*Supporting Information*

# Organocatalytic Insertion into C-B Bond by *In Situ* Generated Carbene: Mechanism, Role of Catalyst, and Origin of Stereoselectivity

Qiao-Yu Zhang,[a] Yang Wang,[b] Shi-jun Li,[a] Yanyan Wang*[a] and Donghui Wei *[a]

[a] Green Catalysis Center, and College of Chemistry, Zhengzhou University, 100 Science Avenue, Zhengzhou, Henan 450001, China

[b] Department of Material and Chemical Engineering, Zhengzhou University of Light Industry, Zhengzhou 450002, China

E-mail: bzzhwangyan@163.com (Y. Wang); donghuiwei@zzu.edu.cn (D. Wei).

## Table of Contents

## Part 1: Computational methods

All theoretical calculations were performed in Gaussian 09[1] and Gaussian 16[2] with "g09default" keyword. All structures were completely optimized by using the B3LYP-D3[3] method and the 6-31G(d, p)[4] basis set (Lanl2DZ[5] basis set for I and Br) in dichloromethane solvent with the (SMD)[6] solvation model. Frequency calculations were carried out at the same level to confirm all the optimized structures as minima (no imaginary frequency) or transition states (only one imaginary frequency), and provided the free energy corrections.

All the energies discussed in the main text are the relative Gibbs free energies (GFE), which are obtained by the addition of the thermal Gibbs free energy corrections (GFEC) at the B3LYP-D3/[Lanl2DZ (I, Br);6-31G(d, p) (others)]/SMD (dichloromethane) (L1) level and the single-point energies (SPE) at a higher computational level of B3LYP-D3/SDD[7] (I, Br); 6-311++G(d, p) (others)/SMD(dichloromethane). To check whether the selected method is reliable, the additional calculations by employing different DFT methods and basis sets (including B3LYP-D3/def2-SVP[8]/SMD(dichloromethane) (L2), M06-2X[9]-D3/[Lanl2DZ(I);6-31G(d, p)(others)]/SMD(dichloromethane) (L3), M06-2X-D3/def2-SVP/SMD(dichloromethane) (L4), ωB97X-D[10]/[Lanl2DZ(I);6-31G(d, p)(others)]/SMD(dichloromethane) (L5) and ωB97X-D/def2-SVP/SMD(dichloromethane) (L6) have been used to reoptimize the key transition states (**TS3S** and **TS3R**) to certificate that the selected method and basis set are suitable and reliable, and the computed results can be found in the **Table S1**. As summarized in **Table S1**, there are tiny differences between the energies calculated by different methods and basis sets. Thus, the selected DFT method is suitable in this work.

**Table S1.** The relative energies (kcal/mol) of transition states **TS3R** and **TS3S** calculated at the six different computational levels

| Level | **TS3S** | **TS3R** |
|---|---|---|
| **L1** | 0.0 | 3.3 |

| | | |
|---|---|---|
| **L2** | 0.0 | 3.6 |
| **L3** | 0.0 | 3.9 |
| **L4** | 0.0 | 3.3 |
| **L5** | 0.0 | 3.3 |
| **L6** | 0.0 | 3.4 |

Bader's quantum theory of atoms in molecules (QTAIM)[11] analyses were plotted using and Multiwfn (version 3.3.8)[12]. Most of the significant three-dimensional structures were illustrated with CYLview[13]. In addition, the extent of enantioselectivity, in terms of enantiomeric excess (*ee*), was calculated by using the Boltzmann distribution of diastereomeric transition states with the following equations:

$$eq.\ 1: \frac{[S]}{[R]} = \frac{exp(-\Delta G^{\neq}_{[S]}/RT)}{exp(-\Delta G^{\neq}_{[R]}/RT)} = exp(\Delta\Delta G^{\neq}_{[R]-[S]}/RT)$$

$$eq.\ 2: ee = \frac{[S]-[R]}{[S]+[R]} \times 100\% = \frac{\frac{[S]}{[R]}-1}{\frac{[S]}{[R]}+1} \times 100\%$$

where $\Delta G^{\neq}$ is the Gibbs free energy barrier of the competing diastereomeric transition state and $\Delta\Delta G^{\neq}$ is the difference between the Gibbs free energy barriers of two diastereomeric transition states.

# Part 2: Additionally computational results

## 2.1 The alcoholysis of Pre-R1

As shown in **Fig. S1**, the alcoholysis of **Pre-R1** initiates two possible pathways (*i.e.,* **Path a** and **Path b**). In **Path a**, the alcoholysis of **Pre-R1** with EtOH to form **R1** and other boronates (*i.e.,* **R1′** and **M7**) is exergonic by only 0.4 kcal/mol. Whereas, the alcoholysis of **Pre-R1** with EtOH to form **R1′** is exergonic by 1.2 kcal/mol in **Path b**. The tiny energy difference (0.8 kcal/mol) means that we cannot confirm which pathway is the energetically dominant one. That is say, both **R1** (transformation from **Path a**) and **R1′** (transformation from **Path b** or **Path a**) are the possible products from the alcoholysis of **Pre-R1**. Therefore, in order to solve the issue, we calculated the complete Gibbs free energy profiles with the **R1** and **R1′** as the starting point in **Fig. 1** (in the main text) and **Fig. S2**, respectively. Then, as shown in **Fig. S2**, the intermediate **M1′** is formed after that the boron atom of the intermediate **R1′** electrophilically attacks the oxygen atom of **Cat**, accompanied by a proton transfer process with the assistance of EtOH via a concerted transition state **TS1′** with an energy barrier of 22.3 kcal/mol, which is higher than that via **TS1** in **Fig. 1** (19.3 kcal/mol). Similarly, the boron atom of **M1′** electrophilically attacks the other hydroxyl oxygen atom of the **Cat** via the other concerted transition state **TS2′** to form vinyl-boronate ester **M2′** with an energy barrier of 24.4 kcal/mol, which is also higher than that via **TS2** in **Fig. 1** (23.0 kcal/mol). Therefore, it could be concluded that **R1** will lead to the formation of **M03** rather than **R1′**.

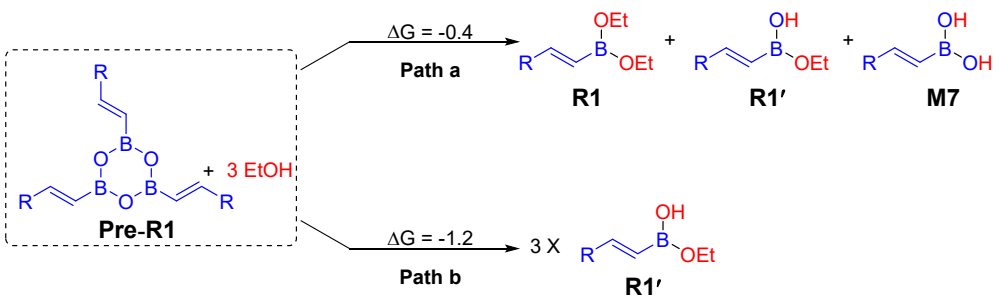



**Fig. S1** The possible pathways for the alcoholysis of **Pre-R1** (Energies are given in

kcal/mol)

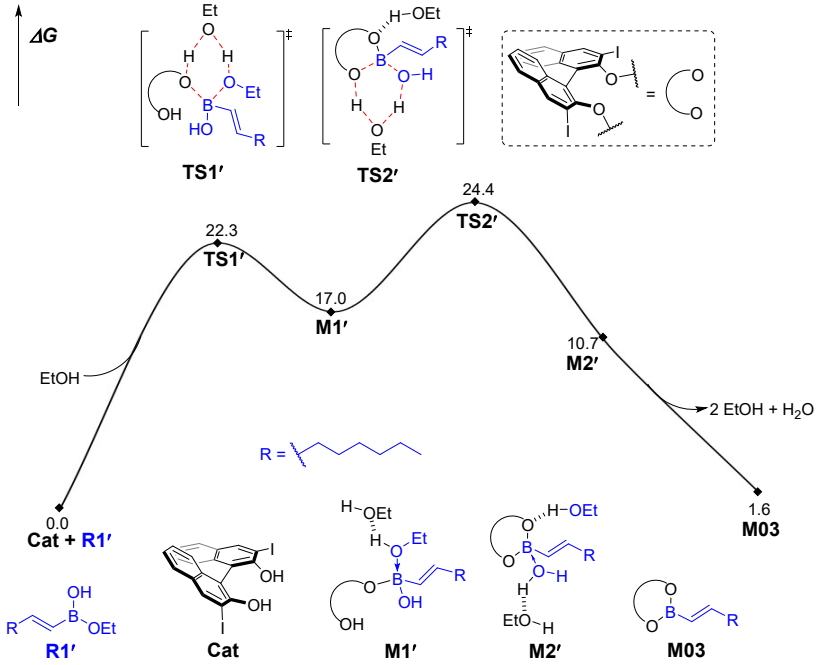



**Fig. S2** The relative Gibbs free energy profile for the other possible pathway of the formation of **M03**.

## 2.2 Different configurations of TS3R and TS3S

To ensure the selected configuration of the stereochemical transition state **TS3R** and **TS3S** with the lowest energy, we have searched multiple possible conformations. By rotating the dihedral angle Φ (C1–B–C2–H) in stereo-controlling transition states **TS3R** and **TS3S**, we have totally constructed 2*3=6 conformations as the initial structures, which have subsequently been optimized at the B3LYP-D3/[Lanl2DZ (I);6-31G(d, p) (others)]/SMD (dichloromethane) level. As depicted in **Fig. S3**, we have located six diastereoselective transition states, and selected the two conformations with the lowest energies (denoted as **TS3R** and **TS3S**) associated with the dihedral angles Φ (C1–B–C2–H) of 75.0°/-79.0°.

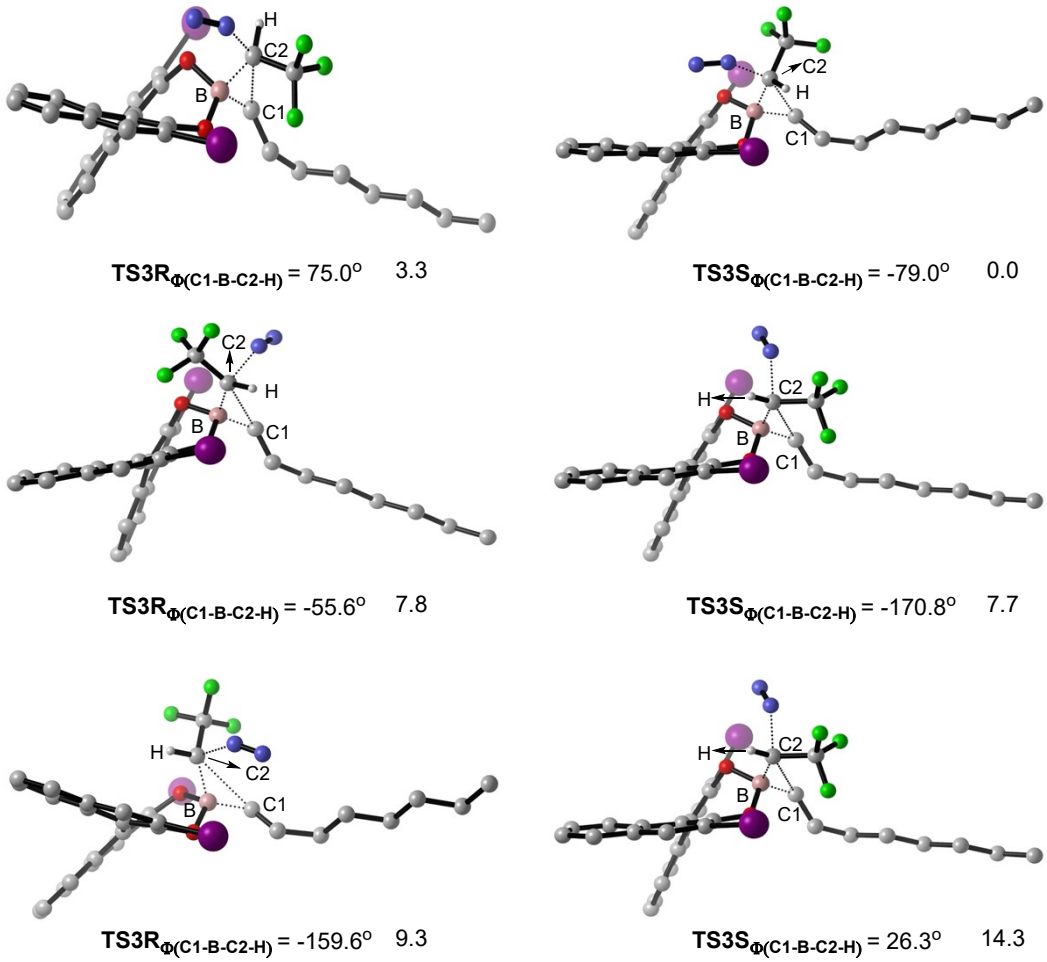
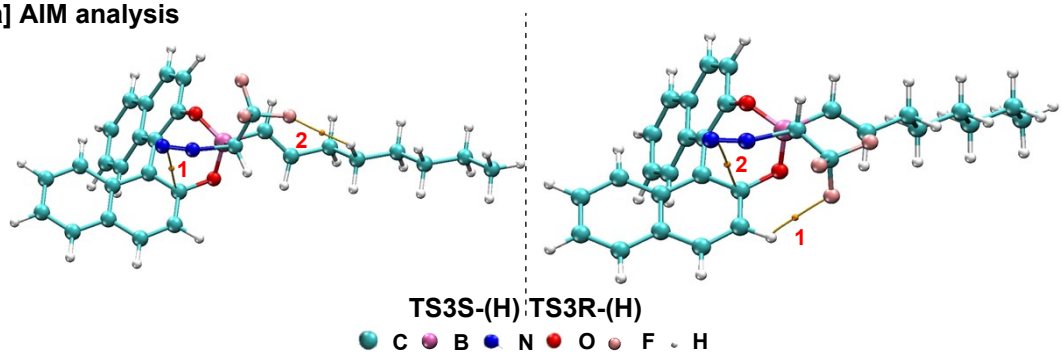



**Fig. S3.** Different configurations of the transition states **TS3R**s and **TS3S**s with different dihedral Φ angles optimized at the B3LYP-D3/[Lanl2DZ (I);6-31G(d, p) (others)]/SMD (dichloromethane) level of theory (energy in kcal/mol)

## 2.3 AIM analyses of the transition states TS3S(H) and TS3R(H)

**[a] AIM analysis**




**[b]**

| **TS3S** (0.0 kcal/mol) | | | **TS3R** (0.7 kcal/mol) | | |
|---|---|---|---|---|---|
| Type | $\nabla^2\rho$ ($10^{-1}$ a.u.) | Distance | Type | $\nabla^2\rho$ ($10^{-1}$ a.u.) | Distance |
| (1) π...π | 0.245 | 3.13 Å | (1) C-H...F | 0.357 | 2.45 Å |
| (2) C-H...F | 0.158 | 2.82 Å | (2) π...π | 0.228 | 3.19 Å |

**Fig. S4** AIM analyses of the transition states **TS3S(H)** and **TS3R(H)**

### 2.4 The bond orders of C1-N1, C1-B, C2-B and C1-C2

As summarized in **Table S2**, the bond orders of C1-N1 and C2-B bonds are reduced from 1.16 and 1.02 to 0.01 and 0.12, respectively, indicating that the breaking of C1-N1 and C2-B bonds. While the bond orders of C1-B and C1-C2 are increased from 0.22 and 0.00 to 0.88 and 0.92, which demonstrates that the C1-B and C1-C2 bonds have been formed finally.

