,3.7333512728,-1.1997503304,1.9392659307
C,0,3.7974754791,-0.8778634742,-0.5384429396
H,0,4.6704516994,-1.7514857771,1.8215641568
H,0,3.96974123,-0.1718923234,2.2439003719
H,0,3.1529961931,-1.6791513839,2.7271597196
H,0,3.7999615798,0.215172304,-0.6496881526
C,0,0.8284161043,-1.3041599637,1.8379965077
H,0,3.1821951075,-2.6124796137,-1.6783381093
H,0,3.6987563749,-1.2318409136,-2.6619709243
H,0,4.8154435497,-1.2461271699,-0.383658118
H,0,0.9726358612,-2.2730508773,2.3296482054
H,0,1.0914502227,-0.5171999681,2.5507031493
H,0,-0.2261153515,-1.1953144221,1.5787545684
```

### Intermediate from equatorial attack with DBU model, orientation B (14) – 6-31+G** Gas Phase

```
E(RB+HF-LYP) = -962.901398516

 Zero-point correction=                           0.450583 (Hartree/Particle)
 Thermal correction to Energy=                    0.474948
 Thermal correction to Enthalpy=                  0.475893
 Thermal correction to Gibbs Free Energy=         0.395875
 Sum of electronic and zero-point Energies=           -962.450816
 Sum of electronic and thermal Energies=              -962.426450
 Sum of electronic and thermal Enthalpies=            -962.425506
 Sum of electronic and thermal Free Energies=         -962.505523

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

```
 Total                   298.035             91.679            168.410

 C,0,-1.2987294015,2.233793169,1.1614978179
 C,0,-0.1652038071,3.2516167367,1.3306588212
 C,0,1.1724267224,2.6291409912,0.9175928995
 C,0,1.1384211135,2.0385656928,-0.5010153975
 C,0,-0.1175048671,1.775398528,-1.0577744227
 C,0,-1.349465635,1.6429113238,-0.2630001739
 O,0,2.2581319237,1.8529794064,-1.0829085751
 O,0,-1.5035907962,0.132694635,-0.1778829554
 O,0,-2.7058039093,-0.2686142188,0.6316685629
 C,0,-3.6431636513,-0.9968234407,-0.1923717179
 C,0,-4.161668138,-0.1267086921,-1.3441000214
 C,0,-3.0015188916,-2.2885123988,-0.7185039539
 C,0,-4.7693119097,-1.3151593077,0.8022479814
 H,0,-0.1714943636,1.5146491864,-2.112674842
 H,0,-2.2499271367,1.9675523065,-0.7964398071
 H,0,-2.265511107,2.6823898481,1.4147573102
 H,0,-1.152637015,1.4107503646,1.8713667041
 H,0,-0.3582104215,4.1322078298,0.7049600832
 H,0,-0.1306469361,3.6019803775,2.3713152042
 H,0,1.9857357956,3.3637615418,0.9347539246
 H,0,1.4565154669,1.842890836,1.6367048385
 H,0,-3.7357774805,-2.8883967956,-1.2673657958
 H,0,-2.17531588,-2.0583089459,-1.3965912098
 H,0,-2.6176568608,-2.8895229054,0.1127290304
 H,0,-4.9210722587,-0.6686176342,-1.9187304998
 H,0,-4.612956976,0.7922782318,-0.9572768989
 H,0,-3.3472770894,0.1429653436,-2.0212449434
 H,0,-5.5627620398,-1.879194539,0.3006128031
 H,0,-4.3914228258,-1.9144296051,1.6364446151
 H,0,-5.199703346,-0.3934155519,1.2050050396
 H,0,0.073510279,-0.854263394,-0.4335591553
 N,0,1.0492750792,-1.1762384339,-0.5227489135
 C,0,1.6486086736,-1.0593259036,-1.8588398447
 C,0,3.070723802,-1.6053275565,-1.8311950741
 H,0,1.0134339939,-1.612577769,-2.5563780877
 H,0,1.6622951284,0.0058720549,-2.1189494194
 C,0,1.7431715214,-1.2087798181,0.6018516232
 N,0,3.0825451417,-1.2410773936,0.6009071369
 C,0,3.8702692644,-1.1802498187,1.8298781221
 C,0,3.8135069167,-0.9730052726,-0.6573379863
 H,0,4.7897769142,-1.7531244292,1.6854262576
 H,0,4.1369750838,-0.1439477876,2.0716976802
 H,0,3.3278324844,-1.6155913216,2.667571297
 H,0,3.8743389057,0.1151765356,-0.7904818397
 C,0,0.9647939029,-1.2397590732,1.8889798319
 H,0,3.0760124789,-2.698241587,-1.7368911577
 H,0,3.5781477719,-1.346084331,-2.7646748312
 H,0,4.816237571,-1.394427057,-0.5477327636
 H,0,1.0976294035,-2.2018863215,2.3951308524
 H,0,1.2952433174,-0.4470188567,2.5644832754
 H,0,-0.0960858431,-1.0953443703,1.6804974842
```

## Intermediate from equatorial attack with DBU model, orientation B (14) – 6-31G* – PCM Dichloroethane

```
E(RB+HF-LYP) =  -962.844738623

Zero-point correction=                           0.453435 (Hartree/Particle)
 Thermal correction to Energy=                    0.477708
 Thermal correction to Enthalpy=                  0.478652
 Thermal correction to Gibbs Free Energy=         0.398080
```

```
Sum of electronic and zero-point Energies=           -962.391304
Sum of electronic and thermal Energies=              -962.367030
Sum of electronic and thermal Enthalpies=            -962.366086
Sum of electronic and thermal Free Energies=         -962.446658

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  299.766             90.837            169.578

C,0,-1.1642170122,2.1940779024,1.1098230122
C,0,-0.0977960122,3.2932129024,1.1339470122
C,0,1.2212999878,2.7518269024,0.5748870122
C,0,1.0633089878,2.1388049024,-0.8259339878
C,0,-0.2186210122,1.7629849024,-1.2193859878
C,0,-1.3683950122,1.6078339024,-0.3027829878
O,0,2.1172259878,2.0493059024,-1.5444049878
O,0,-1.5278410122,0.1222549024,-0.2145859878
O,0,-2.6726910122,-0.2332510976,0.6738410122
C,0,-3.6250290122,-1.0296260976,-0.0658919878
C,0,-4.2103750122,-0.2356610976,-1.2393259878
C,0,-2.9731630122,-2.3334410976,-0.5451239878
C,0,-4.6976140122,-1.3133600976,0.9946620122
H,0,-0.3598850122,1.4196939024,-2.2447209878
H,0,-2.3189190122,1.9535079024,-0.7321259878
H,0,-2.1183820122,2.5607069024,1.5056660122
H,0,-0.8471960122,1.3812709024,1.7747560122
H,0,-0.4272660122,4.1467519024,0.5254170122
H,0,0.0317099878,3.6670489024,2.1592520122
H,0,1.9839269878,3.5383259024,0.5030960122
H,0,1.6343119878,1.9943499024,1.2620470122
H,0,-3.7157720122,-2.9839730976,-1.0210519878
H,0,-2.1850000122,-2.1257180976,-1.2746279878
H,0,-2.5332270122,-2.8736930976,0.3007090122
H,0,-4.9728700122,-0.8258800976,-1.7607129878
H,0,-4.6753900122,0.6896149024,-0.8822589878
H,0,-3.4257290122,0.0220279024,-1.9561219878
H,0,-5.4990260122,-1.9240050976,0.5645990122
H,0,-4.2685530122,-1.8540790976,1.8449060122
H,0,-5.1338570122,-0.3782480976,1.3615880122
H,0,0.0868799878,-0.8339340976,-0.3965069878
N,0,1.0673949878,-1.1378490976,-0.4544529878
C,0,1.6938379878,-1.0802780976,-1.7830669878
C,0,3.1166339878,-1.6202750976,-1.6973539878
H,0,1.0766989878,-1.6765940976,-2.4631889878
H,0,1.7018059878,-0.0332580976,-2.1092509878
C,0,1.7243329878,-1.2056390976,0.6917910122
N,0,3.0593559878,-1.2259370976,0.7264070122
C,0,3.8286659878,-1.3062230976,1.9670290122
C,0,3.8133849878,-0.9519350976,-0.5148399878
H,0,4.6981909878,-1.9483990976,1.8007320122
H,0,4.1793639878,-0.3125810976,2.2725720122
H,0,3.2337369878,-1.7377820976,2.7709470122
H,0,3.8474499878,0.1347429024,-0.6721779878
C,0,0.9074829878,-1.2773340976,1.9531080122
H,0,3.1228099878,-2.7093870976,-1.5682389878
H,0,3.6545519878,-1.3873270976,-2.6218289878
H,0,4.8289729878,-1.3308760976,-0.3756349878
H,0,1.0211399878,-2.2602600976,2.4249990122
H,0,1.2244109878,-0.5173380976,2.6735120122
H,0,-0.1481250122,-1.1244930976,1.7219250122
```

## Intermediate from equatorial attack with DBU model, orientation B (14) – 6-31+G** - PCM Dichloroethane

E(RB+HF-LYP) = -962.926817039

| | |
|---|---|
| Zero-point correction= | 0.449737 (Hartree/Particle) |
| Thermal correction to Energy= | 0.473501 |
| Thermal correction to Enthalpy= | 0.474446 |
| Thermal correction to Gibbs Free Energy= | 0.394925 |
| Sum of electronic and zero-point Energies= | -962.477080 |
| Sum of electronic and thermal Energies= | -962.453316 |
| Sum of electronic and thermal Enthalpies= | -962.452371 |
| Sum of electronic and thermal Free Energies= | -962.531892 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 297.127 | 89.656 | 167.366 |

C,0,-1.3397017083,2.1094979925,1.2619632696
C,0,-0.4133704163,3.325105907,1.3588546156
C,0,0.9517119602,2.9996899247,0.7421696994
C,0,0.8426872009,2.4749083463,-0.6929303309
C,0,-0.3758630653,1.9414892129,-1.0997983006
C,0,-1.4987969016,1.6061559023,-0.1864521289
O,0,1.8874893316,2.5871979256,-1.4382083283
O,0,-1.5087649183,0.1096303062,-0.2001388042
O,0,-2.6115343631,-0.4142150651,0.6499317873
C,0,-3.4934774289,-1.2445538634,-0.1507829066
C,0,-4.1470705423,-0.4267231193,-1.2705653409
C,0,-2.7288839272,-2.4498009475,-0.7127544431
C,0,-4.5361154288,-1.6926819814,0.8820924347
H,0,-0.489315584,1.6501908196,-2.1440391511
H,0,-2.4801407513,1.884659166,-0.5924964719
H,0,-2.3222857109,2.3283847929,1.6941014337
H,0,-0.9144646077,1.2935970383,1.8593199451
H,0,-0.8571911939,4.1780855418,0.82746759
H,0,-0.3049786039,3.6274879518,2.4092398245
H,0,1.6023650834,3.8824612624,0.7196256191
H,0,1.4732242016,2.2503152072,1.3593315722
H,0,-3.4149813789,-3.123739164,-1.2373161835
H,0,-1.9623311289,-2.1267559718,-1.4223823435
H,0,-2.24783091,-3.0101447811,0.0958262219
H,0,-4.8539648611,-1.049600522,-1.8296130525
H,0,-4.693056191,0.4267730185,-0.8560923368
H,0,-3.3925011272,-0.0551099971,-1.9687394915
H,0,-5.2786579066,-2.3385930293,0.4018653623
H,0,-4.0627894995,-2.2545246767,1.6936089757
H,0,-5.0546182334,-0.8291794737,1.3103102019
H,0,0.1802146782,-0.6962535351,-0.4209129204
N,0,1.1658404576,-0.9737168813,-0.5005136878
C,0,1.7991971123,-0.7337277022,-1.8045485678
C,0,3.2010131213,-1.3322398034,-1.8114214648
H,0,1.171978839,-1.2083722954,-2.5664134436
H,0,1.7973782916,0.347662709,-1.9812219752
C,0,1.8087710982,-1.2568874373,0.6204278945
N,0,3.1418160351,-1.3506543612,0.6522160338
C,0,3.8975310532,-1.6542681166,1.8694755469
C,0,3.9336180921,-0.9496037665,-0.5296651317
H,0,4.7127827924,-2.3368642951,1.6155009357
H,0,4.3241503959,-0.7384527313,2.2958116253
H,0,3.2682433506,-2.1361340349,2.6151871708
H,0,4.1068338142,0.133658578,-0.4856062947
C,0,0.9797865785,-1.4845639139,1.8547410581
H,0,3.1492149553,-2.4248827412,-1.888603441

H,0,3.7593208134,-0.962198161,-2.676570604
H,0,4.9016716335,-1.4532519836,-0.4649328992
H,0,1.0517938085,-2.5296135888,2.174917618
H,0,1.3188302433,-0.8517452114,2.6795425462
H,0,-0.0662318529,-1.2589463314,1.6438548843

## Ts 2 from equatorial attack with DBU model, orientation B – (15) 6-31G* - Gas Phase

E(RB+HF-LYP) = -962.818858563

| | |
|---|---|
| Zero-point correction= | 0.452404 (Hartree/Particle) |
| Thermal correction to Energy= | 0.476295 |
| Thermal correction to Enthalpy= | 0.477239 |
| Thermal correction to Gibbs Free Energy= | 0.398459 |
| Sum of electronic and zero-point Energies= | -962.366455 |
| Sum of electronic and thermal Energies= | -962.342564 |
| Sum of electronic and thermal Enthalpies= | -962.341620 |
| Sum of electronic and thermal Free Energies= | -962.420399 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 298.879 | 89.806 | 165.806 |

C,0,-1.7784212684,2.4891694415,0.8793995587
C,0,-0.5461741999,3.3014396919,1.3044072713
C,0,0.7590857554,2.5795378235,0.9472114063
C,0,0.8629425568,2.2826220247,-0.5525154573
C,0,-0.3703982321,2.1127656683,-1.2556528332
C,0,-1.6216033992,1.855341119,-0.5137854685
O,0,1.9922522157,2.1986288249,-1.0868802981
O,0,-1.2109693024,0.4891640888,-0.4738367932
O,0,-2.2318442746,-0.69227017,0.6178503676
C,0,-3.1427490038,-1.4513428374,-0.1266151337
C,0,-4.2280076608,-0.5581546466,-0.7619349048
C,0,-2.4370804859,-2.2733016816,-1.2263225302
C,0,-3.8021607759,-2.4114314148,0.8929407427
H,0,-0.344514838,1.9622977935,-2.32975375
H,0,-2.5295559165,1.9678982515,-1.1169012691
H,0,-2.6650737804,3.1353516902,0.8889292143
H,0,-1.9767304731,1.6657023872,1.5737251557
H,0,-0.5555286212,4.2717514822,0.79000828
H,0,-0.5859120698,3.5179184925,2.3799605154
H,0,1.641826316,3.1663343152,1.2260806903
H,0,0.8182003996,1.63122012,1.5020723998
H,0,-3.1409476885,-2.902726463,-1.7859594905
H,0,-1.9453923738,-1.5966684454,-1.9337548319
H,0,-1.675351184,-2.9267691318,-0.7827904282
H,0,-5.0151569837,-1.1509997956,-1.2454441441
H,0,-4.6900264231,0.0697485919,0.0080408035
H,0,-3.783752706,0.0972827176,-1.5183162854
H,0,-4.5528951198,-3.0519201537,0.4116928505
H,0,-3.0434586336,-3.0538099854,1.3543590757
H,0,-4.2903771433,-1.8369177107,1.6872353027
H,0,0.0864823488,-0.6862118626,-0.5954932567
N,0,1.0712207556,-0.993220304,-0.5839861043
C,0,1.8229780562,-0.7951537142,-1.8291028773
C,0,3.2607102375,-1.268366762,-1.6472885771
H,0,1.3103566215,-1.3587659884,-2.6149160705
H,0,1.8005449152,0.2734761056,-2.0705280552
C,0,1.6016375377,-1.1514593137,0.6143226306
N,0,2.9326720425,-1.15152492,0.7835252335
C,0,3.5708040253,-1.3031662974,2.086271798
C,0,3.7956208299,-0.709430694,-0.330764882