**Table.S2** Bond orders of C1-N1, C1-B, C2-B, and C1-C2 for the key structures along the IRC results of **TS3S**

| SP | C1-N1 | C1-B | C2-B | C1-C2 |
|---|---|---|---|---|
| **IRC-R-40** | 1.16 | 0.22 | 1.02 | 0.00 |
| **IRC-R-6** | 0.88 | 0.51 | 0.92 | 0.04 |
| **IRC-1** | 0.46 | 0.65 | 0.82 | 0.18 |
| **IRC-F-6** | 0.17 | 0.76 | 0.67 | 0.18 |
| **IRC-F-12** | 0.06 | 0.82 | 0.50 | 0.63 |
| **IRC-F-18** | 0.02 | 0.87 | 0.32 | 0.79 |
| **IRC-F-24** | 0.01 | 0.88 | 0.17 | 0.89 |
| **IRC-F-30** | 0.01 | 0.88 | 0.12 | 0.92 |

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## Part 3: Energy values and Cartesian coordinates of all the optimized structures

### 3.1 Absolute SPE and GFE of the optimized structures by using B3LYP-D3 method

| SP | SPE (a.u.) | GFEC (a.u.) | GFE (a.u.) |
|---|---|---|---|
| **Pre-R1** | -1242.354607 | 0.593265 | -1241.761342 |
| **R1** | -647.807162 | 0.310647 | -647.496515 |
| **Cat** | -942.650877 | 0.211805 | -942.439072 |
| **Cat-Br** | -1283.885345 | 0.396843 | -1283.488502 |
| **Cat-H** | -1258.767439 | 0.423063 | -1258.344376 |
| **Cat+R1** | -1590.479375 | 0.544893 | -1589.934482 |
| **EtOH** | -155.05289 | 0.054451 | -154.998439 |
| **$H_2O$** | -76.425144 | 0.002837 | -76.422307 |
| **$N_2$** | -109.515631 | -0.012836 | -109.528467 |
| **R2** | -485.772834 | 0.006137 | -485.766696 |
| **TS1** | -1745.535972 | 0.621118 | -1744.914854 |
| **M1** | -1745.548419 | 0.622357 | -1744.926062 |
| **TS2** | -1745.53112 | 0.62066 | -1744.91046 |
| **M2** | -1745.555164 | 0.626999 | -1744.928165 |
| **M03** | -1280.321708 | 0.394028 | -1279.92768 |
| **Pre-TS3S** | -1766.11425 | 0.421785 | -1765.692465 |
| **TS3R** | -1766.083318 | 0.424426 | -1765.658892 |
| **TS3S** | -1766.087898 | 0.423809 | -1765.66409 |
| **TS3R-Br** | -1769.647135 | 0.425886 | -1769.221249 |
| **TS3S-Br** | -1769.650187 | 0.424831 | -1769.225356 |
| **TS3R-H** | -1744.527719 | 0.452834 | -1744.074885 |
| **TS3S-H** | -1744.527115 | 0.451481 | -1744.075635 |

| | | | |
|---|---|---|---|
| **M3R** | -1656.677219 | 0.421688 | -1656.255531 |
| **M3S** | -1656.676266 | 0.418655 | -1656.257611 |
| **M04R** | -1966.841958 | 0.574899 | -1966.267059 |
| **M04S** | -1966.844734 | 0.576881 | -1966.267853 |
| **TS4R** | -1966.826835 | 0.574747 | -1966.252088 |
| **TS4S** | -1966.829195 | 0.575923 | -1966.253272 |
| **M4R** | -1966.829172 | 0.575401 | -1966.253771 |
| **M4S** | -1966.829462 | 0.576632 | -1966.25283 |
| **TS5R** | -2121.905743 | 0.654709 | -2121.251034 |
| **TS5S** | -2121.894601 | 0.650723 | -2121.243878 |
| **PR/S** | -1024.166341 | 0.337427 | -1023.828913 |
| **Pre-TS6** | -1728.143334 | 0.622026 | -1727.521308 |
| **TS6** | -1728.106571 | 0.62267 | -1727.483901 |
| **M6** | -1618.709281 | 0.620775 | -1618.088506 |
| **Pre-TS7** | -1133.592227 | 0.338951 | -1133.253276 |
| **TS7** | -1133.548032 | 0.34104 | -1133.206992 |
| **M7** | -490.551455 | 0.205992 | -490.345463 |
| **R1′** | -569.179123 | 0.257732 | -568.921391 |
| **Cat+R1′** | -1511.860384 | 0.494522 | -1511.365861 |
| **TS1′** | -1666.904247 | 0.564564 | -1666.339683 |
| **M1′** | -1666.916862 | 0.56888 | -1666.347981 |
| **TS2′** | -1666.908824 | 0.568613 | -1666.340211 |
| **M2′** | -1666.932411 | 0.572343 | -1666.360068 |

### 3.2 Absolute SPE and GFE of the optimized structures by using other DFT methods

**Table S3.** Absolute SPE and GFE of the optimized structures obtained at the M06-2X-D3/[Lanl2DZ(I);6-31G(d, p)(others)]/SMD(dichloromethane) level.

| | SPE(a.u.) | GFEC(a.u.) | CFE(a.u.) | ΔΔG≠ |
|---|---|---|---|---|
| **TS3R** | -1765.235791 | 0.430187 | -1764.805604 | 3.9 |
| **TS3S** | -1765.240806 | 0.428966 | -1764.81184 | 0.0 |

**Table S4.** Absolute SPE and GFE of the optimized structures obtained at the M06-2X-D3/def2-SVP/SMD(dichloromethane) level.

| | SPE(a.u.) | GFEC(a.u.) | CFE(a.u.) | ΔΔG≠ |
|---|---|---|---|---|
| **TS3R** | -2336.524622 | 0.428577 | -2336.096045 | 3.3 |
| **TS3S** | -2336.528803 | 0.427455 | -2336.101348 | 0.0 |

**Table S5.** Absolute SPE and GFE of the optimized structures obtained at the ωB97X-D/[Lanl2DZ(I);6-31G(d, p)(others)]/SMD(dichloromethane) level.

| | SPE(a.u.) | GFEC(a.u.) | CFE(a.u.) | ΔΔG≠ |
|---|---|---|---|---|
| **TS3R** | -1765.489903 | 0.430957 | -1765.058947 | 3.3 |
| **TS3S** | -1765.494845 | 0.430615 | -1765.06423 | 0.0 |

**Table S6.** Absolute SPE and GFE of the optimized structures obtained at the ωB97X-D/def2-SVP/SMD(dichloromethane) level.

| | SPE(a.u.) | GFEC(a.u.) | CFE(a.u.) | ΔΔG≠ |
|---|---|---|---|---|
| **TS3R** | -2336.986441 | 0.429321 | -2336.55712 | 3.3 |
| **TS3S** | -2336.990893 | 0.42839 | -2336.562503 | 0.0 |

**Table S7.** Absolute SPE and GFE of the optimized structures obtained at the B3LYP-D3/def2-SVP/SMD(dichloromethane) level.

| | SPE(a.u.) | GFEC(a.u.) | CFE(a.u.) | ΔΔG≠ |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| **TS3R** | -2337.631487 | 0.423716 | -2337.207772 | 3.6 |
| **TS3S** | -2337.635789 | 0.422296 | -2337.213492 | 0.0 |

**Table S8** Absolute SPE and GFE of the different conformers of **TS3R**s and **TS3S**s

| | **SPE(a.u.)** | **GFEC(a.u.)** | **CFE(a.u.)** |
|---|---|---|---|
| **TS3R**$_{\Phi(C1\text{-}B\text{-}C2\text{-}H)\ =160°}$ | -1766.071071 | 0.421834 | -1765.649237 |
| **TS3R**$_{\Phi(C1\text{-}B\text{-}C2\text{-}H)\ =75°}$ | -1766.083318 | 0.424426 | -1765.658892 |
| **TS3R**$_{\Phi(C1\text{-}B\text{-}C2\text{-}H)\ =-56°}$ | -1766.073452 | 0.421867 | -1765.651585 |
| **TS3S**$_{\Phi(C1\text{-}B\text{-}C2\text{-}H)\ =26°}$ | -1766.087898 | 0.423809 | -1765.66409 |
| **TS3S**$_{\Phi(C1\text{-}B\text{-}C2\text{-}H)\ =-160°}$ | -1766.061309 | 0.420021 | -1765.641288 |
| **TS3S**$_{\Phi(C1\text{-}B\text{-}C2\text{-}H)\ =-170°}$ | -1766.074724 | 0.422831 | -1765.651893 |

### 3.3 Cartesian coordinates and vibrational frequencies of all the stationary points

**Pre-R1**

Cartesian coordinates

Zero-point correction= 0.669876

Thermal correction to Energy= 0.706700

Thermal correction to Enthalpy= 0.707644

Thermal correction to Gibbs Free Energy= 0.593265

Sum of electronic and zero-point Energies= -1241.684730

Sum of electronic and thermal Energies= -1241.647907

Sum of electronic and thermal Enthalpies= -1241.646963

Sum of electronic and thermal Free Energies= -1241.761342

Cartesian coordinates

| | | | |
|---|---|---|---|
| B | -1.096371 | -2.325779 | -0.120135 |
| B | -2.766728 | -1.122174 | 1.136757 |
| B | -0.637455 | -0.091824 | 0.665480 |
| O | -2.347189 | -2.262939 | 0.468351 |
| O | -0.251747 | -1.230102 | -0.020341 |
| O | -1.902407 | -0.045620 | 1.232408 |
| C | 0.333368 | 1.102010 | 0.801328 |
| C | 0.014595 | 2.227073 | 1.466509 |
| H | 1.322963 | 1.032150 | 0.345542 |
| H | -0.973214 | 2.294413 | 1.927895 |
| C | 0.900158 | 3.419569 | 1.670698 |
| C | 1.164136 | 3.704294 | 3.162960 |
| H | 0.413462 | 4.303737 | 1.231752 |
| H | 1.851505 | 3.280932 | 1.142205 |
| C | 2.011511 | 4.961227 | 3.390280 |
| H | 0.203584 | 3.810779 | 3.685740 |

| | | | |
|---|---|---|---|
| H | 1.664692 | 2.835422 | 3.610717 |
| H | 2.970206 | 4.853871 | 2.863093 |
| H | 1.506775 | 5.825239 | 2.934721 |
| C | 2.276599 | 5.251637 | 4.872145 |
| C | 3.118052 | 6.512315 | 5.105566 |
| H | 2.783127 | 4.388330 | 5.327337 |
| H | 1.316921 | 5.354519 | 5.399106 |
| C | 3.371410 | 6.798198 | 6.588592 |
| H | 4.078758 | 6.408007 | 4.582390 |
| H | 2.612733 | 7.373636 | 4.647063 |
| H | 3.975112 | 7.702244 | 6.726727 |
| H | 2.428804 | 6.941672 | 7.130577 |
| H | 3.902938 | 5.966587 | 7.067002 |
| C | -4.176771 | -1.048420 | 1.763489 |
| C | -5.052851 | -2.067667 | 1.701663 |
| H | -4.480905 | -0.133090 | 2.275244 |
| H | -4.745253 | -2.985285 | 1.195260 |
| C | -6.432257 | -2.090553 | 2.288602 |
| C | -6.591151 | -3.179353 | 3.369106 |
| H | -7.157050 | -2.291770 | 1.485312 |
| H | -6.682503 | -1.108891 | 2.709392 |
| C | -8.018216 | -3.266050 | 3.922406 |
| H | -6.301632 | -4.152322 | 2.948924 |
| H | -5.888888 | -2.975292 | 4.188282 |
| H | -8.311903 | -2.286663 | 4.326142 |
| H | -8.713313 | -3.477966 | 3.097400 |
| C | -8.180607 | -4.333211 | 5.011047 |
| C | -9.610019 | -4.434404 | 5.557638 |
| H | -7.490929 | -4.115921 | 5.839371 |
| H | -7.876955 | -5.311148 | 4.610318 |

| | | | |
|---|---|---|---|
| C | -9.760071 | -5.503308 | 6.643450 |
| H | -9.914383 | -3.457933 | 5.959206 |
| H | -10.298776 | -4.652752 | 4.729732 |
| H | -10.788977 | -5.556870 | 7.016813 |
| H | -9.492613 | -6.495871 | 6.261215 |
| H | -9.106418 | -5.293006 | 7.498683 |
| C | -0.650549 | -3.597725 | -0.874992 |
| C | 0.535988 | -3.687251 | -1.502791 |
| H | -1.323267 | -4.456976 | -0.908812 |
| H | 1.206671 | -2.825789 | -1.466164 |
| C | 1.063030 | -4.875401 | -2.250004 |
| C | 2.407314 | -5.372318 | -1.682679 |
| H | 1.216883 | -4.593082 | -3.302743 |
| H | 0.326676 | -5.688603 | -2.240617 |
| C | 2.990801 | -6.550258 | -2.471156 |
| H | 3.126559 | -4.541662 | -1.681004 |
| H | 2.269110 | -5.663318 | -0.632783 |
| H | 2.272320 | -7.382264 | -2.467094 |
| H | 3.113186 | -6.256293 | -3.523491 |
| C | 4.336149 | -7.037083 | -1.920950 |
| C | 4.927400 | -8.212304 | -2.709133 |
| H | 4.214551 | -7.331095 | -0.868419 |
| H | 5.052615 | -6.202911 | -1.923763 |
| C | 6.273318 | -8.687879 | -2.155479 |
| H | 4.212706 | -9.046893 | -2.704326 |
| H | 5.046425 | -7.918003 | -3.761167 |
| H | 6.673737 | -9.526308 | -2.736477 |
| H | 7.017485 | -7.882448 | -2.177387 |
| H | 6.178068 | -9.020026 | -1.114604 |

Vibrational frequencies

| | | |
|---|---|---|
| 11.2218 | 12.4659 | 14.4495 |
| 25.8649 | 29.9481 | 31.9345 |
| 46.7065 | 54.3664 | 55.3923 |
| 56.1675 | 61.4685 | 63.4214 |
| 73.6695 | 74.6378 | 88.5062 |
| 99.0761 | 101.8615 | 105.4293 |
| 128.6046 | 130.9881 | 131.9534 |
| 147.0618 | 149.0002 | 154.8633 |
| 159.5720 | 162.7914 | 165.0997 |
| 172.4009 | 174.8440 | 190.1236 |
| 216.6855 | 218.4066 | 228.3247 |
| 264.4514 | 272.1513 | 273.9934 |
| 278.5381 | 279.8039 | 289.4090 |
| 333.5327 | 334.5680 | 359.0680 |
| 373.8636 | 375.0327 | 425.3729 |
| 446.4218 | 448.2196 | 473.8657 |
| 487.5169 | 488.9230 | 514.4572 |
| 567.6407 | 568.3319 | 629.2725 |
| 631.5710 | 695.4700 | 711.5441 |
| 745.8193 | 746.5169 | 747.9466 |
| 757.9858 | 759.8064 | 761.9481 |
| 800.7648 | 801.8832 | 803.1285 |
| 810.1354 | 842.0850 | 843.3266 |
| 846.5572 | 878.2304 | 878.9518 |
| 907.7792 | 908.8211 | 909.6013 |
| 910.5427 | 915.5786 | 917.1396 |
| 991.1904 | 993.7784 | 994.3424 |
| 1013.3975 | 1014.2798 | 1016.1627 |
| 1029.1803 | 1029.4662 | 1030.0686 |

| | | |
|---|---|---|
| 1041.8885 | 1042.1484 | 1042.4465 |
| 1057.1233 | 1058.8652 | 1059.1590 |
| 1067.9145 | 1068.3039 | 1070.7841 |
| 1075.0968 | 1076.6544 | 1077.2600 |
| 1133.5783 | 1134.1021 | 1135.5114 |
| 1140.1816 | 1140.6385 | 1141.7034 |
| 1184.4122 | 1212.1031 | 1212.6581 |
| 1218.5297 | 1232.0103 | 1233.1920 |
| 1240.5790 | 1253.3970 | 1254.4744 |
| 1256.7474 | 1278.2328 | 1279.5735 |
| 1283.1715 | 1305.8043 | 1307.1285 |
| 1310.6046 | 1314.7277 | 1315.9294 |
| 1321.2373 | 1327.3518 | 1328.8153 |
| 1335.5513 | 1335.9990 | 1338.5154 |
| 1339.5503 | 1341.1811 | 1342.1877 |
| 1344.1637 | 1346.9829 | 1348.6700 |
| 1357.4789 | 1365.9085 | 1367.6489 |
| 1377.5368 | 1377.8725 | 1379.6574 |
| 1400.6188 | 1402.2360 | 1403.4330 |
| 1417.6801 | 1419.0063 | 1419.3123 |
| 1421.2108 | 1423.1451 | 1423.7225 |
| 1474.6005 | 1475.5648 | 1477.6153 |
| 1483.2229 | 1483.4079 | 1483.6139 |
| 1487.9253 | 1487.9412 | 1488.4898 |
| 1496.3088 | 1497.7570 | 1497.7868 |
| 1497.9801 | 1499.6439 | 1501.8124 |
| 1507.2213 | 1507.7459 | 1508.4299 |
| 1513.7393 | 1514.4331 | 1514.7598 |
| 1697.5092 | 1698.1461 | 1701.0747 |
| 3008.9063 | 3009.7405 | 3009.8179 |

| | | |
|---|---|---|
| 3011.2743 | 3011.5882 | 3011.7766 |
| 3013.6550 | 3014.4932 | 3014.5295 |
| 3020.9245 | 3022.1849 | 3022.5109 |
| 3025.5708 | 3025.8993 | 3026.3486 |
| 3032.8888 | 3032.9816 | 3033.4550 |
| 3034.5551 | 3034.9976 | 3035.2532 |
| 3045.7308 | 3046.3750 | 3046.8145 |
| 3058.2438 | 3058.8081 | 3058.8932 |
| 3066.5933 | 3066.9770 | 3067.0255 |
| 3079.0346 | 3079.1087 | 3079.4177 |
| 3099.7229 | 3100.4874 | 3100.6520 |
| 3104.1802 | 3104.9236 | 3104.9614 |
| 3127.8602 | 3128.5810 | 3129.5805 |
| 3135.3624 | 3135.8919 | 3136.3543 |

**R1**

Zero-point correction= 0.361327

Thermal correction to Energy= 0.380680

Thermal correction to Enthalpy= 0.381625

Thermal correction to Gibbs Free Energy= 0.310647

Sum of electronic and zero-point Energies= -647.445836

Sum of electronic and thermal Energies= -647.426482

Sum of electronic and thermal Enthalpies= -647.425538

Sum of electronic and thermal Free Energies= -647.496515

Cartesian coordinates

| | | | |
|---|---|---|---|
| B | 7.418520 | 7.971453 | 0.330976 |
| O | 6.833105 | 9.149763 | 0.720493 |
| C | 8.915229 | 7.740047 | 0.715144 |
| C | 9.625883 | 8.623895 | 1.436712 |

| | | | |
|---|---|---|---|
| H | 9.426648 | 6.825308 | 0.408842 |
| H | 9.135193 | 9.543199 | 1.763478 |
| C | 11.051035 | 8.465035 | 1.880830 |
| C | 11.185753 | 8.435960 | 3.416350 |
| H | 11.644361 | 9.309201 | 1.497827 |
| H | 11.481966 | 7.550766 | 1.453139 |
| C | 12.639651 | 8.327978 | 3.890122 |
| H | 10.730406 | 9.343462 | 3.836578 |
| H | 10.605964 | 7.590089 | 3.809718 |
| H | 13.094958 | 7.423764 | 3.461366 |
| H | 13.214353 | 9.177341 | 3.493592 |
| C | 12.777085 | 8.290255 | 5.416550 |
| C | 14.229560 | 8.181970 | 5.896806 |
| H | 12.201054 | 7.441398 | 5.812616 |
| H | 12.320882 | 9.194381 | 5.845106 |
| C | 14.355234 | 8.149502 | 7.422598 |
| H | 14.683915 | 7.276120 | 5.471955 |
| H | 14.806322 | 9.028490 | 5.499011 |
| H | 15.401287 | 8.068656 | 7.739179 |
| H | 13.941258 | 9.059526 | 7.873667 |
| H | 13.812393 | 7.295714 | 7.846052 |
| C | 5.450786 | 9.421145 | 0.459759 |
| C | 4.554875 | 8.777364 | 1.508684 |
| H | 5.177781 | 9.071181 | -0.542568 |
| H | 5.341584 | 10.511209 | 0.478530 |
| H | 3.506896 | 9.044461 | 1.331843 |
| H | 4.644997 | 7.687409 | 1.469805 |
| H | 4.833226 | 9.114007 | 2.512925 |
| C | 7.048370 | 4.768948 | 0.290813 |
| C | 7.120498 | 5.807137 | -0.818975 |

| | | | |
|---|---|---|---|
| H | 7.361262 | 3.787966 | -0.083573 |
| H | 7.702378 | 5.045331 | 1.124565 |
| H | 6.024775 | 4.684827 | 0.670845 |
| H | 8.142218 | 5.890390 | -1.209409 |
| H | 6.476113 | 5.515741 | -1.655690 |
| O | 6.646471 | 7.079899 | -0.370494 |

Vibrational frequencies

| | | |
|---|---|---|
| 17.5342 | 27.2928 | 42.6921 |
| 52.4075 | 61.5628 | 68.8618 |
| 94.7043 | 107.7291 | 120.6539 |
| 123.5348 | 153.7805 | 156.2350 |
| 166.8779 | 193.0523 | 222.4818 |
| 256.9132 | 264.3001 | 278.3989 |
| 286.5189 | 327.9797 | 363.4171 |
| 414.3621 | 424.9166 | 451.6878 |
| 474.8261 | 522.4124 | 581.1628 |
| 635.0149 | 733.3778 | 745.3736 |
| 761.9279 | 808.5735 | 821.3487 |
| 826.5926 | 844.5670 | 903.6243 |
| 908.6768 | 910.4758 | 938.3136 |
| 991.7414 | 1013.2918 | 1029.5558 |
| 1041.5493 | 1054.3976 | 1060.9072 |
| 1065.2137 | 1072.6388 | 1085.4367 |
| 1121.2502 | 1130.0244 | 1136.0550 |
| 1144.8320 | 1184.7592 | 1193.6374 |
| 1218.3761 | 1245.8398 | 1257.3483 |
| 1281.0071 | 1305.7816 | 1309.0070 |
| 1317.9155 | 1329.0471 | 1335.9701 |
| 1339.9996 | 1344.3259 | 1347.0297 |

| | | |
|---|---|---|
| 1362.8342 | 1373.1981 | 1401.9285 |
| 1402.8473 | 1412.0824 | 1419.2187 |
| 1420.3367 | 1431.8755 | 1446.9389 |
| 1477.3771 | 1482.6197 | 1483.2980 |
| 1485.7651 | 1487.4208 | 1496.5197 |
| 1496.9080 | 1497.3895 | 1497.9458 |
| 1507.2098 | 1513.7369 | 1522.8979 |
| 1537.0666 | 1700.1797 | 3008.0333 |
| 3010.6665 | 3013.2497 | 3021.3219 |
| 3024.0993 | 3031.7923 | 3033.6978 |
| 3043.4245 | 3044.3711 | 3044.8611 |
| 3045.3503 | 3047.4699 | 3055.8126 |
| 3064.4666 | 3075.8039 | 3084.5762 |
| 3088.4775 | 3099.4391 | 3102.1913 |
| 3118.6515 | 3122.6176 | 3122.7508 |
| 3125.8814 | 3130.6233 | 3135.6946 |

**R2**

Zero-point correction= 0.038009

Thermal correction to Energy= 0.044438

Thermal correction to Enthalpy= 0.045382

Thermal correction to Gibbs Free Energy= 0.006137

Sum of electronic and zero-point Energies= -485.734825

Sum of electronic and thermal Energies= -485.728396

Sum of electronic and thermal Enthalpies= -485.727451

Sum of electronic and thermal Free Energies= -485.766696

Cartesian coordinates

| | | | |
|---|---|---|---|
| N | -2.709336 | 0.245102 | 0.000503 |
| N | -1.687109 | -0.260679 | 0.009737 |
| C | -0.529898 | -0.843867 | 0.008470 |

| | | | |
|---|---|---|---|
| H | -0.490740 | -1.922592 | 0.066890 |
| C | 0.697029 | -0.010806 | -0.002633 |
| F | 1.557267 | -0.405060 | -0.972300 |
| F | 0.408463 | 1.293157 | -0.206641 |
| F | 1.394632 | -0.091226 | 1.160087 |

Vibrational frequencies

| | | |
|---|---|---|
| 22.0517 | 160.3658 | 298.7580 |
| 360.1570 | 468.3251 | 479.7928 |
| 532.2593 | 545.7893 | 588.9027 |
| 693.7306 | 865.8827 | 1122.3672 |
| 1150.1250 | 1198.9763 | 1254.7438 |
| 1449.3951 | 2225.7778 | 3266.5702 |

**Cat**

Zero-point correction= 0.262578

Thermal correction to Energy= 0.282406

Thermal correction to Enthalpy= 0.283350

Thermal correction to Gibbs Free Energy= 0.211805

Sum of electronic and zero-point Energies= -942.388300

Sum of electronic and thermal Energies= -942.368472

Sum of electronic and thermal Enthalpies= -942.367527

Sum of electronic and thermal Free Energies= -942.439072

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | 0.636941 | -1.890802 | -0.255739 |
| C | -0.452876 | -1.710576 | -1.047369 |
| O | 0.703073 | 0.896723 | -0.189035 |
| C | -1.427772 | -0.751677 | -0.770556 |
| C | -0.599897 | -2.562607 | -2.177925 |
| C | -0.307857 | 0.906013 | 0.732150 |

| | | | |
|---|---|---|---|
| C | -1.368464 | 0.036792 | 0.499284 |
| C | -1.658291 | -2.432811 | -3.039904 |
| C | -2.503958 | -0.548963 | -1.698616 |
| C | -2.621771 | -1.409953 | -2.837480 |
| C | -0.282700 | 1.725605 | 1.894068 |
| C | -2.393626 | -0.095070 | 1.493789 |
| C | -1.287219 | 1.656200 | 2.825483 |
| C | -2.354870 | 0.737398 | 2.659819 |
| H | -1.760790 | -3.090338 | -3.896845 |
| H | -1.268361 | 2.287963 | 3.707020 |
| C | -3.373706 | 0.621619 | 3.645351 |
| C | -4.391928 | -0.292153 | 3.498313 |
| C | -4.422941 | -1.133379 | 2.358958 |
| C | -3.454849 | -1.037700 | 1.383135 |
| H | -3.327132 | 1.266114 | 4.519113 |
| H | -5.165798 | -0.377455 | 4.255505 |
| H | -5.218533 | -1.865577 | 2.254424 |
| H | -3.491465 | -1.695982 | 0.523263 |
| C | -3.692566 | -1.224340 | -3.754279 |
| C | -4.613166 | -0.218034 | -3.567750 |
| C | -4.491916 | 0.647531 | -2.453568 |
| C | -3.469057 | 0.486841 | -1.543879 |
| H | -3.765308 | -1.891084 | -4.609548 |
| H | -5.425945 | -0.080748 | -4.274864 |
| H | -5.211219 | 1.450065 | -2.316910 |
| H | -3.388958 | 1.164100 | -0.701596 |
| H | 1.392538 | 1.541247 | 0.048313 |
| H | 0.964056 | -1.014428 | 0.012916 |
| I | 1.339997 | 3.101212 | 2.204834 |
| I | 0.874370 | -4.076034 | -2.542093 |

Vibrational frequencies

| | | |
|---|---|---|
| 25.7744 | 40.3368 | 42.6807 |
| 85.4492 | 96.9753 | 100.9774 |
| 109.8375 | 129.8634 | 145.7257 |
| 159.9808 | 184.3187 | 197.8160 |
| 217.4126 | 253.4753 | 284.1113 |
| 294.3435 | 334.3435 | 339.0103 |
| 354.9183 | 378.1468 | 393.8443 |
| 433.9805 | 440.3509 | 451.9661 |
| 457.7296 | 467.6979 | 524.6085 |
| 550.0754 | 558.2812 | 565.2593 |
| 569.5487 | 582.4573 | 610.1240 |
| 613.2100 | 650.0925 | 691.5309 |
| 708.9545 | 722.3745 | 732.0523 |
| 753.4349 | 767.9866 | 768.6080 |
| 785.6317 | 797.8713 | 825.5487 |
| 874.0851 | 876.1211 | 880.1698 |
| 905.6917 | 908.9536 | 948.2807 |
| 969.2231 | 972.4451 | 974.5119 |
| 1001.5194 | 1005.3156 | 1017.5542 |
| 1060.4136 | 1062.6988 | 1096.8009 |
| 1165.0518 | 1174.9291 | 1185.9126 |
| 1191.2321 | 1228.2671 | 1234.5948 |
| 1242.5495 | 1249.6555 | 1278.4122 |
| 1292.3009 | 1303.9226 | 1334.2680 |
| 1358.2754 | 1367.5111 | 1406.6224 |
| 1409.0790 | 1413.4857 | 1427.4965 |
| 1458.5422 | 1470.5852 | 1481.9332 |
| 1490.4760 | 1544.9753 | 1547.4898 |

| | | |
|---|---|---|
| 1603.6825 | 1617.6193 | 1624.7051 |
| 1626.1534 | 1666.7748 | 1669.1244 |
| 3183.2242 | 3187.6085 | 3192.6195 |
| 3196.0019 | 3207.3666 | 3210.4835 |
| 3210.6114 | 3212.8760 | 3225.0976 |
| 3227.9186 | 3679.5387 | 3706.7863 |