H,0,4.4574516542,-1.9359430726,1.9786663684
H,0,3.883700991,-0.3296731841,2.4849889854
H,0,2.8957186723,-1.7757110979,2.7976356012
H,0,3.7986281442,0.3879105667,-0.3581276094
C,0,0.6563315976,-1.3529774708,1.7658190086
H,0,3.3182855133,-2.3634789687,-1.6339188508
H,0,3.8745550663,-0.9103218545,-2.4791904274
H,0,4.8081910176,-1.0674411165,-0.1260304962
H,0,0.7813248347,-2.3611183562,2.1795754256
H,0,0.8601605821,-0.6334741698,2.5651019922
H,0,-0.3846052413,-1.2324521579,1.4308736775

## Ts 2 from equatorial attack with DBU model, orientation B (15) – 6-31+G** - Gas Phase

E(RB+HF-LYP) = -962.896635434

| | |
|---|---|
| Zero-point correction= | 0.448498 (Hartree/Particle) |
| Thermal correction to Energy= | 0.472774 |
| Thermal correction to Enthalpy= | 0.473718 |
| Thermal correction to Gibbs Free Energy= | 0.392929 |
| Sum of electronic and zero-point Energies= | -962.448138 |
| Sum of electronic and thermal Energies= | -962.423861 |
| Sum of electronic and thermal Enthalpies= | -962.422917 |
| Sum of electronic and thermal Free Energies= | -962.503707 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 296.670 | 90.442 | 170.036 |

C,0,-1.8094453258,2.4324443434,0.9926855973
C,0,-0.7133727884,3.4761568336,1.2500887743
C,0,0.6499761371,2.9890164645,0.7442354721
C,0,0.6241634699,2.6478000117,-0.7490698287
C,0,-0.6297869248,2.2400802374,-1.2952166656
C,0,-1.7515452382,1.8339078608,-0.4274580862
O,0,1.6795975156,2.754339233,-1.4187553394
O,0,-1.2829276892,0.4670045248,-0.4536221276
O,0,-2.2054680773,-0.6954172661,0.6282451163
C,0,-3.0033412663,-1.5679861885,-0.1412383936
C,0,-4.0672329145,-0.7972765934,-0.9459372878
C,0,-2.1440403915,-2.4270982525,-1.0911125615
C,0,-3.7008706072,-2.4777329971,0.8973097262
H,0,-0.7024918199,2.0769888339,-2.3652339442
H,0,-2.728350061,1.8744802635,-0.9202864974
H,0,-2.7962957051,2.8805391987,1.157205142
H,0,-1.7273754576,1.5998102231,1.69930523
H,0,-0.9639713503,4.4104202866,0.7308942599
H,0,-0.6659540572,3.7156619655,2.3203122758
H,0,1.4352706575,3.7379072058,0.892221483
H,0,0.9579441105,2.0929150073,1.3053460031
H,0,-2.7578115841,-3.1414802953,-1.6531892296
H,0,-1.6228263871,-1.7835575444,-1.8062940993
H,0,-1.3973012981,-2.9925808863,-0.5215290914
H,0,-4.7470553985,-1.4822350157,-1.4670151727
H,0,-4.6592284131,-0.1640865558,-0.276798971
H,0,-3.5875276452,-0.1586644698,-1.6933499276
H,0,-4.3580972565,-3.2013332984,0.3992115676
H,0,-2.9581023768,-3.0294873047,1.4828587482
H,0,-4.3016822253,-1.8746212627,1.5848386689
H,0,0.2187028207,-0.2167692317,-0.3785818361
N,0,1.1901874753,-0.6104243889,-0.3959812974
C,0,1.953542157,-0.4290757029,-1.6351936127
C,0,3.1348604607,-1.3920440725,-1.6491075413

```
H,0,1.2697557244,-0.6240033101,-2.4651560249
H,0,2.2640186631,0.6207073938,-1.7074618135
C,0,1.680562493,-1.0950922259,0.7238503674
N,0,2.9718142311,-1.4688260523,0.8167559236
C,0,3.595999678,-1.9294364005,2.053776677
C,0,3.8890402421,-1.2965463174,-0.3251278907
H,0,3.9810933698,-2.9475794567,1.9262326067
H,0,4.4332132623,-1.2706037213,2.3117920574
H,0,2.889129223,-1.9232569196,2.8795139432
H,0,4.3954221703,-0.3263820265,-0.232721655
C,0,0.7424293567,-1.223936029,1.892345394
H,0,2.7873523106,-2.4212190842,-1.7980208852
H,0,3.8102038465,-1.1467937882,-2.473528377
H,0,4.6510238832,-2.0789673865,-0.2527553497
H,0,0.7784948419,-2.2361830545,2.3057550853
H,0,1.0183537844,-0.5211331702,2.685987635
H,0,-0.2851647961,-1.0202372704,1.5691037501
```

## Ts 2 from equatorial attack with DBU model, orientation B (15) – 6-31G* - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.839393931

 Zero-point correction=                           0.451344 (Hartree/Particle)
 Thermal correction to Energy=                    0.475543
 Thermal correction to Enthalpy=                  0.476487
 Thermal correction to Gibbs Free Energy=         0.396066
 Sum of electronic and zero-point Energies=           -962.388050
 Sum of electronic and thermal Energies=              -962.363851
 Sum of electronic and thermal Enthalpies=            -962.362907
 Sum of electronic and thermal Free Energies=         -962.443328

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 298.408             89.980            169.259

 C,0,-2.3183927364,1.508897509,1.5507654899
 C,0,-1.5950335369,2.8345919201,1.8286398022
 C,0,-0.3505748721,2.9976885015,0.9456738617
 C,0,-0.7067335341,2.948992127,-0.5444472822
 C,0,-1.8131178658,2.1271373488,-0.9073748864
 C,0,-2.4150968512,1.1716687903,0.049309272
 O,0,-0.0507918878,3.6382737886,-1.3608020478
 O,0,-1.4700723296,0.2082089529,-0.3958409381
 O,0,-1.6415964787,-1.4148453529,0.5517816994
 C,0,-2.1059858798,-2.4131600558,-0.3191787492
 C,0,-3.5049429624,-2.0659059382,-0.8673612662
 C,0,-1.1293534194,-2.6444518581,-1.4904440512
 C,0,-2.1966370262,-3.6958492648,0.5408526571
 H,0,-2.1127928255,2.0892530159,-1.9510552783
 H,0,-3.4271676989,0.8508520437,-0.2242920753
 H,0,-3.3275833272,1.5452404425,1.9804054048
 H,0,-1.8041263069,0.6707775488,2.0327269701
 H,0,-2.2769667028,3.6713909425,1.6238778137
 H,0,-1.3267026292,2.9037927287,2.8911004753
 H,0,0.158243726,3.9506377166,1.1325241341
 H,0,0.3748692768,2.2018584104,1.171537696
 H,0,-1.4705067313,-3.4492537425,-2.1544732763
 H,0,-1.0353659099,-1.7265529323,-2.0794268468
 H,0,-0.1361938283,-2.9137894532,-1.1111872928
 H,0,-3.9188358264,-2.8811369351,-1.4747620696
 H,0,-4.1937988846,-1.8687126664,-0.0377901138
 H,0,-3.4500112497,-1.1671221285,-1.4895767307
 H,0,-2.5753018826,-4.5420632581,-0.0471188817
```

```
H,0,-1.209380191,-3.9637699961,0.9339540919
H,0,-2.8702943341,-3.5345446259,1.3898526302
H,0,0.253853118,-0.0798312067,-0.1583695435
N,0,1.2810284586,-0.078580344,-0.2890048885
C,0,1.7896330125,0.6334962259,-1.4649514517
C,0,3.1432291773,0.0516391919,-1.8556607762
H,0,1.0502880122,0.511615144,-2.2605450233
H,0,1.8545749735,1.705744568,-1.2463133021
C,0,2.0446572533,-0.6871838497,0.6022601074
N,0,3.3779141039,-0.6659953999,0.5030819028
C,0,4.2700360701,-1.2601656349,1.4991745262
C,0,4.0533846325,-0.0065261536,-0.6328829063
H,0,4.7028375751,-2.1940721148,1.1212951121
H,0,5.0816757393,-0.5549583512,1.7041897987
H,0,3.7456575092,-1.4570663827,2.4323220841
H,0,4.3640446143,0.999206692,-0.3195789913
C,0,1.3538118027,-1.4004707044,1.7305655225
H,0,3.0116151628,-0.9570134118,-2.265166299
H,0,3.6117796175,0.6676573944,-2.6293040775
H,0,4.9585306832,-0.5822426323,-0.8520268347
H,0,1.7685593334,-2.4040188302,1.8649855537
H,0,1.4882329871,-0.8503376844,2.6697329786
H,0,0.284054047,-1.4849981285,1.5031938664
```

## Ts 2 from equatorial attack with DBU model, orientation B (15) – 6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.922272222

 Zero-point correction=                           0.448187 (Hartree/Particle)
 Thermal correction to Energy=                    0.472561
 Thermal correction to Enthalpy=                  0.473505
 Thermal correction to Gibbs Free Energy=         0.388791
 Sum of electronic and zero-point Energies=           -962.474085
 Sum of electronic and thermal Energies=              -962.449711
 Sum of electronic and thermal Enthalpies=            -962.448767
 Sum of electronic and thermal Free Energies=         -962.533481

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 296.537             90.503            178.296

 C,0,1.9871922011,-0.8460887035,1.841496618
 C,0,1.8943454287,-2.3792649957,1.8511410075
 C,0,1.4846233556,-2.9297903375,0.4783925451
 C,0,2.4769569361,-2.5080368179,-0.6080473744
 C,0,3.0921810815,-1.2528925727,-0.4536414388
 C,0,2.6242810342,-0.2731982589,0.5556887283
 O,0,2.7263631064,-3.3238359288,-1.5527339979
 O,0,1.6480304573,0.3173001781,-0.3317881537
 O,0,0.8016662272,1.6013035823,0.42157712
 C,0,1.1236400565,2.8357799235,-0.23272268
 C,0,2.6162005772,3.1590328019,-0.0704180533
 C,0,0.7403378825,2.7881240327,-1.7212402669
 C,0,0.2732225564,3.8878556554,0.5055846274
 H,0,3.8063307508,-0.9209240592,-1.2039645643
 H,0,3.3832530567,0.4821598466,0.7933630018
 H,0,2.559168789,-0.5051255698,2.7133346085
 H,0,0.9896521735,-0.4047324239,1.9358611155
 H,0,2.8726687268,-2.8040196022,2.1132322195
 H,0,1.1913459105,-2.7087668226,2.6277649116
 H,0,1.4373998714,-4.0248216273,0.4844703777
 H,0,0.4811845726,-2.5674751107,0.2110922505
```

H,0,0.9893378619,3.7327723798,-2.2174783766
H,0,1.2788026146,1.9796083716,-2.2223040782
H,0,-0.3363088794,2.6203386601,-1.8393699628
H,0,2.8463208776,4.1437108883,-0.4925974763
H,0,2.8921489179,3.1637671829,0.9892393534
H,0,3.2262828537,2.4129867722,-0.5863325951
H,0,0.4555239946,4.8828113278,0.0834036333
H,0,-0.7947318393,3.6675789217,0.406563145
H,0,0.528266574,3.9117813564,1.5699065443
H,0,-0.5992427379,0.6914923691,-0.029719101
N,0,-1.4360735842,0.1229476288,-0.2805933446
C,0,-1.4488782636,-0.5577141309,-1.5773893165
C,0,-2.8824845097,-0.618579895,-2.0943885035
H,0,-0.7924585965,-0.002891032,-2.2498122255
H,0,-1.0290021802,-1.565528241,-1.4642250988
C,0,-2.4486377827,0.0841765698,0.5687162684
N,0,-3.571110818,-0.5848923938,0.2903194364
C,0,-4.700787158,-0.6924860115,1.2169063854
C,0,-3.784784726,-1.2266484151,-1.0257781673
H,0,-5.4926158909,0.0149187908,0.9438621053
H,0,-5.0995845554,-1.7087885556,1.1536885521
H,0,-4.3923712399,-0.5133476656,2.2445381245
H,0,-3.6050828129,-2.3044966246,-0.9189628292
C,0,-2.2857023329,0.8175583655,1.8698308365
H,0,-3.2294573309,0.390478774,-2.3469713294
H,0,-2.9345380026,-1.2274400296,-3.0018092201
H,0,-4.8392321448,-1.0878576043,-1.2858163996
H,0,-3.1078189779,1.5213403537,2.0279012282
H,0,-2.271290271,0.1148286373,2.7096539188
H,0,-1.3423776181,1.3641477777,1.8621784811

## Ts 1 from gauche axial attack with DBU model – 6-31G* - Gas Phase

E(RB+HF-LYP) = -962.820402562

| | |
|---|---|
| Zero-point correction= | 0.453043 (Hartree/Particle) |
| Thermal correction to Energy= | 0.476616 |
| Thermal correction to Enthalpy= | 0.477560 |
| Thermal correction to Gibbs Free Energy= | 0.400048 |
| Sum of electronic and zero-point Energies= | -962.367360 |
| Sum of electronic and thermal Energies= | -962.343787 |
| Sum of electronic and thermal Enthalpies= | -962.342843 |
| Sum of electronic and thermal Free Energies= | -962.420354 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 299.081 | 89.260 | 163.137 |

C,0,-1.5318480328,2.2492504134,1.310174344
C,0,-0.2013863006,2.1428523152,2.065514524
C,0,0.9626916449,2.723670573,1.2506511531
C,0,0.9967274084,2.2615377466,-0.218611864
C,0,-0.2368796847,1.9621060162,-0.826771409
C,0,-1.4353800731,1.6986147779,-0.1026741545
O,0,2.1186998799,2.2349519972,-0.8002337283
O,0,-1.6478620577,-0.0124510679,0.1998599098
O,0,-2.0101398078,-0.5971813404,-1.0871304695
C,0,-3.2534642447,-1.321223621,-0.9641071808
C,0,-3.1022631903,-2.459302078,0.0541756782
C,0,-4.3951732046,-0.374725312,-0.5752692767
C,0,-3.4534625288,-1.8728044577,-2.381200519
H,0,-0.2374599191,1.776643524,-1.8974982065
H,0,-2.3615594491,1.7989344664,-0.6684782085