**Cat-Br**

Zero-point correction= 0.461312

Thermal correction to Energy= 0.491149

Thermal correction to Enthalpy= 0.492094

Thermal correction to Gibbs Free Energy= 0.396843

Sum of electronic and zero-point Energies= -1283.424033

Sum of electronic and thermal Energies= -1283.394196

Sum of electronic and thermal Enthalpies= -1283.393252

Sum of electronic and thermal Free Energies= -1283.488502

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.028832 | 0.073240 | -1.997082 |
| B | 0.429715 | 1.138763 | -1.224999 |
| C | -1.026248 | -0.723699 | -1.498089 |
| O | -0.474027 | 1.925165 | -0.523623 |
| C | -2.267372 | -0.212302 | -1.140412 |
| C | -0.751402 | -2.106560 | -1.332491 |
| C | -1.701940 | 2.205512 | -1.062093 |
| C | -2.585756 | 1.208923 | -1.455228 |
| C | -1.665131 | -2.962444 | -0.778596 |
| C | -3.202968 | -1.063121 | -0.453907 |
| C | -2.901441 | -2.455744 | -0.299925 |
| C | -2.045995 | 3.572449 | -1.231935 |
| C | -3.774064 | 1.575348 | -2.179747 |

| | | | |
|---|---|---|---|
| C | -3.220335 | 3.951608 | -1.824313 |
| C | -4.099486 | 2.962356 | -2.337287 |
| H | -1.444573 | -4.018696 | -0.667905 |
| H | -3.473294 | 5.000141 | -1.938375 |
| C | -5.283125 | 3.335678 | -3.031250 |
| C | -6.105599 | 2.379967 | -3.582273 |
| C | -5.765890 | 1.010282 | -3.469288 |
| C | -4.634854 | 0.618085 | -2.786803 |
| H | -5.516617 | 4.392528 | -3.128542 |
| H | -7.004527 | 2.672508 | -4.116737 |
| H | -6.400835 | 0.259538 | -3.930790 |
| H | -4.387964 | -0.434497 | -2.722805 |
| C | -3.829493 | -3.311287 | 0.354816 |
| C | -5.001499 | -2.810426 | 0.873511 |
| C | -5.283650 | -1.427319 | 0.765602 |
| C | -4.412124 | -0.577787 | 0.119430 |
| H | -3.585623 | -4.365976 | 0.449181 |
| H | -5.702861 | -3.468433 | 1.377943 |
| H | -6.195253 | -1.029122 | 1.201737 |
| H | -4.644028 | 0.478345 | 0.058310 |
| C | 1.929360 | 1.458082 | -1.148071 |
| C | 2.854974 | 0.705427 | -1.773167 |
| H | 2.254694 | 2.334025 | -0.585127 |
| H | 2.516800 | -0.168696 | -2.331281 |
| C | 4.335130 | 0.930426 | -1.763493 |
| C | 5.102769 | -0.285844 | -1.207065 |
| H | 4.580275 | 1.829033 | -1.184416 |
| H | 4.672075 | 1.108961 | -2.795976 |
| C | 6.623132 | -0.093533 | -1.233132 |
| H | 4.772318 | -0.478343 | -0.177860 |

| | | | |
|---|---|---|---|
| H | 4.835491 | -1.178388 | -1.789267 |
| H | 6.944564 | 0.109139 | -2.264747 |
| H | 6.885789 | 0.799965 | -0.649161 |
| C | 7.394836 | -1.301219 | -0.688787 |
| C | 8.916424 | -1.110078 | -0.706067 |
| H | 7.135219 | -2.193423 | -1.276779 |
| H | 7.067904 | -1.508422 | 0.340346 |
| C | 9.680188 | -2.323847 | -0.168907 |
| H | 9.242133 | -0.897100 | -1.733622 |
| H | 9.175526 | -0.221928 | -0.113273 |
| H | 10.763332 | -2.158630 | -0.189278 |
| H | 9.397035 | -2.543126 | 0.867780 |
| H | 9.469252 | -3.220070 | -0.764799 |
| Br | -0.793893 | 4.958066 | -0.605664 |
| Br | 0.994329 | -2.813355 | -1.911552 |

Vibrational frequencies

| | | |
|---|---|---|
| 10.4154 | 15.8549 | 28.9724 |
| 36.2442 | 44.6182 | 56.8989 |
| 64.2357 | 70.8040 | 86.4599 |
| 89.4256 | 101.8634 | 110.4859 |
| 116.3228 | 131.9886 | 133.7540 |
| 155.9559 | 161.4737 | 169.2352 |
| 172.5180 | 187.1505 | 200.9662 |
| 214.5002 | 240.2389 | 251.3577 |
| 276.8178 | 278.8211 | 285.5989 |
| 298.2776 | 320.3569 | 334.2932 |
| 340.5611 | 354.4688 | 387.1979 |
| 395.6695 | 433.0841 | 447.9289 |
| 455.6089 | 461.2628 | 479.1717 |

| | | |
|---|---|---|
| 511.2052 | 517.7754 | 526.1846 |
| 554.9054 | 561.2475 | 573.7289 |
| 588.3622 | 590.8176 | 609.5469 |
| 633.1486 | 649.3718 | 657.2723 |
| 678.1323 | 712.5107 | 736.3815 |
| 746.6733 | 747.8645 | 758.8024 |
| 759.7192 | 767.9461 | 769.5054 |
| 780.1736 | 797.4932 | 806.8826 |
| 830.7791 | 846.1614 | 863.7624 |
| 874.3079 | 876.2606 | 884.3387 |
| 899.0660 | 902.9754 | 908.6387 |
| 911.4368 | 953.0451 | 974.1033 |
| 976.6372 | 978.9212 | 996.9791 |
| 1004.0993 | 1005.6546 | 1013.5409 |
| 1023.1678 | 1029.0531 | 1046.2628 |
| 1060.2925 | 1062.0958 | 1065.5771 |
| 1071.1671 | 1078.7273 | 1107.2031 |
| 1135.4668 | 1141.7042 | 1165.2089 |
| 1184.1551 | 1191.0277 | 1198.5969 |
| 1209.0847 | 1228.8893 | 1235.0903 |
| 1239.6821 | 1252.8027 | 1257.8418 |
| 1261.8555 | 1277.0253 | 1286.1560 |
| 1287.6977 | 1303.3287 | 1309.1179 |
| 1320.7784 | 1337.6676 | 1341.2348 |
| 1346.6060 | 1349.5039 | 1356.5883 |
| 1368.4123 | 1375.6436 | 1402.5452 |
| 1403.0000 | 1406.5442 | 1407.3898 |
| 1418.4334 | 1423.2037 | 1429.0962 |
| 1453.8132 | 1457.6396 | 1476.1635 |
| 1479.4302 | 1483.1314 | 1485.9305 |

| | | |
|---|---|---|
| 1487.9334 | 1498.3538 | 1500.5212 |
| 1508.1310 | 1514.5211 | 1543.7994 |
| 1545.4326 | 1603.9340 | 1614.1173 |
| 1626.5650 | 1629.1999 | 1668.3859 |
| 1669.4473 | 1693.5665 | 3010.7062 |
| 3012.3203 | 3014.8429 | 3022.5883 |
| 3027.9209 | 3033.4268 | 3035.7569 |
| 3047.5894 | 3060.7416 | 3068.9048 |
| 3082.2897 | 3101.1385 | 3104.2658 |
| 3142.9062 | 3158.6855 | 3187.9365 |
| 3188.8803 | 3197.0916 | 3197.7282 |
| 3210.5750 | 3211.4465 | 3214.7746 |
| 3218.5287 | 3233.1809 | 3236.3092 |

**Cat-H**

Zero-point correction= 0.482015

Thermal correction to Energy= 0.508579

Thermal correction to Enthalpy= 0.509524

Thermal correction to Gibbs Free Energy= 0.423063

Sum of electronic and zero-point Energies= -1258.285424

Sum of electronic and thermal Energies= -1258.258860

Sum of electronic and thermal Enthalpies= -1258.257916

Sum of electronic and thermal Free Energies= -1258.344376

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.058167 | 0.444712 | -2.259642 |
| B | 0.445623 | 1.432461 | -1.418713 |
| C | -0.961101 | -0.455846 | -1.722671 |
| O | -0.395553 | 2.170288 | -0.607230 |
| C | -2.165345 | -0.045603 | -1.169671 |
| C | -0.566111 | -1.813377 | -1.755251 |

| | | | |
|---|---|---|---|
| C | -1.715612 | 2.396882 | -0.943953 |
| C | -2.589705 | 1.376238 | -1.290353 |
| C | -1.359657 | -2.772922 | -1.178413 |
| C | -2.947638 | -1.027898 | -0.460744 |
| C | -2.547949 | -2.406489 | -0.490777 |
| C | -2.111609 | 3.754733 | -0.915902 |
| C | -3.890542 | 1.748666 | -1.790481 |
| C | -3.381793 | 4.109487 | -1.293214 |
| C | -4.292894 | 3.126447 | -1.765006 |
| H | -1.068963 | -3.819405 | -1.209959 |
| H | -3.693573 | 5.149959 | -1.265309 |
| C | -5.583548 | 3.490515 | -2.237137 |
| C | -6.444058 | 2.545563 | -2.748639 |
| C | -6.034554 | 1.192716 | -2.820601 |
| C | -4.796290 | 0.805605 | -2.355051 |
| H | -5.872420 | 4.537694 | -2.196485 |
| H | -7.426334 | 2.835334 | -3.110460 |
| H | -6.700767 | 0.451328 | -3.252813 |
| H | -4.500719 | -0.233527 | -2.431685 |
| C | -3.328167 | -3.378906 | 0.192776 |
| C | -4.443598 | -3.014669 | 0.912585 |
| C | -4.815404 | -1.650846 | 0.984138 |
| C | -4.091258 | -0.686876 | 0.316132 |
| H | -3.014458 | -4.418676 | 0.146324 |
| H | -5.028796 | -3.764648 | 1.436818 |
| H | -5.677935 | -1.358925 | 1.576648 |
| H | -4.388456 | 0.351700 | 0.394170 |
| C | 1.958493 | 1.724229 | -1.376449 |
| C | 2.859733 | 0.979938 | -2.043892 |
| H | 2.318614 | 2.564847 | -0.780510 |

| | | | |
|---|---|---|---|
| H | 2.499290 | 0.135758 | -2.635364 |
| C | 4.345305 | 1.176277 | -2.038848 |
| C | 5.093214 | -0.045475 | -1.467461 |
| H | 4.605629 | 2.074547 | -1.465741 |
| H | 4.687494 | 1.340545 | -3.071692 |
| C | 6.616058 | 0.128989 | -1.481534 |
| H | 4.752620 | -0.224180 | -0.439012 |
| H | 4.819946 | -0.939888 | -2.043989 |
| H | 6.950491 | 0.311448 | -2.512750 |
| H | 6.882436 | 1.028954 | -0.909254 |
| C | 7.369113 | -1.077286 | -0.908663 |
| C | 8.892462 | -0.899598 | -0.907482 |
| H | 7.109556 | -1.976149 | -1.486402 |
| H | 7.026437 | -1.265575 | 0.119009 |
| C | 9.638022 | -2.111206 | -0.340814 |
| H | 9.234489 | -0.705323 | -1.933411 |
| H | 9.150835 | -0.004629 | -0.324712 |
| H | 10.722708 | -1.955363 | -0.348295 |
| H | 9.338374 | -2.311953 | 0.694978 |
| H | 9.427935 | -3.014826 | -0.925734 |
| H | -1.383461 | 4.491640 | -0.592977 |
| H | 0.370271 | -2.062875 | -2.243414 |

Vibrational frequencies

| | | |
|---|---|---|
| 10.1211 | 17.5940 | 38.2977 |
| 57.2227 | 59.0733 | 64.7191 |
| 69.2972 | 76.7672 | 84.3315 |
| 116.7543 | 130.6240 | 135.9056 |
| 155.1327 | 161.6232 | 161.8637 |
| 171.9548 | 184.4126 | 202.5536 |

| | | |
|---|---|---|
| 230.3646 | 252.4379 | 276.6745 |
| 280.4437 | 311.5475 | 327.2012 |
| 333.6613 | 352.8539 | 377.4769 |
| 390.2402 | 425.3830 | 430.6599 |
| 442.3665 | 455.7362 | 471.1811 |
| 478.5068 | 497.8319 | 517.2467 |
| 530.0983 | 542.8909 | 546.4012 |
| 547.9387 | 571.8382 | 589.2939 |
| 630.4355 | 647.5847 | 648.0016 |
| 675.0166 | 681.1544 | 712.6805 |
| 719.2706 | 740.0656 | 746.5246 |
| 758.9860 | 768.9161 | 770.9261 |
| 780.5642 | 798.3551 | 806.7007 |
| 806.8670 | 835.3420 | 839.2607 |
| 844.9832 | 859.0107 | 867.0882 |
| 886.1118 | 886.8925 | 907.9471 |
| 909.5968 | 943.7072 | 963.2415 |
| 964.7980 | 965.9175 | 976.0548 |
| 976.8456 | 994.0651 | 1000.0158 |
| 1002.8397 | 1010.2571 | 1015.5946 |
| 1028.4534 | 1042.7806 | 1058.1995 |
| 1061.3191 | 1063.0281 | 1068.8044 |
| 1076.4932 | 1095.2512 | 1134.6519 |
| 1141.7644 | 1153.9282 | 1171.5974 |
| 1174.1688 | 1188.6213 | 1190.0840 |
| 1209.1940 | 1220.5849 | 1229.5993 |
| 1238.3363 | 1239.2398 | 1245.9276 |
| 1253.8501 | 1269.9390 | 1274.6483 |
| 1284.0996 | 1292.0727 | 1303.3450 |
| 1307.9452 | 1320.8038 | 1336.9806 |

| | | |
|---|---|---|
| 1339.0693 | 1346.0638 | 1349.2943 |
| 1364.7863 | 1366.9906 | 1373.7818 |
| 1398.8284 | 1402.1362 | 1404.8923 |
| 1413.6867 | 1418.4643 | 1421.9935 |
| 1437.0741 | 1465.2351 | 1467.9546 |
| 1477.2783 | 1483.1286 | 1488.0577 |
| 1498.6421 | 1499.8805 | 1499.9765 |
| 1505.1262 | 1508.3742 | 1514.6399 |
| 1554.5346 | 1555.7266 | 1618.7382 |
| 1624.8057 | 1643.8972 | 1647.3723 |
| 1670.2719 | 1672.6056 | 1695.5243 |
| 3011.4870 | 3012.8352 | 3014.9415 |
| 3022.8250 | 3027.6038 | 3033.3957 |
| 3035.6869 | 3047.6230 | 3060.5689 |
| 3068.4791 | 3081.5768 | 3101.1162 |
| 3104.2504 | 3133.1232 | 3139.9704 |
| 3183.2673 | 3183.3089 | 3192.3451 |
| 3192.6402 | 3194.0008 | 3194.5026 |
| 3208.0455 | 3208.3512 | 3217.1465 |
| 3218.7640 | 3232.6265 | 3234.9660 |

**Cat+R1**

Zero-point correction= 0.624736

Thermal correction to Energy= 0.665895

Thermal correction to Enthalpy= 0.666839

Thermal correction to Gibbs Free Energy= 0.544893

Sum of electronic and zero-point Energies= -1589.854638

Sum of electronic and thermal Energies= -1589.813480

Sum of electronic and thermal Enthalpies= -1589.812536

Sum of electronic and thermal Free Energies= -1589.934482

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.574891 | -1.041846 | -1.040462 |
| B | 0.495496 | 1.851414 | -2.690475 |
| C | 0.066270 | -1.066147 | 0.155591 |
| O | -1.271335 | 1.899710 | 0.166278 |
| C | -0.618730 | -0.567229 | 1.260327 |
| C | 1.378022 | -1.596715 | 0.327266 |
| C | -2.306716 | 1.083715 | 0.482074 |
| C | -2.038997 | -0.137951 | 1.087725 |
| C | 2.007304 | -1.573370 | 1.547724 |
| C | 0.022784 | -0.511741 | 2.533349 |
| C | 1.357123 | -1.014964 | 2.676458 |
| C | -3.662611 | 1.467205 | 0.257907 |
| C | -3.109020 | -0.991117 | 1.503680 |
| C | -4.710456 | 0.665555 | 0.637047 |
| C | -4.462225 | -0.577700 | 1.276139 |
| H | 3.006216 | -1.979352 | 1.663352 |
| H | -5.736853 | 0.971869 | 0.463783 |
| C | -5.532093 | -1.418474 | 1.689276 |
| C | -5.281341 | -2.626916 | 2.299695 |
| C | -3.944884 | -3.045414 | 2.515560 |
| C | -2.887297 | -2.251884 | 2.127025 |
| H | -6.552352 | -1.087770 | 1.512402 |
| H | -6.104137 | -3.262836 | 2.613407 |
| H | -3.753316 | -4.002552 | 2.992560 |
| H | -1.869003 | -2.585143 | 2.294061 |
| C | 2.001327 | -0.953615 | 3.943096 |
| C | 1.357632 | -0.409675 | 5.031523 |
| C | 0.037872 | 0.090655 | 4.894556 |

| | | | |
|---|---|---|---|
| C | -0.613668 | 0.039912 | 3.681930 |
| H | 3.012042 | -1.343383 | 4.032053 |
| H | 1.856181 | -0.362101 | 5.995208 |
| H | -0.462862 | 0.522153 | 5.756725 |
| H | -1.621149 | 0.430801 | 3.587344 |
| I | -4.074530 | 3.356905 | -0.679308 |
| I | 2.390229 | -2.505972 | -1.338797 |
| H | -1.216118 | 2.023272 | -0.812475 |
| O | -0.867882 | 1.978187 | -2.486124 |
| C | 1.369939 | 2.293894 | -1.477810 |
| C | 2.306927 | 1.510868 | -0.920277 |
| H | 1.063318 | 3.184623 | -0.924202 |
| H | 2.590552 | 0.584849 | -1.421915 |
| C | 2.938629 | 1.726136 | 0.429617 |
| C | 4.295864 | 1.032472 | 0.599392 |
| H | 2.249176 | 1.318758 | 1.183501 |
| H | 3.018666 | 2.799980 | 0.644258 |
| C | 4.836098 | 1.128406 | 2.029605 |
| H | 4.185003 | -0.026285 | 0.327170 |
| H | 5.024279 | 1.457020 | -0.105334 |
| H | 4.988111 | 2.184517 | 2.294258 |
| H | 4.073777 | 0.747597 | 2.723753 |
| C | 6.141992 | 0.354986 | 2.240036 |
| C | 6.670180 | 0.428061 | 3.677581 |
| H | 6.909339 | 0.736932 | 1.551122 |
| H | 5.986065 | -0.699192 | 1.966802 |
| C | 7.975356 | -0.347348 | 3.876933 |
| H | 6.822215 | 1.480518 | 3.954218 |
| H | 5.904047 | 0.040102 | 4.363424 |
| H | 8.330417 | -0.280046 | 4.911495 |

| | | | |
|---|---|---|---|
| H | 7.845018 | -1.410092 | 3.639004 |
| H | 8.769043 | 0.040529 | 3.226868 |
| C | -1.844686 | 1.495502 | -3.430538 |
| C | -2.204619 | 2.583568 | -4.426453 |
| H | -2.715782 | 1.200883 | -2.838698 |
| H | -1.455734 | 0.607488 | -3.937579 |
| H | -2.985934 | 2.230334 | -5.108460 |
| H | -2.575138 | 3.471430 | -3.904536 |
| H | -1.328743 | 2.864938 | -5.019570 |
| C | 2.622851 | -0.091631 | -4.816719 |
| C | 2.251904 | 1.306193 | -4.355459 |
| H | 3.634181 | -0.092151 | -5.237357 |
| H | 2.596109 | -0.797024 | -3.981042 |
| H | 1.927984 | -0.441557 | -5.587222 |
| H | 2.937645 | 1.662120 | -3.580337 |
| H | 2.300612 | 2.010646 | -5.194913 |
| O | 0.900926 | 1.314509 | -3.874102 |
| H | 0.010092 | -1.365678 | -1.745484 |