H,0,-1.8207413974,3.3074434604,1.2261278145
H,0,-2.3330572106,1.7455705012,1.8639112502
H,0,-0.280123392,2.6428296436,3.040735255
H,0,-0.008408835,1.0832143717,2.2804010738
H,0,0.893665187,3.8223032984,1.2436347068
H,0,1.932270982,2.4879516238,1.7080787388
H,0,-5.3452283925,-0.9184327418,-0.5148203506
H,0,-4.1942512752,0.0819708341,0.3972140263
H,0,-4.5014659519,0.4224057145,-1.3190110928
H,0,-4.0191287209,-3.0572121452,0.1120597433
H,0,-2.2774904904,-3.1209462074,-0.2351109474
H,0,-2.8897366732,-2.0516369032,1.0461301537
H,0,-4.3791195599,-2.4560510782,-2.4353044593
H,0,-3.5153771863,-1.0549194076,-3.1063925354
H,0,-2.6183132488,-2.522610467,-2.6637646283
H,0,-0.1386487313,-0.8470574541,0.1974894197
N,0,0.8246289878,-1.2155379401,0.3973982288
C,0,1.1021022829,-1.5652867962,1.7882860709
C,0,2.3776402416,-0.8701576745,2.256089272
H,0,0.2345494678,-1.2629756005,2.3794787002
H,0,1.1994062362,-2.6558507199,1.875429836
C,0,1.7819897832,-0.9186355493,-0.4709300199
N,0,3.0760477573,-0.9473765246,-0.13031415
C,0,4.0978165968,-0.4219869797,-1.047234667
C,0,3.5054502668,-1.1499584284,1.2671034725
H,0,4.0331460178,0.6719409269,-1.0679679819
H,0,5.0779905062,-0.7457918049,-0.6912882782
H,0,3.9568638516,-0.8159500311,-2.0544551407
H,0,3.8796404262,-2.177143915,1.3735007872
C,0,1.3884922646,-0.5872974654,-1.8772305175
H,0,2.2026061438,0.2081808957,2.3158620272
H,0,2.6682313518,-1.2221676013,3.2509985985
H,0,4.3430981301,-0.4724326369,1.4544985572
H,0,1.6979748473,0.4443121235,-2.0863826012
H,0,1.8834044146,-1.2758847365,-2.5719944739
H,0,0.3086221636,-0.6787142739,-1.990425469

## Ts 1 from gauche axial attack with DBU model – 6-31+G** - Gas Phase

E(RB+HF-LYP) = -962.897285038

| | |
|---|---|
| Zero-point correction= | 0.450208 (Hartree/Particle) |
| Thermal correction to Energy= | 0.473932 |
| Thermal correction to Enthalpy= | 0.474876 |
| Thermal correction to Gibbs Free Energy= | 0.396692 |
| Sum of electronic and zero-point Energies= | -962.447077 |
| Sum of electronic and thermal Energies= | -962.423353 |
| Sum of electronic and thermal Enthalpies= | -962.422409 |
| Sum of electronic and thermal Free Energies= | -962.500593 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 297.397 | 89.900 | 164.553 |

C,0,-1.6417667502,2.2198364349,1.2647475416
C,0,-0.3723778897,2.1222387601,2.1209270556
C,0,0.8452038499,2.7132095211,1.3959005447
C,0,0.9952921093,2.250819771,-0.0641670495
C,0,-0.1822878012,1.9437009658,-0.7690976623
C,0,-1.4344145981,1.6593293378,-0.1332661925
O,0,2.1651918111,2.2233543127,-0.556403363
O,0,-1.6209814257,-0.0306896228,0.1577773553
O,0,-2.0065967819,-0.6508424774,-1.1048516107

```
C,0,-3.2960248046,-1.3018516494,-0.9754366054
C,0,-3.2236808259,-2.4109835198,0.0823899169
C,0,-4.3894193047,-0.2818654075,-0.636095788
C,0,-3.5083187289,-1.8897410548,-2.3762108921
H,0,-0.0974258879,1.7546841362,-1.8351033234
H,0,-2.3137940103,1.7571635985,-0.7692392317
H,0,-1.9228156694,3.2763349813,1.1479936575
H,0,-2.4822047192,1.7186688724,1.7579071774
H,0,-0.5286859957,2.6245890047,3.0848284079
H,0,-0.1867457007,1.0648826736,2.352487355
H,0,0.7651160284,3.8102109288,1.3727222942
H,0,1.7775432252,2.4920993385,1.9290545466
H,0,-5.3654423347,-0.7760398788,-0.5775107593
H,0,-4.1845328917,0.1911841531,0.3273613351
H,0,-4.4433331203,0.49601725,-1.4042822308
H,0,-4.1744297856,-2.9526719969,0.1370207742
H,0,-2.4333458648,-3.126660333,-0.1684678247
H,0,-3.0111224283,-1.984802892,1.0661443281
H,0,-4.4665286194,-2.4175947909,-2.419184852
H,0,-3.51494821,-1.0969378159,-3.1305089784
H,0,-2.7120531054,-2.5986015901,-2.6246696771
H,0,-0.0755880946,-0.8731166417,0.1814356552
N,0,0.8919931465,-1.2167444372,0.3783352516
C,0,1.2038873041,-1.5312670553,1.771224448
C,0,2.4694238539,-0.7911014415,2.1963606735
H,0,0.342104831,-1.2399225567,2.3753287923
H,0,1.3325683142,-2.6166657477,1.8774412498
C,0,1.8318573626,-0.9320172341,-0.5145013343
N,0,3.1307485718,-0.9483582674,-0.1975306272
C,0,4.1450807146,-0.4862459244,-1.154319404
C,0,3.589454478,-1.0762050348,1.2008699764
H,0,4.1422044968,0.6093275342,-1.1887972278
H,0,5.1188834012,-0.8534987761,-0.8247983183
H,0,3.9534413583,-0.884775655,-2.1502851492
H,0,4.0006876299,-2.0845358951,1.3414727985
C,0,1.4085003776,-0.6389492361,-1.9204531935
H,0,2.2701940066,0.2834966113,2.2232820992
H,0,2.7825238057,-1.104525016,3.1968056735
H,0,4.4039738574,-0.3603525366,1.3417129774
H,0,1.7483080381,0.3645585807,-2.1916659925
H,0,1.8494615476,-1.3760483008,-2.6005966013
H,0,0.3234289618,-0.6887694067,-1.9989325899
```

## Ts 1 from gauche axial attack with DBU model B – 6-31G* - PCM Dichloroethane

E(RB+HF-LYP) = -962.838975684

| | |
|---|---|
| Zero-point correction= | 0.451263 (Hartree/Particle) |
| Thermal correction to Energy= | 0.475426 |
| Thermal correction to Enthalpy= | 0.476370 |
| Thermal correction to Gibbs Free Energy= | 0.395813 |
| Sum of electronic and zero-point Energies= | -962.387713 |
| Sum of electronic and thermal Energies= | -962.363550 |
| Sum of electronic and thermal Enthalpies= | -962.362606 |
| Sum of electronic and thermal Free Energies= | -962.443163 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 298.334 | 89.629 | 169.547 |

```
C,0,-1.3941410854,2.6197879512,1.2183860244
C,0,0.0907269146,2.7195179512,1.5882610244
C,0,0.9068949146,3.3506629512,0.4535430244
```

```
C,0,0.6193699146,2.7476139512,-0.9300529756
C,0,-0.6611650854,2.1795979512,-1.1448509756
C,0,-1.5900460854,1.9438099512,-0.1202329756
O,0,1.5053379146,2.8486589512,-1.8184289756
O,0,-1.5245430854,0.1339429512,0.4912610244
O,0,-2.0505650854,-0.6410140488,-0.6237809756
C,0,-3.1305910854,-1.4844530488,-0.1709799756
C,0,-2.6234540854,-2.4684650488,0.8921370244
C,0,-4.2860130854,-0.6328310488,0.3697750244
C,0,-3.5432260854,-2.2221450488,-1.4504789756
H,0,-0.8803470854,1.8222209512,-2.1498309756
H,0,-2.6247540854,1.7865369512,-0.4143789756
H,0,-1.8264070854,3.6313209512,1.1527910244
H,0,-1.9554150854,2.0863929512,1.9933360244
H,0,0.2155259146,3.2907709512,2.5176120244
H,0,0.4721169146,1.7096389512,1.7870800244
H,0,0.6844489146,4.4283079512,0.3922210244
H,0,1.9844469146,3.2714929512,0.6423710244
H,0,-5.1188310854,-1.2672330488,0.6952330244
H,0,-3.9460550854,-0.0373860488,1.2209910244
H,0,-4.6549110854,0.0475529512,-0.4062489756
H,0,-3.4217060854,-3.1502960488,1.2075930244
H,0,-1.7959500854,-3.0659490488,0.4923920244
H,0,-2.2641800854,-1.9208070488,1.7676100244
H,0,-4.3760090854,-2.9037390488,-1.2456429756
H,0,-3.8600420854,-1.5094660488,-2.2195889756
H,0,-2.7061670854,-2.8076790488,-1.8462159756
H,0,-0.0335640854,-0.5036380488,0.4519980244
N,0,0.9388589146,-0.9308870488,0.5497890244
C,0,1.3803839146,-1.2498330488,1.9085810244
C,0,2.8895259146,-1.0688710488,2.0238310244
H,0,0.8410199146,-0.5910490488,2.5952960244
H,0,1.0924279146,-2.2820060488,2.1483600244
C,0,1.7172399146,-1.0184400488,-0.5128609756
N,0,2.9996389146,-1.4037900488,-0.4207559756
C,0,3.8445449146,-1.5972000488,-1.6016759756
C,0,3.5784519146,-1.8019590488,0.8764200244
H,0,4.8829999146,-1.4151810488,-1.3153129756
H,0,3.7626499146,-2.6205670488,-1.9890559756
H,0,3.5824809146,-0.8911750488,-2.3893279756
H,0,3.4871589146,-2.8907890488,0.9931310244
C,0,1.1201599146,-0.6628970488,-1.8448839756
H,0,3.1430959146,-0.0029600488,1.9838470244
H,0,3.2501899146,-1.4633860488,2.9789580244
H,0,4.6446719146,-1.5584370488,0.8506240244
H,0,1.4690149146,0.3280579512,-2.1634969756
H,0,1.3950319146,-1.4012800488,-2.6031259756
H,0,0.0337659146,-0.6326100488,-1.7543619756
```

## Ts 1 from gauche axial attack with DBU model B – 6-31+G** - PCM Dichloroethane

```
E(RB+HF-LYP) = -962.921673226

 Zero-point correction=                           0.447355 (Hartree/Particle)
 Thermal correction to Energy=                    0.471892
 Thermal correction to Enthalpy=                  0.472836
 Thermal correction to Gibbs Free Energy=         0.390338
 Sum of electronic and zero-point Energies=           -962.474319
 Sum of electronic and thermal Energies=              -962.449781
 Sum of electronic and thermal Enthalpies=            -962.448837
 Sum of electronic and thermal Free Energies=         -962.531335

                    E (Thermal)             CV                S
```

| | KCal/Mol | Cal/Mol-Kelvin | Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 296.117 | 90.569 | 173.633 |

C,0,-2.1503100427,2.0673620061,1.2675990366
C,0,-0.7943060427,2.6780060061,1.6398630366
C,0,-0.3307390427,3.6772430061,0.5728850366
C,0,-0.4676170427,3.1703720061,-0.8657049634
C,0,-1.3687670427,2.1098270061,-1.1230779634
C,0,-2.1138200427,1.4651850061,-0.1180039634
O,0,0.1822859573,3.7780140061,-1.7679929634
O,0,-1.3615060427,-0.2348869939,0.3793590366
O,0,-1.6992790427,-1.1728519939,-0.6789699634
C,0,-2.5286880427,-2.2460859939,-0.1673369634
C,0,-1.7716210427,-3.0323299939,0.9111100366
C,0,-3.8547660427,-1.6994209939,0.3765220366
C,0,-2.7631150427,-3.1107839939,-1.4120799634
H,0,-1.4780270427,1.7881650061,-2.1578329634
H,0,-3.0122320427,0.9416720061,-0.4305159634
H,0,-2.9242450427,2.8513750061,1.2757070366
H,0,-2.4568800427,1.3113090061,1.9971830366
H,0,-0.8485920427,3.1652260061,2.6213980366
H,0,-0.0567300427,1.8702060061,1.7262650366
H,0,-0.9273270427,4.6003780061,0.6401390366
H,0,0.7125159573,3.9760530061,0.7299870366
H,0,-4.4867100427,-2.5194749939,0.7356750366
H,0,-3.6705140427,-1.0143279939,1.2080870366
H,0,-4.4015380427,-1.1633069939,-0.4065629634
H,0,-2.3659410427,-3.8874369939,1.2520320366
H,0,-0.8226770427,-3.4069649939,0.5123420366
H,0,-1.5603410427,-2.3914259939,1.7710280366
H,0,-3.3897190427,-3.9725319939,-1.1590919634
H,0,-3.2685060427,-2.5336139939,-2.1932149634
H,0,-1.8132280427,-3.4797879939,-1.8122829634
H,0,0.2154559573,-0.4439929939,0.4043480366
N,0,1.2597499573,-0.6466009939,0.5178360366
C,0,1.7589509573,-0.8988339939,1.8701910366
C,0,3.2038169573,-0.4230369939,1.9788520366
H,0,1.1061879573,-0.3711939939,2.5706700366
H,0,1.6856769573,-1.9717409939,2.0933230366
C,0,2.0403019573,-0.6406789939,-0.5470149634
N,0,3.3602079573,-0.8600989939,-0.4558339634
C,0,4.2538949573,-0.9086449939,-1.6148669634
C,0,4.0259039573,-1.0383449939,0.8512080366
H,0,4.8402149573,0.0149050061,-1.6867899634
H,0,4.9400309573,-1.7519789939,-1.4919499634
H,0,3.6993509573,-1.0528229939,-2.5396029634
H,0,4.1889039573,-2.1114329939,1.0183550366
C,0,1.3955979573,-0.3845219939,-1.8803719634
H,0,3.2411589573,0.6708110061,1.9128920366
H,0,3.6318739573,-0.7141959939,2.9427420366
H,0,5.0079839573,-0.5586989939,0.7854640366
H,0,1.8631229573,0.4666440061,-2.3835459634
H,0,1.4945999573,-1.2627939939,-2.5268439634
H,0,0.3361139573,-0.1761929939,-1.7412219634

## Intermediate from gauche axial attack with DBU model – 6-31G* - Gas Phase

E(RB+HF-LYP) = -962.825878133

| | |
|---|---|
| Zero-point correction= | 0.454975 (Hartree/Particle) |
| Thermal correction to Energy= | 0.478533 |
| Thermal correction to Enthalpy= | 0.479477 |
| Thermal correction to Gibbs Free Energy= | 0.402756 |
| Sum of electronic and zero-point Energies= | -962.370904 |

```
Sum of electronic and thermal Energies=             -962.347345
Sum of electronic and thermal Enthalpies=           -962.346401
Sum of electronic and thermal Free Energies=        -962.423122

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  300.284             90.134            161.473

C,0,-0.8308554138,2.9623179239,0.7709786372
C,0,0.5873233122,2.7510073155,1.3125038486
C,0,1.6145347965,2.6735709827,0.1747708287
C,0,1.1893951663,1.8069470107,-1.0241561936
C,0,-0.1610139715,1.5358035357,-1.1963143136
C,0,-1.2184208877,1.8747887618,-0.2343303174
O,0,2.1261772563,1.4384161614,-1.8172293224
O,0,-1.6217409521,0.7233163925,0.69679726
O,0,-2.0272956845,-0.4021613873,-0.1465516074
C,0,-3.3655913643,-0.8239469221,0.2193025174
C,0,-3.3970995057,-1.2725447676,1.6854945622
C,0,-4.366764088,0.3065261693,-0.0400033424
C,0,-3.611254407,-2.0047339769,-0.7278286098
H,0,-0.4666786436,1.0320544943,-2.109768905
H,0,-2.1640634465,2.1293817769,-0.7285181645
H,0,-0.8888780816,3.9253299032,0.2462597901
H,0,-1.5603151907,2.9989384606,1.5906440576
H,0,0.8477472507,3.5548332397,2.0151620101
H,0,0.5982825791,1.818529534,1.8928257526
H,0,1.8161176227,3.6836535903,-0.2136151153
H,0,2.5829970001,2.3043745161,0.5400040427
H,0,-5.3863464928,-0.0284033899,0.1826433475
H,0,-4.1395991986,1.1688257544,0.5915424324
H,0,-4.3267595379,0.6211803668,-1.0878835655
H,0,-4.3959705864,-1.632110926,1.9575502077
H,0,-2.6840211017,-2.0878856708,1.8550024714
H,0,-3.1363747258,-0.4392527148,2.3427078379
H,0,-4.6114887539,-2.4180512106,-0.5606227418
H,0,-3.5398315101,-1.6836885634,-1.7720715351
H,0,-2.8803237457,-2.8032532529,-0.5574928471
H,0,-0.3761439825,-1.3403087759,-0.1560558193
N,0,0.5707120215,-1.5816230944,0.1556965367
C,0,0.7767088342,-1.5031411749,1.6045821209
C,0,2.1474191065,-0.907084641,1.9053803495
H,0,-0.023591271,-0.8742402041,2.0013541344
H,0,0.6808318881,-2.5069640113,2.0387233712
C,0,1.5382942895,-1.474131926,-0.7494176261
N,0,2.8263846236,-1.4975236355,-0.3964995545
C,0,3.8658682225,-1.1065408899,-1.3663952091
C,0,3.2044985073,-1.569591355,1.026202851
H,0,3.7338426047,-0.0431505268,-1.6072440774
H,0,4.8406634975,-1.2961398096,-0.9144137221
H,0,3.7930413376,-1.7077387807,-2.2753330172
H,0,3.3475922308,-2.6223117463,1.3062863905
C,0,1.1622777217,-1.3322260652,-2.1871145748
H,0,2.1334221002,0.1672615045,1.7002446648
H,0,2.3989311079,-1.0493647199,2.9610858659
H,0,4.1653068422,-1.0633023917,1.1398799697
H,0,1.4689338193,-0.3091081734,-2.4878082555
H,0,1.6787061092,-2.0781900776,-2.7995538233
H,0,0.0852468946,-1.4455603043,-2.3119774472
```

## Intermediate from gauche axial attack with DBU model – 6-31+G** - Gas Phase

E(RB+HF-LYP) = -962.901682774

```
Zero-point correction=                           0.451487 (Hartree/Particle)
Thermal correction to Energy=                    0.475532
Thermal correction to Enthalpy=                  0.476477
Thermal correction to Gibbs Free Energy=         0.397937
Sum of electronic and zero-point Energies=           -962.450196
Sum of electronic and thermal Energies=              -962.426150
Sum of electronic and thermal Enthalpies=            -962.425206
Sum of electronic and thermal Free Energies=         -962.503746

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  298.401             91.174            165.300

C,0,-0.8971873686,2.9994145981,0.7821362374
C,0,0.4988611654,2.8163147239,1.389789456
C,0,1.5765273862,2.7283237189,0.3000217396
C,0,1.2201760718,1.8200430581,-0.8888164041
C,0,-0.1217251658,1.5527245198,-1.1365614804
C,0,-1.2265110938,1.8967929534,-0.2276545199
O,0,2.2010853558,1.409647742,-1.608465838
O,0,-1.6555821253,0.749094562,0.7022984583
O,0,-2.0299160328,-0.3963428619,-0.1279405639
C,0,-3.3863020063,-0.8124959742,0.1927482045
C,0,-3.4756799056,-1.2295601477,1.6661134298
C,0,-4.3784438576,0.3095127958,-0.1312390786
C,0,-3.5932359827,-2.0145204706,-0.7371743286
H,0,-0.3765886158,1.0193230686,-2.0480689702
H,0,-2.1512435386,2.132326241,-0.7670109034
H,0,-0.9444919803,3.9545097734,0.242894662
H,0,-1.6625805782,3.0346333041,1.5674840241
H,0,0.7182424303,3.6402813122,2.0820844718
H,0,0.499251433,1.8972000028,1.9907689788
H,0,1.770560781,3.7277862915,-0.1168253065
H,0,2.5355828364,2.3939576896,0.7165165765
H,0,-5.4033507076,-0.0273602125,0.0586372944
H,0,-4.182594079,1.1856475129,0.4910906925
H,0,-4.2992885715,0.6016826081,-1.1827496832
H,0,-4.4839648279,-1.5876597099,1.9005644057
H,0,-2.768058213,-2.0374567419,1.8823334766
H,0,-3.2480029372,-0.3821354036,2.3168551759
H,0,-4.5961645043,-2.4281391446,-0.5918197481
H,0,-3.4918621301,-1.716317921,-1.7851599775
H,0,-2.8659037992,-2.8053833863,-0.5254413171
H,0,-0.3545914912,-1.3215092534,-0.1364675334
N,0,0.5941901347,-1.5863292061,0.1467658764
C,0,0.8607855888,-1.5311084398,1.5862883823
C,0,2.2065767971,-0.8567207394,1.8291085849
H,0,0.0436799414,-0.9665428494,2.0405493799
H,0,0.8507780862,-2.5488177396,1.9977741254
C,0,1.5409909415,-1.5140815793,-0.7844701181
N,0,2.8359963438,-1.5501954458,-0.4667559979
C,0,3.8658619931,-1.2744425368,-1.4820690787
C,0,3.2721894637,-1.4941375382,0.9431008482
H,0,3.8550187284,-0.2026276004,-1.7148952315
H,0,4.8320194197,-1.5787061102,-1.0766336108
H,0,3.6829540832,-1.8537395063,-2.3874963679
H,0,3.5154781478,-2.5106949095,1.2799358542
C,0,1.1216423645,-1.4023271059,-2.2154680613
H,0,2.1278131519,0.2069116712,1.5901048094
H,0,2.4966425671,-0.9518544089,2.8796804856
H,0,4.190257419,-0.9030044242,0.9757313964
H,0,1.4521919567,-0.4127527023,-2.5660743083
H,0,1.5774712981,-2.1920277292,-2.8197140698
```

H,0,0.0375824141,-1.4734437117,-2.2969772602

## Intermediate from gauche axial attack with DBU model B – 6-31G* - PCM Dichloroethane

E(RB+HF-LYP) = -962.845136389

| | |
|---|---|
| Zero-point correction= | 0.454455 (Hartree/Particle) |
| Thermal correction to Energy= | 0.478157 |
| Thermal correction to Enthalpy= | 0.479101 |
| Thermal correction to Gibbs Free Energy= | 0.401697 |
| Sum of electronic and zero-point Energies= | -962.390681 |
| Sum of electronic and thermal Energies= | -962.366980 |
| Sum of electronic and thermal Enthalpies= | -962.366035 |
| Sum of electronic and thermal Free Energies= | -962.443439 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 300.048 | 90.218 | 162.910 |

C,0,-0.8072824052,2.9422553416,0.796111605
C,0,0.6420295601,2.7169602498,1.2387144427
C,0,1.5986994685,2.7220733176,0.0394281517
C,0,1.1043285987,1.9358373721,-1.186513934
C,0,-0.2403033836,1.6167550951,-1.2708201744
C,0,-1.2500882715,1.8889903805,-0.2248225926
O,0,1.9900993871,1.6688409629,-2.0849446715
O,0,-1.5795659996,0.7104147959,0.6610297289
O,0,-2.0036358227,-0.395698243,-0.1987848595
C,0,-3.3324912464,-0.8406319815,0.1930569064
C,0,-3.3244459461,-1.3198190607,1.6489291732
C,0,-4.3514613317,0.2830355703,-0.019547992
C,0,-3.5847073835,-2.0040616522,-0.7732250834
H,0,-0.5868366512,1.1113831621,-2.1703646096
H,0,-2.2197373917,2.1684696527,-0.6583160296
H,0,-0.9035187904,3.9262219318,0.3168679135
H,0,-1.4860318594,2.9382574042,1.6589689992
H,0,0.938100913,3.4789914914,1.9728010027
H,0,0.6978773549,1.7491516519,1.7527561151
H,0,1.7849535027,3.7590931475,-0.2843548904
H,0,2.5819216348,2.3221186828,0.3227332743
H,0,-5.3602878679,-0.0713845633,0.2203115103
H,0,-4.1232299501,1.1352219306,0.6259231813
H,0,-4.3418863472,0.6190156653,-1.0617318821
H,0,-4.314282398,-1.6953679051,1.9318320273
H,0,-2.6015115682,-2.1322944256,1.7863568196
H,0,-3.0602928726,-0.4989708946,2.3207550275
H,0,-4.5778874365,-2.4283811464,-0.5920475315
H,0,-3.5391918467,-1.6620804003,-1.8124654253
H,0,-2.8438060369,-2.7991975322,-0.6339051525
H,0,-0.3809736728,-1.3573721603,-0.0415421185
N,0,0.5718354138,-1.5786708352,0.2640231302
C,0,0.7924178351,-1.6093095945,1.7134637478
C,0,2.1722304176,-1.0498495995,2.0453244632
H,0,0.0023744562,-1.0077447035,2.1695327126
H,0,0.6917493927,-2.6418003656,2.0713803646
C,0,1.5313442676,-1.4403440723,-0.6431251952
N,0,2.8199764506,-1.4569585553,-0.3007203725
C,0,3.8541390188,-1.1529816603,-1.3018587908
C,0,3.2178277824,-1.6474093609,1.1076073976
H,0,3.6620926631,-0.1620521354,-1.7281798815
H,0,4.8233466778,-1.1592328035,-0.8023631343
H,0,3.8728710993,-1.9070629516,-2.0949397306
H,0,3.3517384459,-2.7204457489,1.2997656172

C,0,1.143736792,-1.2857353723,-2.0795961474
H,0,2.1688166092,0.0394873172,1.9344721797
H,0,2.432032169,-1.2825703908,3.0827279768
H,0,4.1841755835,-1.158391732,1.2510627107
H,0,1.4450706571,-0.2790760544,-2.4188129399
H,0,1.6443060983,-2.0461098014,-2.6889782869
H,0,0.0643412266,-1.3915205523,-2.1905225731

## Intermediate from gauche axial attack with DBU model B – 6-31+G** - PCM Dichloroethane

E(RB+HF-LYP) = -962.926189324

Zero-point correction= 0.450342 (Hartree/Particle)
Thermal correction to Energy= 0.474668
Thermal correction to Enthalpy= 0.475612
Thermal correction to Gibbs Free Energy= 0.395179
Sum of electronic and zero-point Energies= -962.475847
Sum of electronic and thermal Energies= -962.451521
Sum of electronic and thermal Enthalpies= -962.450577
Sum of electronic and thermal Free Energies= -962.531010

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 297.859 | 91.300 | 169.286 |

C,0,-1.4383120854,2.7529750854,1.0564830305
C,0,0.0031489146,2.7307310854,1.5782460305
C,0,0.9992769146,3.0868500854,0.4666970305
C,0,0.7296519146,2.4036080854,-0.8794729695
C,0,-0.5148260854,1.8473510854,-1.1145229695
C,0,-1.6189440854,1.7926890854,-0.1237109695
O,0,1.7033769146,2.4267550854,-1.7366469695
O,0,-1.7680120854,0.4659400854,0.5787750305
O,0,-1.8948590854,-0.5815579146,-0.4355469695
C,0,-3.1335160854,-1.3279339146,-0.2342269695
C,0,-3.1327230854,-1.9928639146,1.1468050305
C,0,-4.3436620854,-0.4063399146,-0.4127499695
C,0,-3.0652900854,-2.3734039146,-1.3540079695
H,0,-0.6961830854,1.3960080854,-2.0882319695
H,0,-2.5946620854,1.9514810854,-0.6005749695
H,0,-1.6937810854,3.7615940854,0.7046170305
H,0,-2.1490560854,2.5025640854,1.8539570305
H,0,0.1106029146,3.4219310854,2.4245580305
H,0,0.2225409146,1.7260640854,1.9610530305
H,0,0.9898879146,4.1738230854,0.2887560305
H,0,2.0257009146,2.8416990854,0.7685870305
H,0,-5.2693840854,-0.9850049146,-0.3254669695
H,0,-4.3525270854,0.3722660854,0.3540790305
H,0,-4.3251900854,0.0685220854,-1.3986329695
H,0,-4.0351550854,-2.6006309146,1.2724790305
H,0,-2.2627260854,-2.6481009146,1.2613710305
H,0,-3.1114100854,-1.2393889146,1.9380810305
H,0,-3.9570190854,-3.0073519146,-1.3192339695
H,0,-3.0230000854,-1.8906519146,-2.3351789695
H,0,-2.1863950854,-3.0163379146,-1.2403179695
H,0,-0.1141680854,-1.1421539146,-0.1322169695
N,0,0.8279739146,-1.3481829146,0.2163610305
C,0,0.9638979146,-1.5822419146,1.6578240305
C,0,2.3068779146,-1.0434069146,2.1380010305
H,0,0.1295439146,-1.0760359146,2.1489170305
H,0,0.8794269146,-2.6574699146,1.8607830305
C,0,1.8465739146,-1.1451299146,-0.6100709695
N,0,3.1110139146,-1.2307949146,-0.1889309695

```
C,0,4.2340079146,-1.0963209146,-1.1263399695
C,0,3.4207269146,-1.5417439146,1.2223340305
H,0,4.1400399146,-0.1853319146,-1.7211869695
H,0,5.1541379146,-1.0311459146,-0.5458689695
H,0,4.3050149146,-1.9628519146,-1.7925159695
H,0,3.5643599146,-2.6254799146,1.3292790305
C,0,1.5446719146,-0.7940399146,-2.0324449695
H,0,2.2923439146,0.0520310854,2.1356250305
H,0,2.5013389146,-1.3743759146,3.1624540305
H,0,4.3659569146,-1.0509299146,1.4680170305
H,0,1.6952249146,0.2901410854,-2.1712119695
H,0,2.1858749146,-1.3467539146,-2.7226059695
H,0.5023369146,-1.0190579146,-2.2570829695
```