Vibrational frequencies

| | | |
|---|---|---|
| 9.5720 | 16.9590 | 20.8027 |
| 25.9717 | 27.8444 | 34.1182 |
| 43.3455 | 46.2589 | 50.4579 |
| 59.2233 | 61.4285 | 69.4437 |
| 72.9287 | 80.0768 | 83.4045 |
| 87.6164 | 96.1489 | 100.5415 |
| 102.9154 | 108.2119 | 114.8366 |
| 129.4079 | 131.2581 | 145.7543 |
| 151.7240 | 164.5889 | 166.1553 |
| 171.2326 | 177.1986 | 189.0334 |

| | | |
|---|---|---|
| 197.9559 | 200.0583 | 216.0145 |
| 225.3780 | 240.6212 | 253.1289 |
| 255.7567 | 261.2947 | 283.4434 |
| 286.2860 | 287.7820 | 318.3183 |
| 333.7466 | 345.3155 | 356.1926 |
| 363.6391 | 372.3345 | 374.2718 |
| 385.7186 | 412.4327 | 441.3885 |
| 444.6020 | 457.3977 | 458.1473 |
| 461.8395 | 477.3557 | 519.6674 |
| 528.2608 | 546.8332 | 555.8201 |
| 556.4549 | 566.0941 | 571.3022 |
| 579.9351 | 603.9590 | 621.8008 |
| 626.4480 | 638.7117 | 648.4700 |
| 695.9258 | 714.1387 | 723.7866 |
| 732.6483 | 733.9211 | 746.1225 |
| 751.2537 | 764.0249 | 765.1887 |
| 766.3182 | 778.9071 | 784.9838 |
| 798.7632 | 821.6983 | 823.5192 |
| 825.5578 | 831.1411 | 872.6789 |
| 874.2248 | 880.8878 | 893.2639 |
| 902.9226 | 906.5636 | 907.0610 |
| 909.1675 | 946.1050 | 949.4621 |
| 967.3982 | 969.8927 | 982.5419 |
| 998.4972 | 998.6816 | 1000.1079 |
| 1011.3339 | 1016.7650 | 1041.6680 |
| 1045.7087 | 1052.5310 | 1055.9832 |
| 1059.1214 | 1061.3630 | 1077.5976 |
| 1081.4137 | 1089.9789 | 1100.4768 |
| 1121.4901 | 1129.4818 | 1137.5885 |
| 1141.6214 | 1163.6505 | 1180.8830 |

| | | |
|---|---|---|
| 1185.4494 | 1186.0010 | 1187.4396 |
| 1188.0055 | 1219.3250 | 1229.1939 |
| 1238.0025 | 1243.6802 | 1251.3414 |
| 1255.6036 | 1278.1940 | 1278.4249 |
| 1286.1219 | 1298.3106 | 1302.0678 |
| 1305.1164 | 1309.5126 | 1319.5668 |
| 1328.3770 | 1334.1354 | 1337.0826 |
| 1344.2026 | 1352.8947 | 1356.8520 |
| 1360.0410 | 1366.3644 | 1374.7058 |
| 1379.4373 | 1404.0501 | 1406.6243 |
| 1408.5425 | 1413.8252 | 1415.1487 |
| 1418.9469 | 1420.3143 | 1423.6789 |
| 1433.8037 | 1435.4447 | 1450.4112 |
| 1455.9890 | 1463.2303 | 1468.1068 |
| 1481.5131 | 1483.2489 | 1484.6678 |
| 1486.6222 | 1489.9974 | 1494.9604 |
| 1495.2614 | 1496.7060 | 1498.2243 |
| 1500.2837 | 1506.4117 | 1514.0226 |
| 1520.2854 | 1531.5489 | 1538.6413 |
| 1545.7514 | 1611.0615 | 1614.7399 |
| 1624.4798 | 1626.5140 | 1667.7675 |
| 1668.2028 | 1705.4757 | 3006.1865 |
| 3013.7380 | 3018.1506 | 3020.6995 |
| 3025.6412 | 3031.6737 | 3032.0964 |
| 3043.1665 | 3046.6193 | 3048.5298 |
| 3052.3237 | 3053.4653 | 3062.4210 |
| 3071.9611 | 3073.5063 | 3098.4349 |
| 3099.8248 | 3103.4975 | 3114.3949 |
| 3119.0877 | 3125.0879 | 3125.1369 |
| 3136.4693 | 3141.5328 | 3148.0304 |

| | | |
|---|---|---|
| 3183.2876 | 3184.4375 | 3191.6410 |
| 3193.1129 | 3206.3547 | 3207.6016 |
| 3211.4299 | 3214.0066 | 3216.6114 |
| 3219.8544 | 3364.1569 | 3724.8319 |

**EtOH**

Zero-point correction= 0.079828

Thermal correction to Energy= 0.084110

Thermal correction to Enthalpy= 0.085054

Thermal correction to Gibbs Free Energy= 0.054451

Sum of electronic and zero-point Energies= -154.973062

Sum of electronic and thermal Energies= -154.968780

Sum of electronic and thermal Enthalpies= -154.967836

Sum of electronic and thermal Free Energies= -154.998439

Cartesian coordinates

| | | | |
|---|---|---|---|
| C | 1.222775 | -0.222867 | 0.000002 |
| C | -0.084653 | 0.548457 | 0.000004 |
| H | 2.074505 | 0.465352 | -0.000004 |
| H | 1.292867 | -0.860461 | 0.887636 |
| H | 1.292860 | -0.860463 | -0.887632 |
| H | -0.135212 | 1.201326 | 0.886461 |
| H | -0.135200 | 1.201349 | -0.886438 |
| O | -1.154163 | -0.399699 | -0.000016 |
| H | -1.985246 | 0.096952 | 0.000072 |

Vibrational frequencies

| | | |
|---|---|---|
| 252.6946 | 298.8427 | 413.7689 |
| 828.4693 | 904.6278 | 1037.0043 |
| 1107.9243 | 1180.3948 | 1274.4536 |
| 1302.9071 | 1402.7983 | 1467.9483 |

| | | |
|---|---|---|
| 1482.5461 | 1495.1947 | 1528.3654 |
| 2980.0347 | 3006.0328 | 3045.7188 |
| 3120.0659 | 3123.5782 | 3786.9481 |

**$H_2O$**

Zero-point correction= 0.021156

Thermal correction to Energy= 0.023991

Thermal correction to Enthalpy= 0.024936

Thermal correction to Gibbs Free Energy= 0.002837

Sum of electronic and zero-point Energies= -76.403987

Sum of electronic and thermal Energies= -76.401152

Sum of electronic and thermal Enthalpies= -76.400208

Sum of electronic and thermal Free Energies= -76.422307

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.582413 | -0.252276 | 0.000000 |
| H | 0.383619 | -0.199784 | 0.000000 |
| H | -0.855490 | 0.675971 | 0.000000 |

Vibrational frequencies

| | | |
|---|---|---|
| 1641.0534 | 3773.6170 | 3871.8283 |

**$N_2$**

Zero-point correction= 0.005613

Thermal correction to Energy= 0.007973

Thermal correction to Enthalpy= 0.008917

Thermal correction to Gibbs Free Energy= -0.012836

Sum of electronic and zero-point Energies= -109.510019

Sum of electronic and thermal Energies= -109.507658

Sum of electronic and thermal Enthalpies= -109.506714

Sum of electronic and thermal Free Energies= -109.528467

Cartesian coordinates

| | | | |
|---|---|---|---|
| N | 6.527998 | -0.432621 | 7.783491 |
| N | 5.858423 | 0.445383 | 7.816395 |

Vibrational frequencies

2463.6046

**R2**

Zero-point correction= 0.038009

Thermal correction to Energy= 0.044438

Thermal correction to Enthalpy= 0.045382

Thermal correction to Gibbs Free Energy= 0.006137

Sum of electronic and zero-point Energies= -485.734825

Sum of electronic and thermal Energies= -485.728396

Sum of electronic and thermal Enthalpies= -485.727451

Sum of electronic and thermal Free Energies= -485.766696

Cartesian coordinates

| | | | |
|---|---|---|---|
| N | -2.709336 | 0.245102 | 0.000503 |
| N | -1.687109 | -0.260679 | 0.009737 |
| C | -0.529898 | -0.843867 | 0.008470 |
| H | -0.490740 | -1.922592 | 0.066890 |
| C | 0.697029 | -0.010806 | -0.002633 |
| F | 1.557267 | -0.405060 | -0.972300 |
| F | 0.408463 | 1.293157 | -0.206641 |
| F | 1.394632 | -0.091226 | 1.160087 |

Vibrational frequencies

| | | |
|---|---|---|
| 22.0517 | 160.3658 | 298.7580 |
| 360.1570 | 468.3251 | 479.7928 |
| 532.2593 | 545.7893 | 588.9027 |

| | | |
|---|---|---|
| 693.7306 | 865.8827 | 1122.3672 |
| 1150.1250 | 1198.9763 | 1254.7438 |
| 1449.3951 | 2225.7778 | 3266.5702 |

**TS1**

Zero-point correction= 0.703629

Thermal correction to Energy= 0.747917

Thermal correction to Enthalpy= 0.748861

Thermal correction to Gibbs Free Energy= 0.621118

Sum of electronic and zero-point Energies= -1744.832343

Sum of electronic and thermal Energies= -1744.788055

Sum of electronic and thermal Enthalpies= -1744.787111

Sum of electronic and thermal Free Energies= -1744.914854

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.212113 | -0.919172 | -0.845837 |
| B | 0.795004 | 0.279768 | -1.262966 |
| C | -0.282980 | -1.397303 | 0.433808 |
| O | -1.026216 | 1.946206 | 1.016575 |
| C | -1.255481 | -0.901988 | 1.288779 |
| C | 0.612781 | -2.410402 | 0.888727 |
| C | -2.230343 | 1.357035 | 0.782889 |
| C | -2.360626 | -0.026056 | 0.790228 |
| C | 0.593571 | -2.840446 | 2.192212 |
| C | -1.286895 | -1.325857 | 2.657203 |
| C | -0.334918 | -2.291971 | 3.114711 |
| C | -3.381940 | 2.158806 | 0.522662 |
| C | -3.600096 | -0.637613 | 0.415549 |
| C | -4.590806 | 1.602766 | 0.186228 |
| C | -4.722176 | 0.191761 | 0.091230 |
| H | 1.278474 | -3.609623 | 2.532756 |

| | | | |
|---|---|---|---|
| H | -5.455068 | 2.226855 | -0.016662 |
| C | -5.950228 | -0.410572 | -0.296897 |
| C | -6.070444 | -1.780550 | -0.369097 |
| C | -4.964297 | -2.604865 | -0.046436 |
| C | -3.763277 | -2.050126 | 0.340605 |
| H | -6.792195 | 0.233143 | -0.537847 |
| H | -7.011028 | -2.232209 | -0.670694 |
| H | -5.064914 | -3.685087 | -0.103212 |
| H | -2.925277 | -2.692333 | 0.587980 |
| C | -0.356927 | -2.710060 | 4.473387 |
| C | -1.285682 | -2.196453 | 5.350534 |
| C | -2.232051 | -1.242965 | 4.900999 |
| C | -2.236077 | -0.820478 | 3.589331 |
| H | 0.373322 | -3.443547 | 4.804882 |
| H | -1.295572 | -2.519257 | 6.387548 |
| H | -2.960787 | -0.840452 | 5.598816 |
| H | -2.961980 | -0.086345 | 3.257850 |
| I | -3.219422 | 4.291189 | 0.705285 |
| I | 1.945994 | -3.380658 | -0.480521 |
| H | -0.524775 | 1.876968 | 0.153949 |
| O | -0.010894 | 1.481633 | -1.393149 |
| C | 1.890440 | 0.503437 | -0.129385 |
| C | 3.169753 | 0.114347 | -0.188984 |
| H | 1.574796 | 1.021896 | 0.781321 |
| H | 3.515065 | -0.413448 | -1.080678 |
| C | 4.208794 | 0.323284 | 0.878325 |
| C | 5.382933 | 1.207114 | 0.417541 |
| H | 4.611613 | -0.653728 | 1.187784 |
| H | 3.742868 | 0.767450 | 1.767864 |
| C | 6.454580 | 1.388704 | 1.498336 |

| | | | |
|---|---|---|---|
| H | 5.838445 | 0.766985 | -0.481081 |
| H | 4.993740 | 2.189050 | 0.115349 |
| H | 5.991928 | 1.825287 | 2.395187 |
| H | 6.834238 | 0.402061 | 1.801129 |
| C | 7.629118 | 2.269095 | 1.055592 |
| C | 8.694861 | 2.454866 | 2.142568 |
| H | 7.250080 | 3.254552 | 0.748256 |
| H | 8.096388 | 1.830172 | 0.161920 |
| C | 9.872017 | 3.321853 | 1.686686 |
| H | 8.230223 | 2.904453 | 3.031117 |
| H | 9.065573 | 1.469450 | 2.457373 |
| H | 10.616481 | 3.441596 | 2.481993 |
| H | 10.378627 | 2.877431 | 0.821278 |
| H | 9.535534 | 4.323469 | 1.392497 |
| C | -1.078546 | 1.504980 | -2.347728 |
| C | -1.364462 | 2.942801 | -2.742539 |
| H | -1.969766 | 1.034558 | -1.914063 |
| H | -0.805228 | 0.917283 | -3.231704 |
| H | -2.200681 | 2.987185 | -3.449158 |
| H | -1.625380 | 3.540464 | -1.864903 |
| H | -0.485616 | 3.394008 | -3.215438 |
| C | 2.605322 | -0.159680 | -4.550972 |
| C | 2.017929 | 0.642182 | -3.402760 |
| H | 3.185628 | 0.488498 | -5.216137 |
| H | 3.263944 | -0.948719 | -4.173027 |
| H | 1.810094 | -0.629248 | -5.142105 |
| H | 2.811385 | 1.119752 | -2.815915 |
| H | 1.368682 | 1.442084 | -3.785091 |
| O | 1.275077 | -0.242065 | -2.560200 |
| H | 0.212925 | -1.259606 | -3.186026 |

| | | | |
|---|---|---|---|
| C | -1.590336 | -3.935684 | -2.486669 |
| C | -0.615755 | -3.185053 | -3.369345 |
| H | -1.629155 | -4.984395 | -2.796459 |
| H | -1.272759 | -3.901136 | -1.439619 |
| H | -2.595491 | -3.510741 | -2.565698 |
| H | 0.406498 | -3.552601 | -3.249351 |
| H | -0.896602 | -3.236215 | -4.424131 |
| O | -0.653947 | -1.768296 | -3.004490 |
| H | -0.599538 | -1.540156 | -1.887222 |