### 3-tert-Butylhydroperoxycyclohexanone - 6-31G* Gas Phase

```
E(RB+HF-LYP) = -617.499588925

 Zero-point correction=                           0.271937 (Hartree/Particle)
 Thermal correction to Energy=                    0.286175
 Thermal correction to Enthalpy=                  0.287119
 Thermal correction to Gibbs Free Energy=         0.230167
 Sum of electronic and zero-point Energies=           -617.227652
 Sum of electronic and thermal Energies=              -617.213414
 Sum of electronic and thermal Enthalpies=            -617.212470
 Sum of electronic and thermal Free Energies=         -617.269422

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 179.577             53.931            119.865

 C,0,-0.2082626084,1.5757296991,1.4395737677
 C,0,1.2443463653,1.3699834312,1.8874995072
 C,0,2.2322231147,2.1438568235,0.9911788145
 C,0,2.0099955034,1.866073017,-0.4895291744
 C,0,0.5571098109,1.9327871165,-0.9581940138
 C,0,-0.4048800636,1.1751473886,-0.0292816389
 O,0,2.9215595296,1.6420022912,-1.2609805007
 O,0,-0.0816237829,-0.2008999151,-0.2507348727
 O,0,-1.0584445429,-0.9868308029,0.5090255164
 C,0,-1.4657809575,-2.1127049523,-0.3061584993
 C,0,-2.173382945,-1.6289823369,-1.5768026125
 C,0,-0.2531198183,-2.9932097222,-0.6294119132
 C,0,-2.4406801424,-2.8355259134,0.6319113739
 H,0,0.2515079185,2.9891123968,-0.9623841121
 H,0,-1.4448413831,1.3460105387,-0.338005399
 H,0,-0.4989721138,2.6304171476,1.5514706131
 H,0,-0.8880969924,0.9870113858,2.0626954063
 H,0,1.3679261529,1.68496584,2.930116725
 H,0,1.4793639128,0.3005607201,1.8465676078
 H,0,2.0836849363,3.2249772353,1.1439418805
 H,0,3.2752669385,1.9188766222,1.2322557013
 H,0,-0.5674105165,-3.8914741127,-1.172753793
 H,0,0.4670732054,-2.4509373743,-1.2476414788
 H,0,0.2480034752,-3.3033063792,0.2934776163
 H,0,-2.538993587,-2.4816052872,-2.1598243459
 H,0,-3.0296853477,-0.995214379,-1.3212972002
 H,0,-1.4873850476,-1.0545924746,-2.2050386172
 H,0,-2.8291718932,-3.7343400653,0.1417817717
 H,0,-1.937084217,-3.1348225288,1.5564965538
 H,0,-3.2856337314,-2.1884813826,0.8891563198
 H,0,0.4971091045,1.5597422032,-1.9842100599
```

## 3-tert-Butylhydroperoxycyclohexanone - 6-31+G** Gas Phase

E(RB+HF-LYP) = -617.545699234

| | |
|---|---|
| Zero-point correction= | 0.269910 (Hartree/Particle) |
| Thermal correction to Energy= | 0.284254 |
| Thermal correction to Enthalpy= | 0.285198 |
| Thermal correction to Gibbs Free Energy= | 0.227904 |
| Sum of electronic and zero-point Energies= | -617.275789 |
| Sum of electronic and thermal Energies= | -617.261446 |
| Sum of electronic and thermal Enthalpies= | -617.260501 |
| Sum of electronic and thermal Free Energies= | -617.317795 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 178.372 | 54.380 | 120.585 |

C,0,-0.183259816,1.5627637924,1.4588934479
C,0,1.274542316,1.3508455338,1.8869814489
C,0,2.2543083871,2.1350640829,0.9904651262
C,0,2.0120019256,1.8932943201,-0.4909086363
C,0,0.5564261304,1.9411318851,-0.9456897961
C,0,-0.4022910763,1.1840064507,-0.0123581808
O,0,2.9208343431,1.7178601991,-1.2834493726
O,0,-0.1082389816,-0.1968822179,-0.2593256987
O,0,-1.0961811041,-0.978594171,0.493144476
C,0,-1.4771604985,-2.1281451846,-0.3098981683
C,0,-2.1676070272,-1.6739625189,-1.6009256695
C,0,-0.2489985817,-3.000268104,-0.5952362615
C,0,-2.4608490154,-2.8445968308,0.6239196662
H,0,0.2485483737,2.9963760415,-0.947247042
H,0,-1.4428595297,1.3742370842,-0.306901344
H,0,-0.4700879223,2.6164503988,1.5857004298
H,0,-0.8569081248,0.9696887394,2.0838692952
H,0,1.4094502202,1.6548372506,2.9308916035
H,0,1.510960701,0.2824631574,1.8335921018
H,0,2.114226065,3.214180477,1.1614825754
H,0,3.299165957,1.9016707817,1.2125120361
H,0,-0.5475914751,-3.9103241844,-1.1263952694
H,0,0.4755837826,-2.4636649153,-1.2122774737
H,0,0.2390498,-3.2889305849,0.3407611383
H,0,-2.5153911334,-2.5427488275,-2.1696713839
H,0,-3.0333855757,-1.04384271,-1.3726900516
H,0,-1.4769910146,-1.1082358449,-2.2310891822
H,0,-2.8299172936,-3.7538744645,0.1392853792
H,0,-1.9712720831,-3.125870451,1.5609033793
H,0,-3.3173300655,-2.2039242151,0.8550484498
H,0,0.4907587946,1.5716412247,-1.9721877411

## 3-tert-Butylhydroperoxycyclohexanone - 6-31G* – PCM Dichloroethane

E(RB+HF-LYP) = -617.507326327

| | |
|---|---|
| Zero-point correction= | 0.271406 (Hartree/Particle) |
| Thermal correction to Energy= | 0.285591 |
| Thermal correction to Enthalpy= | 0.286536 |
| Thermal correction to Gibbs Free Energy= | 0.229988 |
| Sum of electronic and zero-point Energies= | -617.235921 |
| Sum of electronic and thermal Energies= | -617.221735 |
| Sum of electronic and thermal Enthalpies= | -617.220791 |
| Sum of electronic and thermal Free Energies= | -617.277338 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 179.211 | 53.947 | 119.014 |

```
C,0,-0.239571168,1.5901028417,1.399131551
C,0,1.2052583881,1.4600889618,1.8970473775
C,0,2.1903522428,2.2263612325,0.9898803048
C,0,2.0190033888,1.8686273337,-0.475996206
C,0,0.584985224,1.8639284651,-0.9894679564
C,0,-0.3810100391,1.1186629849,-0.0537066734
O,0,2.9649575136,1.6344514327,-1.2113560377
O,0,-0.0072379256,-0.2583554863,-0.2071409459
O,0,-0.9764272294,-1.053330703,0.5495393715
C,0,-1.4742180058,-2.1148996739,-0.3062355902
C,0,-2.2117102976,-1.5351306357,-1.5177246933
C,0,-0.3200982002,-3.0306106781,-0.7291420668
C,0,-2.4419912121,-2.8427792312,0.6349526332
H,0,0.2481628079,2.9096777081,-1.0475477474
H,0,-1.4143232771,1.2477254384,-0.4019991922
H,0,-0.5705364949,2.6371440595,1.4536938029
H,0,-0.9162732735,1.0055547425,2.0304402591
H,0,1.2886726771,1.8347254,2.9236985571
H,0,1.4835419273,0.4000016412,1.9188982128
H,0,1.9931654937,3.3068740061,1.0803044017
H,0,3.2334398956,2.0556249362,1.2748041027
H,0,-0.6994033781,-3.8799430476,-1.3084013709
H,0,0.3995637846,-2.4865712248,-1.3471218076
H,0,0.2016685967,-3.4177512808,0.1526602032
H,0,-2.6440511715,-2.3415345578,-2.1205535487
H,0,-3.0239466372,-0.8749911489,-1.1941416111
H,0,-1.5271886422,-0.9651716986,-2.15218678
H,0,-2.8904034998,-3.6961613816,0.115567889
H,0,-1.9162087348,-3.2140374821,1.5207530597
H,0,-3.2459632025,-2.1741755454,0.9602802291
H,0,0.5637423361,1.4447778839,-1.9999198457
```

## 3-tert-Butylhydroperoxycyclohexanone - 6-31+G** – PCM Dichloroethane

```
E(RB+HF-LYP) = -617.507326327

 Zero-point correction=                           0.271406 (Hartree/Particle)
 Thermal correction to Energy=                    0.285591
 Thermal correction to Enthalpy=                  0.286536
 Thermal correction to Gibbs Free Energy=         0.229988
 Sum of electronic and zero-point Energies=           -617.235921
 Sum of electronic and thermal Energies=              -617.221735
 Sum of electronic and thermal Enthalpies=            -617.220791
 Sum of electronic and thermal Free Energies=         -617.277338

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 179.211             53.947            119.014

 C,0,-0.239571168,1.5901028417,1.399131551
 C,0,1.2052583881,1.4600889618,1.8970473775
 C,0,2.1903522428,2.2263612325,0.9898803048
 C,0,2.0190033888,1.8686273337,-0.475996206
 C,0,0.584985224,1.8639284651,-0.9894679564
 C,0,-0.3810100391,1.1186629849,-0.0537066734
 O,0,2.9649575136,1.6344514327,-1.2113560377
 O,0,-0.0072379256,-0.2583554863,-0.2071409459
 O,0,-0.9764272294,-1.053330703,0.5495393715
 C,0,-1.4742180058,-2.1148996739,-0.3062355902
 C,0,-2.2117102976,-1.5351306357,-1.5177246933
 C,0,-0.3200982002,-3.0306106781,-0.7291420668
 C,0,-2.4419912121,-2.8427792312,0.6349526332
 H,0,0.2481628079,2.9096777081,-1.0475477474
```

H,0,-1.4143232771,1.2477254384,-0.4019991922
H,0,-0.5705364949,2.6371440595,1.4536938029
H,0,-0.9162732735,1.0055547425,2.0304402591
H,0,1.2886726771,1.8347254,2.9236985571
H,0,1.4835419273,0.4000016412,1.9188982128
H,0,1.9931654937,3.3068740061,1.0803044017
H,0,3.2334398956,2.0556249362,1.2748041027
H,0,-0.6994033781,-3.8799430476,-1.3084013709
H,0,0.3995637846,-2.4865712248,-1.3471218076
H,0,0.2016685967,-3.4177512808,0.1526602032
H,0,-2.6440511715,-2.3415345578,-2.1205535487
H,0,-3.0239466372,-0.8749911489,-1.1941416111
H,0,-1.5271886422,-0.9651716986,-2.15218678
H,0,-2.8904034998,-3.6961613816,0.115567889
H,0,-1.9162087348,-3.2140374821,1.5207530597
H,0,-3.2459632025,-2.1741755454,0.9602802291
H,0,0.5637423361,1.4447778839,-1.9999198457

## 4-methylcyclohexanone - 6-31G* (23) – Gas Phase

E(RB+HF-LYP) = -347.980744335

| | |
|---|---|
| Zero-point correction= | 0.156050 (Hartree/Particle) |
| Thermal correction to Energy= | 0.163560 |
| Thermal correction to Enthalpy= | 0.164504 |
| Thermal correction to Gibbs Free Energy= | 0.124308 |
| Sum of electronic and zero-point Energies= | -347.824695 |
| Sum of electronic and thermal Energies= | -347.817185 |
| Sum of electronic and thermal Enthalpies= | -347.816241 |
| Sum of electronic and thermal Free Energies= | -347.856437 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 102.635 | 28.716 | 84.599 |

C,0,1.1433816996,-0.8306667622,-0.7395299599
C,0,1.2882869758,-0.3730695756,0.6606748757
O,0,2.0838156571,-1.3013899787,-1.3621464531
C,0,0.2694103419,0.1708578191,1.3477646884
H,0,2.2652852311,-0.5272332609,1.1119048551
C,0,-1.100121889,0.4365782326,0.7678127753
H,0,0.4194909833,0.4477260008,2.3919762562
C,0,-1.0408612492,0.464512258,-0.7697757737
H,0,-1.7504530945,-0.4023148929,1.0723949654
C,0,-1.710821402,1.7250663912,1.3422013502
C,0,-0.2567218083,-0.7273326899,-1.3348954015
H,0,-2.0564339386,0.4848613222,-1.183285482
H,0,-0.5538636378,1.3988800059,-1.0828214716
H,0,-0.780991019,-1.6655377967,-1.0944463058
H,0,-0.1657761198,-0.6857533773,-2.4246203906
H,0,-2.7153025075,1.8919097154,0.9375088309
H,0,-1.7919147028,1.6761344331,2.4342964847
H,0,-1.0958824648,2.5967736405,1.0887485554

## 4-methylcyclohexanone - 6-31+G** (23) – Gas Phase

E(RB+HF-LYP) = -348.009396968

| | |
|---|---|
| Zero-point correction= | 0.155072 (Hartree/Particle) |
| Thermal correction to Energy= | 0.162610 |
| Thermal correction to Enthalpy= | 0.163554 |
| Thermal correction to Gibbs Free Energy= | 0.123301 |
| Sum of electronic and zero-point Energies= | -347.854325 |

```
 Sum of electronic and thermal Energies=              -347.846787
 Sum of electronic and thermal Enthalpies=            -347.845843
 Sum of electronic and thermal Free Energies=         -347.886096

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  102.039             28.902             84.719

 C,0,1.1400632479,-0.834609228,-0.7372552061
 C,0,1.2911594603,-0.373285447,0.6602899178
 O,0,2.0792070737,-1.3180921218,-1.358813902
 C,0,0.2719902635,0.1777336548,1.3459295997
 H,0,2.2671883781,-0.5280908334,1.1122553579
 C,0,-1.0978757523,0.441575688,0.7670003285
 H,0,0.425607335,0.4564032362,2.3887482321
 C,0,-1.0401947168,0.4677761209,-0.7706086726
 H,0,-1.7432632548,-0.4002158007,1.0731331877
 C,0,-1.7136861602,1.7271041217,1.3438048909
 C,0,-0.2546078609,-0.7227756002,-1.337764273
 H,0,-2.0557775171,0.4838355995,-1.1829089688
 H,0,-0.556745821,1.4030510621,-1.0854956806
 H,0,-0.7780963185,-1.662396086,-1.1036036644
 H,0,-0.1581703281,-0.6758780155,-2.4262408166
 H,0,-2.719197168,1.8891124896,0.9412840489
 H,0,-1.7928768141,1.6764840215,2.4352796062
 H,0,-1.1034159708,2.6013154405,1.0896804022
```

## 4-methylcyclohexanone - 6-31G* (23) – PCM Dichloroethane

```
E(RB+HF-LYP) = -347.989066368

 Zero-point correction=                           0.155427 (Hartree/Particle)
 Thermal correction to Energy=                    0.162939
 Thermal correction to Enthalpy=                  0.163884
 Thermal correction to Gibbs Free Energy=         0.123705
 Sum of electronic and zero-point Energies=           -347.833640
 Sum of electronic and thermal Energies=              -347.826127
 Sum of electronic and thermal Enthalpies=            -347.825183
 Sum of electronic and thermal Free Energies=         -347.865362

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  102.246             28.759             84.564

 C,0,1.1398854117,-0.8285043728,-0.7352892412
 C,0,1.289515269,-0.3730669931,0.6585378103
 O,0,2.0826850675,-1.3097501121,-1.3608497736
 C,0,0.2680757345,0.1714205618,1.345989099
 H,0,2.265901811,-0.5290211857,1.1158492643
 C,0,-1.0993418167,0.4382375486,0.7665626595
 H,0,0.4204350109,0.4424944326,2.393157612
 C,0,-1.0415935739,0.4665666457,-0.7706573894
 H,0,-1.746950693,-0.4034857614,1.0743016819
 C,0,-1.7099098441,1.7265325427,1.3422086785
 C,0,-0.2540138842,-0.7235591551,-1.3348810355
 H,0,-2.0571734784,0.4785362316,-1.1839442562
 H,0,-0.5584274184,1.402375745,-1.086471517
 H,0,-0.77739545,-1.6632081758,-1.0946776718
 H,0,-0.1630018213,-0.6804912379,-2.4254297566
 H,0,-2.7163000088,1.8882141447,0.9400843376
 H,0,-1.785854733,1.6771244013,2.4345879432
 H,0,-1.0984175376,2.5997016355,1.0845170645
```

## 4-methylcyclohexanone - 6-31+G** (23) – PCM Dichloroethane

E(RB+HF-LYP) = -348.019873307

| | |
|---|---|
| Zero-point correction= | 0.154314 (Hartree/Particle) |
| Thermal correction to Energy= | 0.161848 |
| Thermal correction to Enthalpy= | 0.162792 |
| Thermal correction to Gibbs Free Energy= | 0.122590 |
| Sum of electronic and zero-point Energies= | -347.865559 |
| Sum of electronic and thermal Energies= | -347.858026 |
| Sum of electronic and thermal Enthalpies= | -347.857082 |
| Sum of electronic and thermal Free Energies= | -347.897283 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 101.561 | 28.938 | 84.612 |

C,0,1.1355633089,-0.8315170423,-0.7319730056
C,0,1.2925892645,-0.3732973896,0.6574686685
O,0,2.0783627762,-1.3276120924,-1.357595329
C,0,0.2700486698,0.1780331543,1.3436939218
H,0,2.2678053035,-0.5303196264,1.1172795649
C,0,-1.0968344984,0.4435218187,0.7655454292
H,0,0.4261362137,0.4491041661,2.3905554502
C,0,-1.0413645412,0.4698633754,-0.7715495147
H,0,-1.7391295179,-0.4017984342,1.0760354845
C,0,-1.7122915229,1.7289197945,1.3437791142
C,0,-0.2512176136,-0.7182942277,-1.3375695455
H,0,-2.0570794983,0.4751069331,-1.1833583439
H,0,-0.5632010584,1.4071112577,-1.0901643053
H,0,-0.7735767161,-1.6597333752,-1.1031582957
H,0,-0.1553935315,-0.6695167738,-2.4270346122
H,0,-2.7194985475,1.8855965478,0.943299295
H,0,-1.7865980577,1.6774411317,2.4355118978
H,0,-1.1053252025,2.6045280126,1.0854260895

## Ts 1 from axial attack on methylcyclohexanone, methyl equatorial (16) – 6-31G* – PCM Dichloroethane

E(RB+HF-LYP) = -1002.15387621

| | |
|---|---|
| Zero-point correction= | 0.478716 (Hartree/Particle) |
| Thermal correction to Energy= | 0.504396 |
| Thermal correction to Enthalpy= | 0.505340 |
| Thermal correction to Gibbs Free Energy= | 0.421847 |
| Sum of electronic and zero-point Energies= | -1001.675160 |
| Sum of electronic and thermal Energies= | -1001.649480 |
| Sum of electronic and thermal Enthalpies= | -1001.648536 |
| Sum of electronic and thermal Free Energies= | -1001.732030 |

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 316.513 | 95.620 | 175.727 |

C,0,-2.1842099755,1.8030370877,1.4032740865
C,0,-0.7615362145,2.1501865956,1.8608758885
C,0,-0.1553594699,3.2632593493,0.9987781492
C,0,-0.3309917374,3.062246211,-0.5130127913
C,0,-1.3891285029,2.2185676291,-0.9513965079
C,0,-2.1763742538,1.4583055314,-0.0754765988
O,0,0.4294410062,3.6952131632,-1.2866471516
O,0,-1.2781716969,-0.2141007365,-0.2373842277
O,0,-1.648955662,-1.4730667735,0.4409164152

```
C,0,-2.2492252546,-2.3940285563,-0.4913454575
C,0,-3.5413877603,-1.8065959191,-1.0731062113
C,0,-1.2580288957,-2.7477033056,-1.6083304951
C,0,-2.5532922273,-3.6185970038,0.3820316345
H,0,-1.5285527471,2.1187088519,-2.0269076972
H,0,-3.1141753892,1.0580572034,-0.4538100633
H,0,-2.7882461323,2.7269073883,1.4743064136
C,0,-2.8580180702,0.7553504505,2.2962718753
H,0,-0.7658122989,2.4457495229,2.9188785236
H,0,-0.1495876611,1.2432386003,1.7823035249
H,0,-0.6296506952,4.2259494978,1.2500143821
H,0,0.9152446888,3.3935547587,1.1999821332
H,0,-1.6981975143,-3.4644393055,-2.3115085998
H,0,-0.9806892252,-1.8440362332,-2.1574470689
H,0,-0.3486414951,-3.1930972796,-1.1883746828
H,0,-4.0437838575,-2.5364184376,-1.719080117
H,0,-4.2288254938,-1.5264267062,-0.2673232812
H,0,-3.3180454094,-0.9156393104,-1.6657912508
H,0,-3.0171066502,-4.4101444702,-0.2172083666
H,0,-1.6334427822,-4.0161451158,0.8249135307
H,0,-3.238993673,-3.3518053302,1.1935808993
H,0,0.3312650327,-0.2301546637,-0.3408662741
N,0,1.3874273794,-0.2156172458,-0.4907571658
C,0,1.8787314915,0.5207810912,-1.6583034982
C,0,3.2483674435,-0.0161891262,-2.0591887097
H,0,1.1432898858,0.3864844618,-2.4566331478
H,0,1.9098135314,1.5927640122,-1.4309122597
C,0,2.1719845794,-0.8079172431,0.3864257155
N,0,3.5083484869,-0.7555789889,0.2873589484
C,0,4.4200558142,-1.3430505103,1.2675509039
C,0,4.1617482846,-0.059740033,-0.8378452562
H,0,4.9251800339,-2.2197276654,0.8444510735
H,0,5.177966906,-0.5994838427,1.5366223634
H,0,3.8937047517,-1.6362801851,2.1736609416
H,0,4.439955353,0.952410975,-0.5138004497
C,0,1.510850119,-1.5555099544,1.5137777757
H,0,3.1470720316,-1.024815239,-2.4779215246
H,0,3.6971573101,0.6207756744,-2.8278037005
H,0,5.0857010742,-0.6019283274,-1.0646037759
H,0,1.9154377158,-2.5692411898,1.5954080781
H,0,1.6829516389,-1.0453046088,2.468626939
H,0,0.4350719548,-1.6205150793,1.3327573061
H,0,-3.8852657349,0.5585578326,1.9640005512
H,0,-2.3182769614,-0.1932272159,2.2714756749
H,0,-2.9065706507,1.1152660794,3.3318341389
```

## Ts 1 from axial attack on methylcyclohexanone, methyl equatorial (16) – 6-31+G** – PCM Dichloroethane

```
E(RB+HF-LYP) = -1002.23909138

 Zero-point correction=                           0.474943 (Hartree/Particle)
 Thermal correction to Energy=                    0.499864
 Thermal correction to Enthalpy=                  0.500808
 Thermal correction to Gibbs Free Energy=         0.420150
 Sum of electronic and zero-point Energies=          -1001.764149
 Sum of electronic and thermal Energies=             -1001.739227
 Sum of electronic and thermal Enthalpies=           -1001.738283
 Sum of electronic and thermal Free Energies=        -1001.818941

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 313.669             94.270            169.759
```

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.360268 | -1.104063 | 1.589092 |
| 2 | 6 | 0 | 1.295824 | -2.210130 | 1.569958 |
| 3 | 6 | 0 | 1.646551 | -3.311414 | 0.562653 |
| 4 | 6 | 0 | 2.086990 | -2.793627 | -0.807195 |
| 5 | 6 | 0 | 2.566463 | -1.460750 | -0.898980 |
| 6 | 6 | 0 | 2.587497 | -0.575093 | 0.185881 |
| 7 | 8 | 0 | 2.066930 | -3.599330 | -1.781663 |
| 8 | 8 | 0 | 1.041275 | 0.579934 | -0.198981 |
| 9 | 8 | 0 | 1.017177 | 1.922499 | 0.387783 |
| 10 | 6 | 0 | 1.278302 | 2.932887 | -0.616706 |
| 11 | 6 | 0 | 2.669565 | 2.739657 | -1.232896 |
| 12 | 6 | 0 | 0.191568 | 2.908673 | -1.700235 |
| 13 | 6 | 0 | 1.216588 | 4.236823 | 0.190166 |
| 14 | 1 | 0 | 2.904801 | -1.120317 | -1.876411 |
| 15 | 1 | 0 | 3.230794 | 0.297583 | 0.121748 |
| 16 | 1 | 0 | 3.322504 | -1.575584 | 1.864652 |
| 17 | 6 | 0 | 2.074497 | -0.026997 | 2.641156 |
| 18 | 1 | 0 | 1.182735 | -2.639598 | 2.573902 |
| 19 | 1 | 0 | 0.331821 | -1.757056 | 1.306106 |
| 20 | 1 | 0 | 2.478786 | -3.919672 | 0.950759 |
| 21 | 1 | 0 | 0.808611 | -4.002567 | 0.412482 |
| 22 | 1 | 0 | 0.365060 | 3.700340 | -2.437705 |
| 23 | 1 | 0 | 0.194078 | 1.945923 | -2.217604 |
| 24 | 1 | 0 | -0.797649 | 3.064959 | -1.256310 |
| 25 | 1 | 0 | 2.886122 | 3.542869 | -1.946219 |
| 26 | 1 | 0 | 3.439427 | 2.754782 | -0.453996 |
| 27 | 1 | 0 | 2.721930 | 1.784130 | -1.760566 |
| 28 | 1 | 0 | 1.399307 | 5.094741 | -0.465591 |
| 29 | 1 | 0 | 0.231913 | 4.360633 | 0.652741 |
| 30 | 1 | 0 | 1.973947 | 4.237668 | 0.980614 |
| 31 | 1 | 0 | -0.465018 | 0.114845 | -0.180365 |
| 32 | 7 | 0 | -1.475923 | -0.237681 | -0.282342 |
| 33 | 6 | 0 | -1.728840 | -1.221948 | -1.336758 |
| 34 | 6 | 0 | -3.157730 | -1.068499 | -1.846959 |
| 35 | 1 | 0 | -0.992949 | -1.054022 | -2.127307 |
| 36 | 1 | 0 | -1.565265 | -2.233174 | -0.942233 |
| 37 | 6 | 0 | -2.424064 | 0.223264 | 0.511397 |
| 38 | 7 | 0 | -3.697238 | -0.185533 | 0.404090 |
| 39 | 6 | 0 | -4.764021 | 0.244549 | 1.309894 |
| 40 | 6 | 0 | -4.124689 | -1.107996 | -0.668215 |
| 41 | 1 | 0 | -5.424677 | 0.964084 | 0.812367 |
| 42 | 1 | 0 | -5.353629 | -0.631707 | 1.597184 |
| 43 | 1 | 0 | -4.360895 | 0.694109 | 2.214571 |
| 44 | 1 | 0 | -4.200484 | -2.121020 | -0.250562 |
| 45 | 6 | 0 | -2.030561 | 1.232783 | 1.554897 |
| 46 | 1 | 0 | -3.260672 | -0.116974 | -2.382117 |
| 47 | 1 | 0 | -3.402691 | -1.873376 | -2.546358 |
| 48 | 1 | 0 | -5.128002 | -0.800961 | -0.981336 |
| 49 | 1 | 0 | -2.687358 | 2.106565 | 1.517991 |
| 50 | 1 | 0 | -2.103400 | 0.796514 | 2.557410 |
| 51 | 1 | 0 | -1.002754 | 1.556314 | 1.381202 |
| 52 | 1 | 0 | 2.846333 | 0.750189 | 2.632939 |
| 53 | 1 | 0 | 1.117301 | 0.464145 | 2.454259 |
| 54 | 1 | 0 | 2.053787 | -0.475404 | 3.641492 |

## Ts 1 from axial attack on methylcyclohexanone, methyl axial (17) – 6-31G* – PCM Dichloroethane

E(RB+HF-LYP) = -1002.15621553

Zero-point correction= 0.479138 (Hartree/Particle)
Thermal correction to Energy= 0.504756