Vibrational frequencies

| | | |
|---|---|---|
| -424.5913 | 11.5522 | 14.3234 |
| 19.6981 | 23.5282 | 28.9096 |
| 32.6869 | 45.7368 | 49.9855 |
| 53.3568 | 59.5630 | 62.7280 |
| 71.0191 | 76.0618 | 76.7909 |
| 82.4880 | 85.3403 | 89.1527 |
| 90.7229 | 99.2661 | 108.4734 |
| 118.1806 | 123.5922 | 131.7502 |
| 145.1831 | 154.9006 | 157.7578 |
| 158.6815 | 163.8731 | 166.4900 |
| 167.7901 | 175.8076 | 179.9609 |
| 193.9023 | 199.1709 | 208.8912 |
| 218.5238 | 232.8529 | 239.1497 |
| 259.6440 | 268.0268 | 271.1780 |
| 277.3516 | 283.8189 | 286.1758 |
| 289.4651 | 306.0915 | 318.1551 |
| 329.2027 | 344.1165 | 354.9142 |
| 364.5483 | 369.6735 | 388.0504 |
| 393.9429 | 403.5207 | 441.9953 |

| | | |
|---|---|---|
| 452.9261 | 455.0217 | 458.1226 |
| 480.5103 | 498.9823 | 501.8659 |
| 511.0439 | 528.6723 | 548.5879 |
| 560.9435 | 563.2140 | 565.4370 |
| 582.8216 | 597.1282 | 626.0283 |
| 630.2052 | 639.2320 | 653.8270 |
| 699.3252 | 713.2905 | 720.5291 |
| 732.0966 | 747.2853 | 748.8317 |
| 754.3401 | 764.5206 | 766.9853 |
| 767.5028 | 775.0684 | 792.5445 |
| 799.1954 | 801.5194 | 809.3782 |
| 824.0415 | 826.7261 | 827.7656 |
| 830.7637 | 841.9190 | 872.7914 |
| 878.0390 | 881.9536 | 893.6801 |
| 900.0687 | 905.4133 | 907.9719 |
| 910.1063 | 910.7651 | 913.9545 |
| 943.8181 | 949.3583 | 970.0325 |
| 971.3699 | 992.3807 | 993.9420 |
| 1000.1579 | 1002.2033 | 1009.2039 |
| 1019.1212 | 1028.3035 | 1034.4604 |
| 1048.5816 | 1054.1781 | 1058.1067 |
| 1058.4503 | 1061.6684 | 1069.2592 |
| 1077.3808 | 1081.7988 | 1092.4972 |
| 1106.8245 | 1117.8043 | 1123.8149 |
| 1131.6758 | 1138.3362 | 1147.2790 |
| 1154.7806 | 1163.4608 | 1173.8770 |
| 1184.4601 | 1185.9740 | 1188.1984 |
| 1190.1434 | 1194.5263 | 1222.5310 |
| 1238.9261 | 1241.6559 | 1255.2462 |
| 1265.2480 | 1270.0066 | 1276.1835 |

| | | |
|---|---|---|
| 1276.9880 | 1282.1177 | 1294.0190 |
| 1307.4396 | 1311.8029 | 1315.7158 |
| 1319.0298 | 1323.9969 | 1329.8800 |
| 1336.9062 | 1339.9222 | 1341.9013 |
| 1344.4779 | 1346.6116 | 1361.0892 |
| 1376.3815 | 1395.3785 | 1403.5352 |
| 1404.7024 | 1405.8191 | 1406.4137 |
| 1408.3099 | 1415.8861 | 1417.5714 |
| 1421.6679 | 1422.9098 | 1432.0846 |
| 1436.3911 | 1437.5405 | 1448.4899 |
| 1464.2204 | 1473.7725 | 1479.6551 |
| 1480.2391 | 1481.0910 | 1483.8998 |
| 1484.5119 | 1487.9622 | 1491.1191 |
| 1491.7241 | 1494.4459 | 1497.3359 |
| 1497.6318 | 1498.0969 | 1500.5464 |
| 1507.6487 | 1514.6375 | 1528.6490 |
| 1533.9695 | 1537.6209 | 1541.9124 |
| 1543.9303 | 1604.2098 | 1612.4797 |
| 1621.4764 | 1623.3833 | 1666.0999 |
| 1667.7312 | 1724.2491 | 1907.2317 |
| 2901.3922 | 3000.3066 | 3010.7548 |
| 3012.4354 | 3019.4118 | 3021.9917 |
| 3026.0350 | 3031.6999 | 3033.6075 |
| 3041.2288 | 3042.1417 | 3043.0742 |
| 3047.4174 | 3052.0655 | 3055.4116 |
| 3062.6426 | 3071.8824 | 3072.1790 |
| 3079.5797 | 3086.7750 | 3093.5270 |
| 3099.5606 | 3101.6323 | 3113.4549 |
| 3117.1149 | 3123.7809 | 3124.7932 |
| 3126.0842 | 3139.0573 | 3139.2848 |

| | | |
|---|---|---|
| 3148.5901 | 3152.9610 | 3183.9535 |
| 3185.4873 | 3192.2350 | 3194.3764 |
| 3206.1714 | 3208.3252 | 3209.7090 |
| 3211.3769 | 3218.5592 | 3221.1202 |

**M1**

Zero-point correction= 0.708069

Thermal correction to Energy= 0.753344

Thermal correction to Enthalpy= 0.754288

Thermal correction to Gibbs Free Energy= 0.622357

Sum of electronic and zero-point Energies= -1744.840350

Sum of electronic and thermal Energies= -1744.795075

Sum of electronic and thermal Enthalpies= -1744.794131

Sum of electronic and thermal Free Energies= -1744.926062

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.202746 | -0.988453 | -0.742416 |
| B | 0.766153 | 0.111801 | -1.049941 |
| C | -0.305029 | -1.463873 | 0.525346 |
| O | -0.881424 | 1.889312 | 1.110326 |
| C | -1.264157 | -0.943748 | 1.385575 |
| C | 0.528036 | -2.532081 | 0.976406 |
| C | -2.115703 | 1.363331 | 0.858285 |
| C | -2.319414 | -0.009520 | 0.884471 |
| C | 0.474000 | -2.988617 | 2.269597 |
| C | -1.335591 | -1.393804 | 2.743152 |
| C | -0.436844 | -2.413473 | 3.193386 |
| C | -3.210413 | 2.225213 | 0.552948 |
| C | -3.584698 | -0.555943 | 0.492364 |
| C | -4.442425 | 1.732276 | 0.202681 |
| C | -4.651885 | 0.329277 | 0.133027 |

| | | | |
|---|---|---|---|
| H | 1.115256 | -3.798736 | 2.600415 |
| H | -5.264431 | 2.400034 | -0.033677 |
| C | -5.902409 | -0.209966 | -0.275981 |
| C | -6.094061 | -1.572152 | -0.338825 |
| C | -5.040381 | -2.451565 | 0.012555 |
| C | -3.820355 | -1.958409 | 0.422348 |
| H | -6.702684 | 0.475354 | -0.542888 |
| H | -7.050703 | -1.975396 | -0.658136 |
| H | -5.197278 | -3.525204 | -0.040969 |
| H | -3.020999 | -2.641170 | 0.688643 |
| C | -0.496954 | -2.857073 | 4.542777 |
| C | -1.410642 | -2.316879 | 5.419879 |
| C | -2.303659 | -1.309539 | 4.978279 |
| C | -2.270417 | -0.861591 | 3.675410 |
| H | 0.192574 | -3.632035 | 4.867360 |
| H | -1.449348 | -2.659331 | 6.449913 |
| H | -3.020703 | -0.885290 | 5.675484 |
| H | -2.954951 | -0.085341 | 3.351313 |
| I | -2.919738 | 4.348771 | 0.665265 |
| I | 1.816535 | -3.541388 | -0.409696 |
| H | -0.399591 | 1.855037 | 0.243184 |
| O | 0.091111 | 1.350346 | -1.360429 |
| C | 1.906309 | 0.369616 | 0.028736 |
| C | 3.187228 | -0.011702 | -0.047538 |
| H | 1.611401 | 0.927134 | 0.922277 |
| H | 3.518598 | -0.579340 | -0.919375 |
| C | 4.257579 | 0.282730 | 0.967943 |
| C | 5.363277 | 1.199470 | 0.411972 |
| H | 4.719757 | -0.660053 | 1.298144 |
| H | 3.810436 | 0.745105 | 1.857607 |

| | | | |
|---|---|---|---|
| C | 6.477575 | 1.484845 | 1.425105 |
| H | 5.796192 | 0.741367 | -0.488962 |
| H | 4.910150 | 2.146235 | 0.087204 |
| H | 6.038864 | 1.934430 | 2.327499 |
| H | 6.928159 | 0.534482 | 1.745887 |
| C | 7.572535 | 2.408529 | 0.880275 |
| C | 8.684901 | 2.703146 | 1.894035 |
| H | 7.119738 | 3.356659 | 0.555684 |
| H | 8.014113 | 1.957911 | -0.020647 |
| C | 9.771789 | 3.627320 | 1.338021 |
| H | 8.243336 | 3.154837 | 2.793289 |
| H | 9.138189 | 1.756334 | 2.219111 |
| H | 10.552915 | 3.824591 | 2.080888 |
| H | 10.254455 | 3.185947 | 0.457501 |
| H | 9.351413 | 4.593454 | 1.033429 |
| C | -1.010009 | 1.341812 | -2.281564 |
| C | -1.233679 | 2.753410 | -2.792480 |
| H | -1.907541 | 0.959432 | -1.783156 |
| H | -0.801531 | 0.665925 | -3.119627 |
| H | -2.080396 | 2.778057 | -3.487204 |
| H | -1.449926 | 3.434633 | -1.964633 |
| H | -0.344135 | 3.119881 | -3.315902 |
| C | 2.952218 | -0.376549 | -4.263437 |
| C | 2.114016 | 0.442783 | -3.304450 |
| H | 3.498941 | 0.293229 | -4.934749 |
| H | 3.674472 | -0.992884 | -3.719986 |
| H | 2.322640 | -1.031155 | -4.875921 |
| H | 2.723443 | 1.082878 | -2.666671 |
| H | 1.379513 | 1.062889 | -3.825832 |
| O | 1.415743 | -0.460127 | -2.395392 |

| | | | |
|---|---|---|---|
| H | 0.757883 | -1.058396 | -2.887408 |
| C | -1.881606 | -3.875150 | -3.345255 |
| C | -0.562653 | -3.202448 | -3.685516 |
| H | -1.873878 | -4.918299 | -3.678953 |
| H | -2.051516 | -3.867410 | -2.261871 |
| H | -2.717313 | -3.359078 | -3.828387 |
| H | 0.275869 | -3.724304 | -3.208110 |
| H | -0.388121 | -3.194074 | -4.765592 |
| O | -0.571807 | -1.816787 | -3.280142 |
| H | -0.846274 | -1.764982 | -2.340823 |

Vibrational frequencies

| | | |
|---|---|---|
| 5.5125 | 11.1935 | 14.7157 |
| 24.9724 | 27.1998 | 32.2572 |
| 39.2694 | 45.9106 | 47.9452 |
| 51.2344 | 56.5209 | 59.1475 |
| 61.7943 | 70.4423 | 75.1726 |
| 83.5204 | 85.3159 | 88.2592 |
| 97.0589 | 104.7396 | 113.1165 |
| 118.8292 | 126.9006 | 137.3186 |
| 139.7582 | 144.3676 | 150.3728 |
| 156.0386 | 161.0245 | 165.2098 |
| 168.1482 | 175.1913 | 186.8369 |
| 189.1122 | 203.9293 | 206.4661 |
| 221.1093 | 225.5645 | 236.2142 |
| 251.4049 | 260.1146 | 263.0523 |
| 275.7937 | 279.8630 | 283.8238 |
| 284.5275 | 302.3216 | 308.1524 |
| 342.1579 | 352.8890 | 360.7881 |
| 368.2216 | 370.3607 | 380.0919 |

| | | |
|---|---|---|
| 391.3186 | 435.2523 | 444.2594 |
| 449.3956 | 457.0985 | 459.6836 |
| 471.2754 | 485.8994 | 502.9860 |
| 528.1322 | 537.4044 | 547.8713 |
| 562.6030 | 565.6863 | 577.3667 |
| 587.2727 | 607.9895 | 615.0921 |
| 630.7940 | 634.0696 | 653.1551 |
| 676.3066 | 698.1630 | 713.5293 |
| 719.8148 | 742.3279 | 745.1406 |
| 749.0573 | 754.7408 | 757.5524 |
| 765.1078 | 767.5276 | 789.0083 |
| 798.4223 | 800.6958 | 820.6909 |
| 823.8564 | 828.1775 | 829.9186 |
| 831.0165 | 832.2704 | 873.8899 |
| 874.3964 | 882.0691 | 898.0948 |
| 902.0176 | 903.9643 | 906.4980 |
| 908.1128 | 908.2776 | 911.9703 |
| 948.7119 | 968.6086 | 969.3756 |
| 982.1661 | 990.1656 | 999.2507 |
| 1000.5576 | 1003.2065 | 1015.8630 |
| 1018.6738 | 1025.2296 | 1033.5836 |
| 1041.9290 | 1049.5174 | 1055.3407 |
| 1056.9834 | 1057.9834 | 1059.5458 |
| 1065.5089 | 1071.2745 | 1078.1908 |
| 1105.2674 | 1111.2312 | 1122.6756 |
| 1128.4882 | 1136.7763 | 1147.2471 |
| 1148.0929 | 1162.4094 | 1162.8604 |
| 1183.9452 | 1185.2966 | 1186.5043 |
| 1188.4182 | 1202.1605 | 1220.3326 |
| 1238.5703 | 1241.3045 | 1248.7828 |

| | | |
|---|---|---|
| 1263.7938 | 1272.9474 | 1275.7777 |
| 1283.0029 | 1297.0562 | 1301.2892 |
| 1304.2714 | 1313.8147 | 1319.9111 |
| 1323.5341 | 1331.9688 | 1334.7660 |
| 1339.8242 | 1342.4455 | 1347.9474 |
| 1359.5634 | 1368.8519 | 1387.7129 |
| 1394.6777 | 1398.7194 | 1400.8160 |
| 1404.0723 | 1406.6051 | 1407.4995 |
| 1409.8497 | 1415.5897 | 1417.5900 |
| 1423.7119 | 1429.9303 | 1431.2497 |
| 1437.5745 | 1442.9243 | 1449.0980 |
| 1458.6217 | 1477.2318 | 1478.4532 |
| 1479.9414 | 1481.7456 | 1481.8511 |
| 1485.6911 | 1488.0408 | 1491.6103 |
| 1493.9988 | 1494.4775 | 1494.9782 |
| 1497.7830 | 1498.4062 | 1506.2763 |
| 1513.3572 | 1518.6064 | 1527.0066 |
| 1535.6070 | 1541.7940 | 1542.6734 |
| 1591.8008 | 1605.0651 | 1609.5021 |
| 1621.6013 | 1622.0144 | 1666.5957 |
| 1667.2848 | 1725.0739 | 2855.3807 |
| 3004.2307 | 3008.4357 | 3010.8138 |
| 3017.5434 | 3020.6884 | 3031.7853 |
| 3032.1973 | 3041.2680 | 3042.7930 |
| 3046.2435 | 3049.4633 | 3051.4665 |
| 3051.6677 | 3054.8423 | 3061.6374 |
| 3071.5106 | 3088.3411 | 3093.5194 |
| 3099.2640 | 3101.8026 | 3102.9495 |
| 3106.0449 | 3118.6849 | 3120.8667 |
| 3122.5963 | 3127.5762 | 3129.7094 |

| | | |
|---|---|---|
| 3135.8136 | 3137.2663 | 3168.3110 |
| 3183.5356 | 3184.0579 | 3191.6088 |
| 3192.7863 | 3206.9356 | 3207.0749 |
| 3209.7328 | 3210.7967 | 3219.1528 |
| 3219.2389 | 3301.6973 | 3579.1803 |

**TS2**

Zero-point correction= 0.703720

Thermal correction to Energy= 0.748629

Thermal correction to Enthalpy= 0.749573

Thermal correction to Gibbs Free Energy= 0.620660

Sum of electronic and zero-point Energies= -1744.827401

Sum of electronic and thermal Energies= -1744.782491

Sum of electronic and thermal Enthalpies= -1744.781547

Sum of electronic and thermal Free Energies= -1744.910460

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.675608 | -0.435910 | -1.453934 |
| B | -0.424153 | -1.241932 | -0.235675 |
| C | -1.853272 | 0.239428 | -1.393480 |
| O | -0.052605 | -0.195879 | 0.926934 |
| C | -1.971610 | 1.318031 | -0.522655 |
| C | -2.972805 | -0.185941 | -2.156682 |
| C | 0.227352 | 1.131354 | 0.690149 |
| C | -0.718560 | 1.914293 | 0.024819 |
| C | -4.209631 | 0.382354 | -1.980739 |
| C | -3.271725 | 1.847255 | -0.232944 |
| C | -4.398339 | 1.376647 | -0.983247 |
| C | 1.451369 | 1.716145 | 1.127760 |
| C | -0.428887 | 3.297545 | -0.251553 |
| C | 1.690097 | 3.058801 | 0.960836 |

| | | | |
|---|---|---|---|
| C | 0.766277 | 3.881210 | 0.274777 |
| H | -5.063149 | 0.052399 | -2.563602 |
| H | 2.616537 | 3.499788 | 1.312100 |
| C | 1.049447 | 5.257119 | 0.050043 |
| C | 0.199433 | 6.033775 | -0.701689 |
| C | -0.958194 | 5.451464 | -1.273048 |
| C | -1.263391 | 4.125387 | -1.058234 |
| H | 1.959280 | 5.675291 | 0.472409 |
| H | 0.421577 | 7.082564 | -0.875351 |
| H | -1.610814 | 6.055686 | -1.896744 |
| H | -2.146078 | 3.705306 | -1.522208 |
| C | -5.693958 | 1.887635 | -0.697332 |
| C | -5.881864 | 2.805629 | 0.311625 |
| C | -4.774863 | 3.251446 | 1.075131 |
| C | -3.503788 | 2.792101 | 0.805687 |
| H | -6.536253 | 1.523126 | -1.279319 |
| H | -6.877156 | 3.180206 | 0.532203 |
| H | -4.930445 | 3.961199 | 1.882652 |
| H | -2.665056 | 3.138157 | 1.399776 |
| I | 3.065476 | 0.574458 | 1.963843 |
| I | -2.710666 | -1.773921 | -3.569582 |
| H | 0.432001 | -0.923419 | 1.782230 |
| O | 0.798039 | -2.002656 | -0.372815 |
| C | -1.709299 | -2.059408 | 0.261426 |
| C | -2.541907 | -1.702234 | 1.248283 |
| H | -1.966543 | -2.965133 | -0.296556 |
| H | -2.323138 | -0.789255 | 1.806868 |
| C | -3.826882 | -2.380793 | 1.638082 |
| C | -5.040220 | -1.476972 | 1.343856 |
| H | -3.817764 | -2.616566 | 2.713345 |

| | | | |
|---|---|---|---|
| H | -3.934455 | -3.332981 | 1.102421 |
| C | -6.375691 | -2.055315 | 1.820579 |
| H | -4.881251 | -0.498085 | 1.816993 |
| H | -5.081914 | -1.285275 | 0.264373 |
| H | -6.531981 | -3.043485 | 1.364515 |
| H | -6.332839 | -2.223108 | 2.906576 |
| C | -7.568746 | -1.149612 | 1.492760 |
| C | -8.908932 | -1.689595 | 2.005162 |
| H | -7.626954 | -1.007768 | 0.403860 |
| H | -7.393551 | -0.150870 | 1.918025 |
| C | -10.089714 | -0.773195 | 1.672151 |
| H | -9.084958 | -2.686297 | 1.577404 |
| H | -8.849321 | -1.830678 | 3.093391 |
| H | -11.035534 | -1.180876 | 2.046536 |
| H | -9.956667 | 0.220325 | 2.117351 |
| H | -10.191672 | -0.637344 | 0.588670 |
| C | 0.808690 | -3.101186 | -1.294433 |
| C | 0.922739 | -4.422877 | -0.549439 |
| H | 1.655822 | -2.952277 | -1.971470 |
| H | -0.095514 | -3.087097 | -1.914293 |
| H | 0.969930 | -5.261577 | -1.253210 |
| H | 1.832220 | -4.443496 | 0.062723 |
| H | 0.058156 | -4.573619 | 0.106440 |
| C | 1.007585 | -3.837584 | 3.738495 |
| C | 0.139642 | -2.716358 | 3.207935 |
| H | 0.438396 | -4.426323 | 4.465178 |
| H | 1.318503 | -4.506431 | 2.928861 |
| H | 1.900758 | -3.442600 | 4.231256 |
| H | -0.756036 | -3.083789 | 2.703986 |
| H | -0.158023 | -2.020771 | 3.995384 |

| | | | |
|---|---|---|---|
| O | 0.913659 | -1.908763 | 2.266187 |
| H | 1.076027 | -2.376992 | 1.405253 |
| C | 2.354980 | 1.544039 | -2.378737 |
| C | 2.529441 | 0.027893 | -2.376282 |
| H | 3.127736 | 2.032807 | -1.774370 |
| H | 2.414168 | 1.935924 | -3.400246 |
| H | 1.379549 | 1.816739 | -1.964833 |
| H | 3.512186 | -0.236593 | -2.787420 |
| H | 2.491737 | -0.356755 | -1.347064 |
| O | 1.560450 | -0.626603 | -3.191272 |
| H | 0.714744 | -0.560252 | -2.713615 |

Vibrational frequencies

| | | |
|---|---|---|
| -660.0282 | 13.0799 | 20.7418 |
| 26.0818 | 28.9735 | 32.3384 |
| 35.5383 | 39.8876 | 43.1433 |
| 48.9585 | 52.5508 | 58.3096 |
| 61.5658 | 65.9918 | 73.2177 |
| 83.4387 | 86.1265 | 90.5259 |
| 94.0765 | 99.5044 | 100.2034 |
| 106.2771 | 108.7410 | 110.6858 |
| 124.8656 | 127.8243 | 144.8496 |
| 149.0416 | 153.7026 | 157.7601 |
| 163.7819 | 165.4286 | 171.2522 |
| 187.8187 | 189.7630 | 201.4719 |
| 212.4199 | 224.3825 | 226.0683 |
| 245.4213 | 256.9275 | 262.8325 |
| 276.7256 | 279.5227 | 283.0635 |
| 296.4781 | 300.8310 | 302.6195 |
| 317.0511 | 336.7271 | 344.6071 |

| | | |
|---|---|---|
| 361.2719 | 381.8206 | 405.2610 |
| 421.1510 | 426.0637 | 430.6823 |
| 439.0607 | 455.3514 | 457.7894 |
| 470.2835 | 480.7836 | 502.8087 |
| 516.1333 | 524.6457 | 550.9519 |
| 558.9934 | 564.3075 | 568.8294 |
| 571.0387 | 584.5359 | 598.9056 |
| 613.6149 | 633.0014 | 654.3222 |
| 657.6271 | 678.7124 | 712.5192 |
| 719.0958 | 740.9324 | 743.4148 |
| 756.3106 | 757.6075 | 765.7552 |
| 767.6274 | 771.8445 | 783.1924 |
| 790.0034 | 803.7164 | 807.9239 |
| 816.2144 | 819.7760 | 827.2315 |
| 830.1700 | 834.9292 | 848.8652 |
| 873.5536 | 875.7204 | 884.0230 |
| 896.9632 | 902.9036 | 904.4959 |
| 907.2689 | 907.7169 | 914.8647 |
| 916.7084 | 955.6825 | 970.3913 |
| 973.2084 | 981.1945 | 986.9741 |
| 998.8004 | 1001.9556 | 1011.2298 |
| 1022.4226 | 1028.0029 | 1030.5370 |
| 1036.5610 | 1046.5098 | 1059.2254 |
| 1059.6695 | 1062.0462 | 1068.1014 |
| 1069.9355 | 1071.1042 | 1075.4444 |
| 1085.4220 | 1099.1750 | 1105.4537 |
| 1108.7777 | 1122.6246 | 1136.6576 |
| 1144.2522 | 1146.3650 | 1149.4678 |
| 1164.8986 | 1184.2902 | 1189.5374 |
| 1194.7002 | 1198.7332 | 1218.3423 |

| | | |
|---|---|---|
| 1238.9541 | 1245.2538 | 1254.5351 |
| 1265.5510 | 1271.2955 | 1277.5153 |
| 1285.3051 | 1289.3706 | 1300.6786 |
| 1305.0268 | 1306.1043 | 1317.2555 |
| 1324.6034 | 1333.0011 | 1338.7722 |
| 1342.4039 | 1343.2073 | 1350.2820 |
| 1355.3267 | 1370.1510 | 1371.6735 |
| 1392.1861 | 1394.2949 | 1397.4042 |
| 1402.3205 | 1406.5288 | 1406.8632 |
| 1411.3268 | 1418.9942 | 1419.3695 |
| 1421.7194 | 1422.3060 | 1422.7269 |
| 1430.7734 | 1441.2280 | 1446.9229 |
| 1454.1775 | 1465.2754 | 1476.0283 |
| 1479.6005 | 1480.3755 | 1482.1103 |
| 1482.2725 | 1484.5753 | 1487.7501 |
| 1490.2763 | 1491.8079 | 1495.5120 |
| 1496.6838 | 1497.9190 | 1498.0814 |
| 1506.7170 | 1512.9203 | 1524.8197 |
| 1524.9078 | 1529.4915 | 1538.3188 |
| 1540.8280 | 1595.4967 | 1606.9285 |
| 1618.2071 | 1621.4430 | 1666.5770 |
| 1668.6467 | 1716.0810 | 1762.1982 |
| 3002.9353 | 3009.6672 | 3012.1808 |
| 3017.8049 | 3020.6933 | 3027.2699 |
| 3031.5045 | 3032.6985 | 3034.6859 |
| 3042.9250 | 3045.1005 | 3052.3036 |
| 3053.5066 | 3054.7642 | 3061.6615 |
| 3062.4608 | 3078.7455 | 3090.5401 |
| 3097.5681 | 3098.4581 | 3100.4150 |
| 3102.9440 | 3109.9806 | 3111.9447 |

| | | |
|---|---|---|
| 3118.0862 | 3120.2290 | 3126.1534 |
| 3133.6919 | 3135.1843 | 3163.7890 |
| 3185.0601 | 3185.5504 | 3193.1667 |
| 3194.4324 | 3207.4501 | 3209.3739 |
| 3211.0070 | 3211.7139 | 3218.9964 |
| 3241.9202 | 3366.1664 | 3675.0082 |

**M2**

Zero-point correction= 0.709272

Thermal correction to Energy= 0.754360

Thermal correction to Enthalpy= 0.755305

Thermal correction to Gibbs Free Energy= 0.626999

Sum of electronic and zero-point Energies= -1744.845892

Sum of electronic and thermal Energies= -1744.800804

Sum of electronic and thermal Enthalpies= -1744.799859

Sum of electronic and thermal Free Energies= -1744.928165

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.860356 | -0.606934 | -1.111664 |
| B | -0.625288 | -1.112681 | 0.262152 |
| C | -2.019684 | 0.103870 | -1.177547 |
| O | -0.239173 | -0.051156 | 1.189016 |
| C | -2.101978 | 1.332410 | -0.529362 |
| C | -3.151508 | -0.437117 | -1.842925 |
| C | 0.012228 | 1.218616 | 0.817156 |
| C | -0.845651 | 1.950102 | -0.013328 |
| C | -4.372578 | 0.185821 | -1.786803 |
| C | -3.389508 | 1.949642 | -0.368410 |
| C | -4.529276 | 1.368292 | -1.015458 |
| C | 1.168564 | 1.860420 | 1.354386 |
| C | -0.477627 | 3.282102 | -0.416227 |

| | | | |
|---|---|---|---|
| C | 1.481327 | 3.162686 | 1.065787 |
| C | 0.678995 | 3.901108 | 0.159036 |
| H | -5.236758 | -0.233289 | -2.291410 |
| H | 2.360421 | 3.632186 | 1.494367 |
| C | 1.040342 | 5.223542 | -0.216663 |
| C | 0.310096 | 5.912592 | -1.157865 |
| C | -0.805992 | 5.290910 | -1.767881 |
| C | -1.189459 | 4.016744 | -1.408667 |
| H | 1.916773 | 5.671926 | 0.244095 |
| H | 0.595942 | 6.919906 | -1.446341 |
| H | -1.363258 | 5.821227 | -2.535053 |
| H | -2.037655 | 3.559051 | -1.902514 |
| C | -5.811163 | 1.961936 | -0.851635 |
| C | -5.976627 | 3.072774 | -0.055760 |
| C | -4.859095 | 3.634681 | 0.608351 |
| C | -3.601639 | 3.091986 | 0.454021 |
| H | -6.661515 | 1.508023 | -1.353630 |
| H | -6.960940 | 3.513668 | 0.072171 |
| H | -4.995662 | 4.499349 | 1.251599 |
| H | -2.760145 | 3.529003 | 0.978559 |
| I | 2.478340 | 0.751844 | 2.641891 |
| I | -2.937801 | -2.274867 | -2.923349 |
| H | 0.917174 | -1.754377 | 2.919142 |
| O | 0.688320 | -1.960267 | 0.081738 |
| C | -1.824372 | -1.988623 | 0.839327 |
| C | -2.637606 | -1.569518 | 1.818850 |
| H | -2.096435 | -2.918613 | 0.332241 |
| H | -2.404585 | -0.624208 | 2.313673 |
| C | -3.943949 | -2.195874 | 2.222862 |
| C | -5.117578 | -1.339919 | 1.702605 |

| | | | |
|---|---|---|---|
| H | -4.015448 | -2.273418 | 3.317623 |
| H | -4.023866 | -3.213384 | 1.818321 |
| C | -6.502647 | -1.854300 | 2.104583 |
| H | -4.995366 | -0.308806 | 2.061856 |
| H | -5.047675 | -1.287260 | 0.608743 |
| H | -6.615743 | -2.898422 | 1.779150 |
| H | -6.587780 | -1.863503 | 3.200800 |
| C | -7.637459 | -1.011392 | 1.509301 |
| C | -9.037454 | -1.485374 | 1.915700 |
| H | -7.556290 | -1.021937 | 0.412609 |
| H | -7.507385 | 0.038056 | 1.810815 |
| C | -10.156002 | -0.637274 | 1.303585 |
| H | -9.165935 | -2.534593 | 1.615536 |
| H | -9.121254 | -1.468697 | 3.011131 |
| H | -11.146266 | -0.994156 | 1.608506 |
| H | -10.071053 | 0.411592 | 1.612775 |
| H | -10.116385 | -0.661441 | 0.207623 |
| C | 0.671266 | -3.120888 | -0.814738 |
| C | 2.093982 | -3.561738 | -1.077667 |
| H | 0.175889 | -2.784088 | -1.723002 |
| H | 0.067583 | -3.905803 | -0.349920 |
| H | 2.084263 | -4.451835 | -1.715559 |
| H | 2.636406 | -2.765545 | -1.591643 |
| H | 2.612394 | -3.815542 | -0.147380 |
| C | 1.119076 | -4.973480 | 2.532355 |
| C | 0.480099 | -3.696833 | 3.039153 |
| H | 0.594251 | -5.840461 | 2.946027 |
| H | 1.067723 | -5.034118 | 1.440865 |
| H | 2.169879 | -5.026078 | 2.833583 |
| H | -0.568767 | -3.622238 | 2.730308 |

| | | | |
|---|---|---|---|
| H | 0.523652 | -3.646210 | 4.133147 |
| O | 1.223619 | -2.574774 | 2.497128 |
| H | 0.981641 | -2.248569 | 1.020531 |
| C | 2.365031 | 1.646405 | -2.200417 |
| C | 2.454933 | 0.173259 | -1.817266 |
| H | 3.068797 | 2.250973 | -1.617138 |
| H | 2.591080 | 1.780503 | -3.264008 |
| H | 1.356857 | 2.028622 | -2.015878 |
| H | 3.464116 | -0.207041 | -2.020527 |
| H | 2.276274 | 0.047890 | -0.739770 |
| O | 1.555218 | -0.630119 | -2.577617 |
| H | 0.671713 | -0.509879 | -2.186528 |