Thermal correction to Enthalpy= 0.505700
Thermal correction to Gibbs Free Energy= 0.422256
Sum of electronic and zero-point Energies= -1001.677077
Sum of electronic and thermal Energies= -1001.651459
Sum of electronic and thermal Enthalpies= -1001.650515
Sum of electronic and thermal Free Energies= -1001.733960

| | | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|---|
| Total | | 316.739 | 95.380 | 175.624 |
| 1 | 6 | 0 | -2.361226 | 1.436353 | 0.939529 |
| 2 | 6 | 0 | -1.086820 | 1.930174 | 1.646304 |
| 3 | 6 | 0 | -0.462927 | 3.147352 | 0.951667 |
| 4 | 6 | 0 | -0.338003 | 3.002315 | -0.570790 |
| 5 | 6 | 0 | -1.233024 | 2.106370 | -1.224416 |
| 6 | 6 | 0 | -2.093028 | 1.246891 | -0.537007 |
| 7 | 8 | 0 | 0.496466 | 3.720929 | -1.171179 |
| 8 | 8 | 0 | -1.141702 | -0.456962 | -0.536525 |
| 9 | 8 | 0 | -1.593186 | -1.498781 | 0.384592 |
| 10 | 6 | 0 | -2.170807 | -2.603793 | -0.345884 |
| 11 | 6 | 0 | -3.382436 | -2.133547 | -1.159502 |
| 12 | 6 | 0 | -1.112913 | -3.243425 | -1.254603 |
| 13 | 6 | 0 | -2.599793 | -3.567678 | 0.767172 |
| 14 | 1 | 0 | -1.182949 | 2.068215 | -2.312175 |
| 15 | 1 | 0 | -2.915025 | 0.804510 | -1.094886 |
| 16 | 6 | 0 | -3.562193 | 2.382206 | 1.145245 |
| 17 | 1 | 0 | -2.628977 | 0.457117 | 1.352089 |
| 18 | 1 | 0 | -1.301595 | 2.158118 | 2.699423 |
| 19 | 1 | 0 | -0.361999 | 1.107954 | 1.639504 |
| 20 | 1 | 0 | -1.064537 | 4.049904 | 1.139802 |
| 21 | 1 | 0 | 0.534524 | 3.364383 | 1.353250 |
| 22 | 1 | 0 | -1.535897 | -4.080806 | -1.821693 |
| 23 | 1 | 0 | -0.732264 | -2.497601 | -1.957436 |
| 24 | 1 | 0 | -0.272912 | -3.621923 | -0.660375 |
| 25 | 1 | 0 | -3.864499 | -2.979876 | -1.662951 |
| 26 | 1 | 0 | -4.119938 | -1.656001 | -0.504561 |
| 27 | 1 | 0 | -3.069265 | -1.409854 | -1.916328 |
| 28 | 1 | 0 | -3.056406 | -4.467260 | 0.339635 |
| 29 | 1 | 0 | -1.736819 | -3.873645 | 1.368855 |
| 30 | 1 | 0 | -3.330118 | -3.090385 | 1.429572 |
| 31 | 1 | 0 | 0.443047 | -0.356593 | -0.373625 |
| 32 | 7 | 0 | 1.509566 | -0.253566 | -0.388117 |
| 33 | 6 | 0 | 2.079078 | 0.490562 | -1.514174 |
| 34 | 6 | 0 | 3.512127 | 0.030121 | -1.757601 |
| 35 | 1 | 0 | 1.439985 | 0.298789 | -2.380747 |
| 36 | 1 | 0 | 2.026270 | 1.566163 | -1.307279 |
| 37 | 6 | 0 | 2.230017 | -0.773841 | 0.583674 |
| 38 | 7 | 0 | 3.564358 | -0.640718 | 0.623997 |
| 39 | 6 | 0 | 4.400636 | -1.146035 | 1.711144 |
| 40 | 6 | 0 | 4.292032 | 0.067765 | -0.446632 |
| 41 | 1 | 0 | 5.015984 | -1.983839 | 1.361665 |
| 42 | 1 | 0 | 5.064073 | -0.344036 | 2.052570 |
| 43 | 1 | 0 | 3.798932 | -1.474630 | 2.555984 |
| 44 | 1 | 0 | 4.475607 | 1.101718 | -0.123980 |
| 45 | 6 | 0 | 1.498976 | -1.531652 | 1.660112 |
| 46 | 1 | 0 | 3.513534 | -0.990986 | -2.157448 |
| 47 | 1 | 0 | 4.001725 | 0.677409 | -2.491935 |
| 48 | 1 | 0 | 5.264583 | -0.422518 | -0.560195 |
| 49 | 1 | 0 | 1.922301 | -2.533800 | 1.783693 |
| 50 | 1 | 0 | 1.579741 | -1.010870 | 2.621074 |
| 51 | 1 | 0 | 0.442263 | -1.624258 | 1.396627 |
| 52 | 1 | 0 | -4.457093 | 1.998920 | 0.639777 |
| 53 | 1 | 0 | -3.797297 | 2.479493 | 2.212483 |

| | | | | | |
|---|---|---|---|---|---|
| 54 | 1 | 0 | -3.363239 | 3.383854 | 0.747921 |

## Ts 1 from axial attack on methylcyclohexanone, methyl axial (17) – 6-31+G** – PCM Dichloroethane

E(RB+HF-LYP) = -1002.24132823

Zero-point correction= 0.475325 (Hartree/Particle)
Thermal correction to Energy= 0.500304
Thermal correction to Enthalpy= 0.501248
Thermal correction to Gibbs Free Energy= 0.420099
Sum of electronic and zero-point Energies= -1001.766004
Sum of electronic and thermal Energies= -1001.741024
Sum of electronic and thermal Enthalpies= -1001.740080
Sum of electronic and thermal Free Energies= -1001.821229

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 313.946 | 94.190 | 170.793 |

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.441810 | -1.285610 | 0.973612 |
| 2 | 6 | 0 | 1.213521 | -1.940950 | 1.627120 |
| 3 | 6 | 0 | 0.744166 | -3.197826 | 0.880325 |
| 4 | 6 | 0 | 0.672964 | -3.034917 | -0.639156 |
| 5 | 6 | 0 | 1.448412 | -2.008884 | -1.242858 |
| 6 | 6 | 0 | 2.198025 | -1.084258 | -0.504550 |
| 7 | 8 | 0 | -0.020441 | -3.863840 | -1.294291 |
| 8 | 8 | 0 | 1.078327 | 0.522375 | -0.501199 |
| 9 | 8 | 0 | 1.459954 | 1.609664 | 0.398141 |
| 10 | 6 | 0 | 1.944349 | 2.758224 | -0.342074 |
| 11 | 6 | 0 | 3.183389 | 2.388213 | -1.166228 |
| 12 | 6 | 0 | 0.832629 | 3.317747 | -1.239619 |
| 13 | 6 | 0 | 2.305322 | 3.752629 | 0.769152 |
| 14 | 1 | 0 | 1.429861 | -1.944143 | -2.330028 |
| 15 | 1 | 0 | 2.979894 | -0.542081 | -1.029164 |
| 16 | 6 | 0 | 3.741888 | -2.087114 | 1.199084 |
| 17 | 1 | 0 | 2.583429 | -0.293837 | 1.417201 |
| 18 | 1 | 0 | 1.427897 | -2.181634 | 2.676696 |
| 19 | 1 | 0 | 0.401645 | -1.205281 | 1.628770 |
| 20 | 1 | 0 | 1.421851 | -4.042765 | 1.073388 |
| 21 | 1 | 0 | -0.242954 | -3.519300 | 1.233318 |
| 22 | 1 | 0 | 1.181795 | 4.205221 | -1.779170 |
| 23 | 1 | 0 | 0.523754 | 2.564468 | -1.968851 |
| 24 | 1 | 0 | -0.038940 | 3.601230 | -0.639618 |
| 25 | 1 | 0 | 3.588453 | 3.275385 | -1.665789 |
| 26 | 1 | 0 | 3.962758 | 1.970145 | -0.520365 |
| 27 | 1 | 0 | 2.925863 | 1.648994 | -1.928856 |
| 28 | 1 | 0 | 2.676718 | 4.686196 | 0.333497 |
| 29 | 1 | 0 | 1.428175 | 3.984397 | 1.382210 |
| 30 | 1 | 0 | 3.083871 | 3.340814 | 1.419540 |
| 31 | 1 | 0 | -0.488810 | 0.345766 | -0.357833 |
| 32 | 7 | 0 | -1.549257 | 0.187584 | -0.381989 |
| 33 | 6 | 0 | -2.082083 | -0.511701 | -1.553411 |
| 34 | 6 | 0 | -3.528615 | -0.090014 | -1.786668 |
| 35 | 1 | 0 | -1.444254 | -0.257682 | -2.404149 |
| 36 | 1 | 0 | -2.003660 | -1.594894 | -1.399698 |
| 37 | 6 | 0 | -2.301148 | 0.596373 | 0.621284 |
| 38 | 7 | 0 | -3.627379 | 0.393080 | 0.640318 |
| 39 | 6 | 0 | -4.492312 | 0.774300 | 1.757561 |
| 40 | 6 | 0 | -4.321466 | -0.251124 | -0.493755 |
| 41 | 1 | 0 | -5.117028 | 1.632017 | 1.482248 |
| 42 | 1 | 0 | -5.144732 | -0.070005 | 2.002136 |
| 43 | 1 | 0 | -3.912708 | 1.024463 | 2.643078 |

| | | | | | |
|---|---|---|---|---|---|
| 44 | 1 | 0 | -4.477975 | -1.311587 | -0.254175 |
| 45 | 6 | 0 | -1.616781 | 1.306129 | 1.757908 |
| 46 | 1 | 0 | -3.563288 | 0.955610 | -2.115388 |
| 47 | 1 | 0 | -3.982695 | -0.702456 | -2.571462 |
| 48 | 1 | 0 | -5.306247 | 0.219022 | -0.582551 |
| 49 | 1 | 0 | -2.089909 | 2.273484 | 1.951525 |
| 50 | 1 | 0 | -1.676062 | 0.711175 | 2.675726 |
| 51 | 1 | 0 | -0.566454 | 1.469759 | 1.509749 |
| 52 | 1 | 0 | 4.596538 | -1.590394 | 0.725381 |
| 53 | 1 | 0 | 3.955634 | -2.170416 | 2.271233 |
| 54 | 1 | 0 | 3.676884 | -3.099217 | 0.785521 |

## Ts 1 from equatorial attack on methylcyclohexanone, methyl equatorial (18) – 6-31+G** – PCM Dichloroethane

E(RB+HF-LYP) = -1002.23994315

Zero-point correction= 0.475475 (Hartree/Particle)
Thermal correction to Energy= 0.501407
Thermal correction to Enthalpy= 0.502351
Thermal correction to Gibbs Free Energy= 0.416572
Sum of electronic and zero-point Energies= -1001.764469
Sum of electronic and thermal Energies= -1001.738536
Sum of electronic and thermal Enthalpies= -1001.737592
Sum of electronic and thermal Free Energies= -1001.823372

| | E (Thermal) KCal/Mol | CV Cal/Mol-Kelvin | S Cal/Mol-Kelvin |
|---|---|---|---|
| Total | 314.637 | 96.134 | 180.538 |

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.188929 | 1.585649 | 0.982730 |
| 2 | 6 | 0 | -1.486108 | 2.886577 | 1.410193 |
| 3 | 6 | 0 | -0.100218 | 3.025198 | 0.771275 |
| 4 | 6 | 0 | -0.169016 | 2.948772 | -0.753173 |
| 5 | 6 | 0 | -1.194653 | 2.139470 | -1.306329 |
| 6 | 6 | 0 | -2.023691 | 1.327728 | -0.512489 |
| 7 | 8 | 0 | 0.670653 | 3.600689 | -1.437252 |
| 8 | 8 | 0 | -1.131034 | -0.368671 | -0.569546 |
| 9 | 8 | 0 | -1.604086 | -1.399560 | 0.356049 |
| 10 | 6 | 0 | -2.240383 | -2.490557 | -0.355776 |
| 11 | 6 | 0 | -3.460136 | -1.989393 | -1.138124 |
| 12 | 6 | 0 | -1.231526 | -3.175403 | -1.287476 |
| 13 | 6 | 0 | -2.666993 | -3.432794 | 0.777413 |
| 14 | 1 | 0 | -1.257250 | 2.072776 | -2.391571 |
| 15 | 1 | 0 | -2.894742 | 0.899556 | -0.999766 |
| 16 | 6 | 0 | -3.673984 | 1.598738 | 1.381162 |
| 17 | 1 | 0 | -1.715952 | 0.746973 | 1.507149 |
| 18 | 1 | 0 | -2.101884 | 3.745508 | 1.107274 |
| 19 | 1 | 0 | -1.412034 | 2.921332 | 2.505083 |
| 20 | 1 | 0 | 0.378155 | 3.971908 | 1.046058 |
| 21 | 1 | 0 | 0.560321 | 2.219591 | 1.126271 |
| 22 | 1 | 0 | -1.696158 | -4.024538 | -1.801019 |
| 23 | 1 | 0 | -0.871111 | -2.468482 | -2.039171 |
| 24 | 1 | 0 | -0.372942 | -3.546201 | -0.717077 |
| 25 | 1 | 0 | -3.973279 | -2.827473 | -1.622890 |
| 26 | 1 | 0 | -4.169458 | -1.492901 | -0.467853 |
| 27 | 1 | 0 | -3.151699 | -1.279658 | -1.909940 |
| 28 | 1 | 0 | -3.161749 | -4.318522 | 0.365050 |
| 29 | 1 | 0 | -1.797316 | -3.762490 | 1.355154 |
| 30 | 1 | 0 | -3.364526 | -2.930745 | 1.455516 |
| 31 | 1 | 0 | 0.461590 | -0.367068 | -0.389359 |
| 32 | 7 | 0 | 1.529204 | -0.338770 | -0.386319 |
| 33 | 6 | 0 | 2.177018 | 0.181607 | -1.593481 |

| | | | | | |
|---|---|---|---|---|---|
| 34 | 6 | 0 | 3.573041 | -0.417242 | -1.721714 |
| 35 | 1 | 0 | 1.544355 | -0.084351 | -2.444586 |
| 36 | 1 | 0 | 2.214177 | 1.276617 | -1.543335 |
| 37 | 6 | 0 | 2.196136 | -0.728474 | 0.683340 |
| 38 | 7 | 0 | 3.534690 | -0.668485 | 0.741911 |
| 39 | 6 | 0 | 4.312466 | -1.040498 | 1.924970 |
| 40 | 6 | 0 | 4.335587 | -0.218936 | -0.415881 |
| 41 | 1 | 0 | 4.815032 | -2.001967 | 1.767123 |
| 42 | 1 | 0 | 5.072245 | -0.272615 | 2.100371 |
| 43 | 1 | 0 | 3.684703 | -1.105965 | 2.810816 |
| 44 | 1 | 0 | 4.603610 | 0.836064 | -0.269275 |
| 45 | 6 | 0 | 1.399831 | -1.245902 | 1.850148 |
| 46 | 1 | 0 | 3.500529 | -1.487330 | -1.950158 |
| 47 | 1 | 0 | 4.119649 | 0.062647 | -2.539080 |
| 48 | 1 | 0 | 5.262443 | -0.801610 | -0.416731 |
| 49 | 1 | 0 | 1.762146 | -2.230778 | 2.159439 |
| 50 | 1 | 0 | 1.487334 | -0.569285 | 2.707235 |
| 51 | 1 | 0 | 0.348671 | -1.330358 | 1.569066 |
| 52 | 1 | 0 | -4.151276 | 0.639134 | 1.156982 |
| 53 | 1 | 0 | -3.785800 | 1.789340 | 2.455097 |
| 54 | 1 | 0 | -4.219950 | 2.384771 | 0.844235 |

## Table of Absolute and Relative Energies

| **gas phase, 6-31G*** | **HF** | **E + zpe** | **Erel vs sep SMs** | **G est (25)** | **Grel vs sep SMs** | | |
|---|---|---|---|---|---|---|---|
| tBuOOH | -308.80215 | -308.66261 | | -308.69353 | | | |
| dbu model (9) | -345.35894 | -345.17863 | | -345.21114 | | | |
| dbumod - HOOtBu complex | -654.1814 | -653.85938 | **-11.4** | -653.90684 | **-1.4** | | |
| cyclohexenone | -308.66613 | -308.53818 | | -308.56809 | | Erel vs complex | Grel vs complex |
| ts Ax A (10) | -962.82403 | -962.37139 | **5.0** | -962.42461 | **30.2** | **16.4** | **31.6** |
| ts Ax B | -962.82376 | -962.37101 | **5.3** | -962.42383 | **30.7** | **16.7** | **32.1** |
| ts Eq A | -962.82071 | -962.36814 | **7.1** | -962.42265 | **31.4** | **18.5** | **32.8** |
| ts Eq B (13) | -962.82235 | -962.36962 | **6.2** | -962.42296 | **31.2** | **17.5** | **32.6** |
| ts gauche | -962.8204 | -962.36736 | **7.6** | -962.42035 | **32.9** | **19.0** | **34.2** |
| int Ax A (11) | -962.8277 | -962.37341 | **3.8** | -962.42699 | **28.7** | **15.2** | **30.1** |
| int Ax B | 962.82696 | -962.37288 | **4.1** | -962.42668 | **28.9** | **15.5** | **30.3** |
| int Eq A | -962.82571 | -962.37184 | **4.8** | -962.42698 | **28.7** | **16.1** | **30.1** |
| int Eq B (14) | -962.82502 | -962.37115 | **5.2** | -962.42511 | **29.9** | **16.6** | **31.3** |
| int gauche | -962.82588 | -962.3709 | **5.3** | -962.42312 | **31.1** | **16.7** | **32.5** |
| ts2 Ax A (12) | -962.82277 | -962.3705 | **5.6** | -962.42427 | **30.4** | **17.0** | **31.8** |
| ts2 Eq A | -962.81723 | -962.36566 | **8.6** | -962.42086 | **32.6** | **20.0** | **33.9** |
| ts2 Eq B (15) | -962.81886 | -962.36646 | **8.1** | -962.4204 | **32.9** | **19.5** | **34.2** |
| t-BuOO-cyclohexanone | -617.49959 | -617.22765 | **-16.9** | -617.26942 | **-4.9** | **-5.5** | **-3.5** |

| **gas phase, 6-31+G**** | **HF** | **E + zpe** | **Erel vs sep SMs** | **G est (25)** | **Grel vs sep SMs** |
|---|---|---|---|---|---|
| tBuOOH | -308.83468 | -308.69606 | | -308.72706 | |
| dbu model (9) | -345.38627 | -345.20726 | | -345.23982 | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| dbumod - HOOtBu complex | -654.23711 | -653.91758 | **-8.9** | -653.96645 | **0.3** | | |
| cyclohexenone | -308.69105 | -308.56388 | | -308.59381 | | Erel vs complex | Grel vs complex |
| ts Ax A (10) | -962.90069 | -962.45176 | **9.7** | -962.50677 | **33.8** | **18.6** | **33.6** |
| ts Ax B | -962.90057 | -962.45155 | **9.8** | -962.50552 | **34.6** | **18.8** | **34.4** |
| ts Eq A | -962.89824 | -962.44934 | **11.2** | -962.50399 | **35.6** | **20.2** | **35.3** |
| ts Eq B (13) | -962.89927 | -962.44994 | **10.8** | -962.50398 | **35.6** | **19.8** | **35.3** |
| ts gauche | -962.89729 | -962.44708 | **12.6** | -962.50059 | **37.7** | **21.6** | **37.4** |
| int Ax A (11) | -962.90386 | -962.45286 | **9.0** | -962.50716 | **33.6** | **17.9** | **33.3** |
| int Ax B | -962.90489 | -962.4545 | **8.0** | -962.5095 | **32.1** | **16.9** | **31.9** |
| int Eq A | -962.90205 | -962.45171 | **9.7** | -962.50745 | **33.4** | **18.7** | **33.1** |
| int Eq B (14) | -962.9014 | -962.45082 | **10.3** | -962.50552 | **34.6** | **19.2** | **34.3** |
| int gauche | -962.90168 | -962.4502 | **10.7** | -962.50375 | **35.7** | **19.6** | **35.5** |
| ts2 Ax A (12) | -962.8998 | -962.45094 | **10.2** | -962.50511 | **34.9** | **19.2** | **34.6** |
| ts2 Eq A | -962.89531 | -962.44708 | **12.6** | -962.50286 | **36.3** | **21.6** | **36.0** |
| ts2 Eq B (15) | -962.89664 | -962.44814 | **12.0** | -962.50371 | **35.8** | **20.9** | **35.5** |
| t-BuOO-cyclohexanone | -617.5457 | -617.27579 | **-9.9** | -617.3178 | **1.9** | **-1.0** | **1.7** |

| **PCM, 6-31G*** | **HF** | **E + zpe** | **Erel vs sep SMs** | **G est (25)** | **Grel vs sep SMs** | | |
|---|---|---|---|---|---|---|---|
| tBuOOH | -308.81112 | -308.67223 | | -308.70304 | | | |
| dbu model (9) | -345.36498 | -345.18494 | | -345.21754 | | | |
| dbumod - HOOtBu complex | -654.18942 | -653.86848 | **-7.1** | -653.91477 | **3.6** | | |
| cyclohexenone | -308.6744 | -308.54703 | | -308.57692 | | Erel vs complex | Grel vs complex |
| ts Ax A (10) | -962.84328 | -962.39251 | **7.3** | -962.44772 | **31.2** | **14.4** | **27.6** |
| ts Ax B | -962.84183 | -962.39121 | **8.2** | -962.44764 | **31.3** | **15.2** | **27.6** |
| ts Eq A | -962.83877 | -962.38809 | **10.1** | -962.44467 | **33.2** | **17.2** | **29.5** |
| ts Eq B (13) | -962.84034 | -962.38903 | **9.5** | -962.44411 | **33.5** | **16.6** | **29.9** |
| ts gauche | -962.83898 | -962.38771 | **10.3** | -962.44316 | **34.1** | **17.4** | **30.5** |
| int Ax A (11) | -962.84922 | -962.39601 | **5.1** | -962.45148 | **28.9** | **12.2** | **25.2** |
| int Ax B | -962.84819 | -962.39561 | **5.4** | -962.4548 | **26.8** | **12.5** | **23.2** |
| int Eq A | -962.84996 | -962.39753 | **4.2** | -962.45404 | **27.3** | **11.3** | **23.6** |
| int Eq B (14) | -962.84474 | -962.3913 | **8.1** | -962.44666 | **31.9** | **15.2** | **28.3** |
| int gauche | -962.84514 | -962.39068 | **8.5** | -962.44344 | **33.9** | **15.6** | **30.3** |
| ts2 Ax A (12) | -962.84303 | -962.39177 | **7.8** | -962.44766 | **31.3** | **14.9** | **27.6** |
| ts2 Ax B | -962.84444 | -962.39286 | **7.1** | -962.44823 | **30.9** | **14.2** | **27.3** |
| ts2 Eq A | -962.83996 | -962.38853 | **9.8** | -962.44445 | **33.3** | **16.9** | **29.6** |
| ts2 Eq B (15) | -962.83939 | -962.38805 | **10.1** | -962.44333 | **34.0** | **17.2** | **30.3** |
| t-BuOO-cyclohexanone | -617.50733 | -617.23592 | **-10.5** | -617.27734 | **1.6** | **-3.4** | **-2.0** |

| **PCM, 6-31+G**** | **HF** | **E + zpe** | **Erel vs sep SMs** | **G est (25)** | **Grel vs sep SMs** | | |
|---|---|---|---|---|---|---|---|
| tBuOOH | -308.84483 | -308.70704 | | -308.73789 | | | |
| dbu model (9) | -345.3937 | -345.21495 | | -345.24762 | | | |
| dbumod - HOOtBu complex | -654.24751 | -653.92875 | **-4.2** | -653.9766 | **5.6** | | |
| cyclohexenone | -308.70146 | -308.575 | | -308.60491 | | Erel vs complex | Grel vs complex |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| ts Ax A (10) | -962.92499 | -962.47762 | **12.1** | -962.53128 | **37.1** | **16.4** | **31.5** |
| ts Ax B | -962.92456 | -962.47751 | **12.2** | -962.53163 | **36.9** | **16.5** | **31.3** |
| ts Eq A | -962.92137 | -962.47415 | **14.3** | -962.52882 | **38.7** | **18.6** | **33.1** |
| ts Eq B (13) | -962.92215 | -962.47451 | **14.1** | -962.53099 | **37.3** | **18.3** | **31.7** |
| ts gauche | -962.92167 | -962.47432 | **14.2** | -962.53134 | **37.1** | **18.5** | **31.5** |
| int Ax A (11) | -962.93282 | -962.48276 | **8.9** | -962.53856 | **32.5** | **13.2** | **26.9** |
| int Ax B | -962.93109 | -962.48135 | **9.8** | -962.53678 | **33.7** | **14.1** | **28.1** |
| int Eq A | -962.92901 | -962.47962 | **10.9** | -962.53544 | **34.5** | **15.1** | **28.9** |
| int Eq B (14) | -962.92682 | -962.47708 | **12.5** | -962.53189 | **36.7** | **16.7** | **31.1** |
| int gauche | -962.92619 | -962.47585 | **13.3** | -962.53101 | **37.3** | **17.5** | **31.7** |
| ts2 Ax A (12) | -962.92686 | -962.47886 | **11.4** | -962.53225 | **36.5** | **15.6** | **30.9** |
| ts2 Ax B | -962.92726 | -962.47937 | **11.0** | -962.53265 | **36.2** | **15.3** | **30.7** |
| ts2 Eq A | -962.92316 | -962.47502 | **13.8** | -962.52812 | **39.1** | **18.0** | **33.5** |
| ts2 Eq B (15) | -962.92227 | -962.47409 | **14.4** | -962.53348 | **35.7** | **18.6** | **30.1** |
| t-BuOO-cyclohexanone | -617.5556 | -617.28626 | **-2.7** | -617.32758 | **9.6** | **1.6** | **4.0** |

# Isotope Effect Results and Calculations

**$^{13}$C Results.** For the $^{13}$C spectra of cyclohexenone the integration of the C6 methylene ring carbon was set at 1000. The average integrations and standard deviations (in parentheses) for the other carbons are shown in Table 1 along with the number of spectra recorded for each sample (n).

**Table 1.** Average $^{13}$C integrations for cyclohexenone, with standard deviations (in parentheses).

| % conversion | C=O | -CH=CH- | -CH=CH- | O=C-CH$_2$ | -CH$_2$-CH$_2$ | =CH-CH$_2$ | n |
|---|---|---|---|---|---|---|---|
| Cyclohexenone | | | | | | | |
| Standard 1 400 MHz | 866.35 (8.0) | 972.25 (8.2) | 945.51 (5.2) | 1000 | 1005.63 (5.1) | 1009.24 (3.5) | 6 |
| Exp. 1A (89.1 ± 3%) | 861.90 (13.4) | 1044.11 (5.9) | 965.74 (8.8) | 1000 | 996.30 (5.2) | 1020.08 (2.7) | 6 |
| Exp. 2A (83.4 ± 3%) | 871.24 (9.9) | 1019.89 (4.9) | 960.82 (5.1) | 1000 | 1004.63 (2.9) | 1011.98 (5.5) | 6 |
| Standard 2 500 MHz | 765.22 (1.1) | 1031.66 (4.4) | 1022.46 (3.2) | 1000 | 990.08 (2.3) | 988.54 (2.9) | 5 |
| Exp. 1B (89.1 ± 3%) | 802.77 (3.1) | 1097.52 (2.9) | 1044.80 (3.1) | 1000 | 997.53 (4.1) | 1006.67 (2.1) | 5 |
| Exp. 2B (83.4 ± 3%) | 790.19 (4.1) | 1100.65 (5.7) | 1041.03 (7.2) | 1000 | 981.61 (5.1) | 992.29 (4.9) | 5 |

The values for $R/R_O$, calculated as the ratio of average integrations in Table 1 relative to standard, are shown in Table 2. The standard deviations were calculated from the formula:

$$\Delta R / R_0 = R / R_0 \times ((\Delta \text{IntSample} / \text{IntSample})^2 + (\Delta \text{IntStandard} / \text{IntStandard})^2)^{1/2} \quad (1)$$

**Table 2.** $R/R_O$ for $^{13}$C.

| | C=O | -CH=CH- | -CH=CH- | O=C-CH$_2$ | -CH$_2$-CH$_2$ | =CH-CH$_2$ |
|---|---|---|---|---|---|---|
| Cyclohexenone | | | | assumed | | |
| Exp. 1A $R/R_0$ | 0.995 | 1.074 | 1.021 | 1.000 | 0.991 | 1.011 |
| Standard dev | 0.008 | 0.007 | 0.005 | 0 | 0.003 | 0.002 |
| Exp. 1B $R/R_0$ | 1.006 | 1.049 | 1.016 | 1.000 | 0.999 | 1.003 |
| Standard dev | 0.008 | 0.007 | 0.004 | 0 | 0.003 | 0.003 |
| Exp. 2A $R/R_0$ | 1.049 | 1.064 | 1.021 | 1.000 | 1.008 | 1.018 |
| Standard dev | 0.003 | 0.004 | 0.002 | 0 | 0.002 | 0.002 |
| Exp. 2B $R/R_0$ | 1.032 | 1.067 | 1.018 | 1.000 | 0.991 | 1.004 |
| Standard dev | 0.004 | 0.006 | 0.005 | 0 | 0.003 | 0.003 |

The $^{13}C$ KIEs for cyclohexenone were then calculated from eq. 2, with the standard deviations calculated from eq. 3, 4, and 5. All of these equations are taken from: Singleton, D. A.; Thomas, A. A. *J. Am. Chem. Soc.* **1995**, 117, 9357, its Supporting Information, and references therein.

$$KIE_{calcd} = \frac{\ln(1 - F)}{\ln[(1 - F)R/R_0]} \quad (2)$$

$$\Delta KIE_F = \frac{\partial KIE}{\partial F}\Delta F = \frac{-\ln(R/R_0)}{(1-F)\ln^2[(1-F)R/R_0]}\Delta F \quad (3)$$

$$\Delta KIE_R = \frac{\partial KIE}{\partial (R/R_0)}\Delta(R/R_0) = \frac{-\ln(1-F)}{(R/R_0)\ln^2[(1-F)R/R_0]}\Delta(R/R_0) \quad (4)$$

$$\Delta KIE = KIE*((\Delta KIE_R/KIE)^2 + (\Delta KIE_F/KIE)^2)^{1/2} \quad (5)$$

**Table 3.** $^{13}C$ KIEs.

| | C=O | -CH=CH- | -CH=CH- | O=C-CH$_2$ | -CH$_2$-CH$_2$ | =CH-CH$_2$ |
|---|---|---|---|---|---|---|
| Cyclohexenone | | | | assumed | | |
| Exp. 1A (89.1 ± 3%) | 0.998 (8) | 1.033 (7) | 1.010 (5) | 1.000 | 0.996 (3) | 1.004 (2) |
| Exp. 1B (83.4 ± 3%) | 1.003 (8) | 1.027 (7) | 1.010 (4) | 1.000 | 0.999 (3) | 1.002 (3) |
| Exp. 2A (89.1 ± 3%)* | 1.022 (3) | 1.028 (4) | 1.010 (2) | 1.000 | 1.003 (2) | 1.008 (2) |
| Exp. 2B (83.4 ± 3%)* | 1.018 (4) | 1.037 (6) | 1.010 (5) | 1.000 | 0.995 (3) | 1.002 (3) |

* Due to time constraints, the recycle time was only 30 s. This did not allow for adequate relaxation of the carbonyl center, but was adequate for all other positions.