Vibrational frequencies

| | | |
|---|---|---|
| 11.8380 | 21.6649 | 27.6150 |
| 32.2735 | 34.8897 | 42.4431 |
| 46.7050 | 50.2077 | 53.7490 |
| 55.3410 | 62.8810 | 70.7464 |
| 75.1502 | 77.5039 | 80.3368 |
| 87.8653 | 91.0185 | 94.8450 |
| 100.1194 | 102.8591 | 109.3456 |
| 111.8927 | 117.2615 | 126.8676 |
| 128.6386 | 133.0760 | 142.8429 |
| 149.9490 | 153.9730 | 158.0529 |
| 163.6345 | 175.2925 | 182.2642 |
| 190.9078 | 199.6782 | 205.6170 |
| 214.8264 | 225.4527 | 244.2251 |
| 260.1545 | 268.9532 | 273.9800 |
| 279.4934 | 286.0227 | 290.4622 |
| 292.7499 | 297.9455 | 316.5806 |

| | | |
|---|---|---|
| 336.3726 | 340.9491 | 354.5754 |
| 379.5113 | 381.7429 | 402.4110 |
| 422.0267 | 427.5547 | 433.5002 |
| 446.9963 | 457.1757 | 462.9681 |
| 475.9220 | 478.0384 | 502.1369 |
| 519.4249 | 521.9425 | 544.4179 |
| 560.4596 | 564.8759 | 568.6311 |
| 580.1169 | 582.8816 | 592.4415 |
| 620.6066 | 636.6097 | 655.8652 |
| 667.1806 | 675.2033 | 720.4441 |
| 734.0198 | 741.4625 | 748.2946 |
| 754.5940 | 759.8886 | 767.2159 |
| 769.0891 | 782.2314 | 784.3186 |
| 807.0211 | 816.2341 | 818.5167 |
| 825.0609 | 826.5508 | 832.0445 |
| 839.5085 | 854.1074 | 875.7782 |
| 876.6701 | 882.3113 | 889.9763 |
| 894.9840 | 902.2101 | 902.8050 |
| 907.6882 | 907.9930 | 912.1924 |
| 948.1266 | 969.7161 | 971.9170 |
| 974.7346 | 980.6138 | 994.3744 |
| 1000.1869 | 1001.2682 | 1013.6666 |
| 1026.8706 | 1029.3908 | 1035.9787 |
| 1044.6773 | 1048.4311 | 1056.9827 |
| 1060.7249 | 1066.6537 | 1067.7497 |
| 1072.5316 | 1073.0741 | 1078.8115 |
| 1088.3807 | 1108.9804 | 1109.9254 |
| 1132.5051 | 1134.2834 | 1137.3247 |
| 1143.2752 | 1143.6024 | 1164.5512 |
| 1183.9334 | 1184.2521 | 1190.4409 |

| | | |
|---|---|---|
| 1194.0934 | 1207.5242 | 1219.2980 |
| 1237.8894 | 1241.1177 | 1252.7509 |
| 1268.4616 | 1272.3138 | 1275.1623 |
| 1285.1755 | 1290.2771 | 1302.2364 |
| 1304.4870 | 1305.3312 | 1309.8995 |
| 1314.7917 | 1328.0059 | 1331.7127 |
| 1333.8981 | 1343.3297 | 1345.1038 |
| 1354.5804 | 1363.9363 | 1366.7233 |
| 1397.4147 | 1398.7818 | 1403.1571 |
| 1403.4833 | 1404.9958 | 1405.5318 |
| 1410.7112 | 1418.0566 | 1422.1169 |
| 1422.9027 | 1427.2358 | 1436.0444 |
| 1443.0219 | 1452.1272 | 1453.7903 |
| 1454.2893 | 1475.0988 | 1480.5241 |
| 1480.9059 | 1481.7978 | 1483.0071 |
| 1484.7655 | 1486.5110 | 1488.9497 |
| 1495.7084 | 1497.6631 | 1498.8715 |
| 1500.3016 | 1500.6848 | 1508.2105 |
| 1515.5027 | 1522.9360 | 1526.9040 |
| 1528.8400 | 1538.8377 | 1540.5961 |
| 1590.2939 | 1604.6371 | 1618.5157 |
| 1623.3999 | 1633.8488 | 1666.8489 |
| 1667.4048 | 1713.1035 | 2722.8529 |
| 3009.6959 | 3011.9042 | 3013.6225 |
| 3021.9678 | 3022.5389 | 3028.6832 |
| 3032.5100 | 3034.0743 | 3043.7194 |
| 3047.2103 | 3051.3215 | 3055.2006 |
| 3055.8997 | 3058.5368 | 3062.1126 |
| 3063.9611 | 3081.6125 | 3088.6546 |
| 3096.0828 | 3098.9358 | 3102.6538 |

| | | |
|---|---|---|
| 3104.7559 | 3112.9663 | 3123.4759 |
| 3129.2592 | 3133.7812 | 3135.8794 |
| 3140.4647 | 3157.3576 | 3184.5263 |
| 3184.6130 | 3190.1712 | 3192.7864 |
| 3193.6014 | 3207.3348 | 3209.3188 |
| 3210.2281 | 3210.2633 | 3225.4651 |
| 3230.2520 | 3667.8431 | 3746.0195 |

**M03**

Zero-point correction= 0.460558

Thermal correction to Energy= 0.490802

Thermal correction to Enthalpy= 0.491746

Thermal correction to Gibbs Free Energy= 0.394028

Sum of electronic and zero-point Energies= -1279.861150

Sum of electronic and thermal Energies= -1279.830906

Sum of electronic and thermal Enthalpies= -1279.829962

Sum of electronic and thermal Free Energies= -1279.927680

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | 0.083357 | 0.299228 | -1.905811 |
| B | 0.532397 | 1.326051 | -1.081314 |
| C | -0.953946 | -0.498764 | -1.489106 |
| O | -0.377746 | 2.077508 | -0.348376 |
| C | -2.194457 | 0.031941 | -1.157541 |
| C | -0.712877 | -1.895808 | -1.391771 |
| C | -1.578303 | 2.428627 | -0.913815 |
| C | -2.464139 | 1.476774 | -1.401973 |
| C | -1.682123 | -2.746439 | -0.923773 |
| C | -3.182111 | -0.825813 | -0.558511 |
| C | -2.924416 | -2.232089 | -0.469847 |
| C | -1.877088 | 3.814866 | -1.004122 |

| | | | |
|---|---|---|---|
| C | -3.610602 | 1.914184 | -2.153196 |
| C | -3.022121 | 4.248453 | -1.622516 |
| C | -3.897715 | 3.315452 | -2.236712 |
| H | -1.500237 | -3.813993 | -0.861252 |
| H | -3.254332 | 5.306427 | -1.681666 |
| C | -5.040371 | 3.760122 | -2.956951 |
| C | -5.857316 | 2.861468 | -3.603945 |
| C | -5.553009 | 1.479282 | -3.562791 |
| C | -4.463648 | 1.017392 | -2.856446 |
| H | -5.245787 | 4.826569 | -2.996468 |
| H | -6.724523 | 3.208762 | -4.157824 |
| H | -6.182605 | 0.774520 | -4.098308 |
| H | -4.243195 | -0.043061 | -2.847599 |
| C | -3.903019 | -3.095075 | 0.096104 |
| C | -5.083118 | -2.590155 | 0.592085 |
| C | -5.323122 | -1.195432 | 0.550322 |
| C | -4.401587 | -0.337447 | -0.009749 |
| H | -3.691783 | -4.160058 | 0.140908 |
| H | -5.823389 | -3.254358 | 1.028221 |
| H | -6.241852 | -0.795395 | 0.969555 |
| H | -4.601511 | 0.726972 | -0.020630 |
| C | 2.030762 | 1.649045 | -0.975436 |
| C | 2.967319 | 0.970523 | -1.665180 |
| H | 2.343836 | 2.475049 | -0.335074 |
| H | 2.644198 | 0.149241 | -2.305875 |
| C | 4.445003 | 1.210163 | -1.631146 |
| C | 5.223764 | -0.051655 | -1.206927 |
| H | 4.682410 | 2.045339 | -0.960956 |
| H | 4.779772 | 1.499585 | -2.639003 |
| C | 6.742991 | 0.149808 | -1.224879 |

| | | | |
|---|---|---|---|
| H | 4.902722 | -0.350945 | -0.200386 |
| H | 4.956525 | -0.881450 | -1.875535 |
| H | 7.054805 | 0.460215 | -2.232444 |
| H | 7.008183 | 0.978513 | -0.553060 |
| C | 7.522354 | -1.105622 | -0.815955 |
| C | 9.043547 | -0.911367 | -0.831755 |
| H | 7.255930 | -1.933668 | -1.488790 |
| H | 7.207713 | -1.417503 | 0.190432 |
| C | 9.812260 | -2.171160 | -0.423097 |
| H | 9.357678 | -0.599706 | -1.837618 |
| H | 9.309190 | -0.084483 | -0.158623 |
| H | 10.895283 | -2.004894 | -0.438510 |
| H | 9.539020 | -2.490049 | 0.590104 |
| H | 9.594164 | -3.005418 | -1.100881 |
| I | -0.514050 | 5.247037 | -0.179323 |
| I | 1.189876 | -2.690918 | -1.970159 |

Vibrational frequencies

| | | |
|---|---|---|
| 10.0577 | 13.5180 | 26.8652 |
| 28.5338 | 40.4678 | 48.5572 |
| 53.0619 | 61.1816 | 83.3070 |
| 85.8293 | 95.3028 | 101.7667 |
| 107.7132 | 123.0590 | 128.7307 |
| 147.5861 | 152.7200 | 157.0306 |
| 168.5579 | 179.0622 | 197.0965 |
| 197.8709 | 219.6211 | 227.1726 |
| 266.2720 | 272.0509 | 280.8631 |
| 291.3080 | 317.0177 | 333.6620 |
| 338.6397 | 353.9433 | 386.7549 |
| 396.5098 | 431.6086 | 447.0077 |

| | | |
|---|---|---|
| 454.1351 | 461.0954 | 478.7154 |
| 509.3890 | 516.0839 | 525.0258 |
| 553.4986 | 560.1555 | 566.1092 |
| 583.9226 | 594.1768 | 607.8279 |
| 632.4236 | 647.8694 | 657.4470 |
| 678.4011 | 714.5464 | 734.7397 |
| 743.9529 | 746.5047 | 750.9874 |
| 756.0676 | 769.3938 | 771.1361 |
| 782.4824 | 799.1392 | 804.9684 |
| 826.9874 | 846.1480 | 863.6771 |
| 878.5365 | 880.4282 | 883.5638 |
| 908.1581 | 911.5744 | 912.0148 |
| 913.3518 | 951.4976 | 974.7982 |
| 977.5513 | 978.1074 | 997.3369 |
| 1003.7464 | 1005.6087 | 1013.7328 |
| 1021.1428 | 1029.9440 | 1048.7003 |
| 1059.6238 | 1062.3406 | 1064.7654 |
| 1071.9518 | 1078.4531 | 1107.3652 |
| 1135.4537 | 1141.3988 | 1164.6096 |
| 1184.8490 | 1190.2367 | 1198.9009 |
| 1207.5045 | 1227.8565 | 1239.9214 |
| 1242.9641 | 1253.6562 | 1255.6398 |
| 1263.2125 | 1276.2737 | 1286.2034 |
| 1286.8172 | 1302.2699 | 1308.2322 |
| 1319.1815 | 1337.8982 | 1338.3622 |
| 1344.6228 | 1347.2631 | 1355.8773 |
| 1363.9517 | 1373.2937 | 1400.5596 |
| 1402.5307 | 1405.6093 | 1408.0662 |
| 1418.8299 | 1423.9811 | 1427.8240 |
| 1450.1567 | 1455.5002 | 1473.8198 |

| | | |
|---|---|---|
| 1475.2733 | 1481.4650 | 1482.1392 |
| 1485.7792 | 1495.2615 | 1500.2376 |
| 1505.5883 | 1512.9706 | 1541.9144 |
| 1543.0160 | 1602.8759 | 1613.1850 |
| 1620.4462 | 1622.6368 | 1667.9117 |
| 1668.7347 | 1694.3225 | 3009.8844 |
| 3011.4840 | 3013.7140 | 3021.2461 |
| 3026.7939 | 3032.2353 | 3034.5890 |
| 3045.6678 | 3058.5745 | 3067.1972 |
| 3080.4253 | 3099.1137 | 3104.1196 |
| 3142.3551 | 3158.2237 | 3186.8618 |
| 3187.9223 | 3196.0317 | 3196.7061 |
| 3209.7148 | 3210.4628 | 3214.9362 |
| 3215.6739 | 3234.0900 | 3234.7470 |

**Pre-TS3S**

Zero-point correction= 0.499844

Thermal correction to Energy= 0.538313

Thermal correction to Enthalpy= 0.539257

Thermal correction to Gibbs Free Energy= 0.421785

Sum of electronic and zero-point Energies= -1765.614406

Sum of electronic and thermal Energies= -1765.575937

Sum of electronic and thermal Enthalpies= -1765.574993

Sum of electronic and thermal Free Energies= -1765.692465

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | 0.012470 | 0.392812 | -2.113200 |
| B | 0.524929 | 1.342421 | -1.227387 |
| C | -0.883397 | -0.534411 | -1.641079 |
| O | -0.311968 | 1.976716 | -0.321686 |

| | | | |
|---|---|---|---|
| C | -2.069616 | -0.152357 | -1.024747 |
| C | -0.548365 | -1.909857 | -1.771670 |
| C | -1.613873 | 2.260986 | -0.640600 |
| C | -2.495939 | 1.274926 | -1.057689 |
| C | -1.340192 | -2.883084 | -1.214418 |
| C | -2.843833 | -1.144915 | -0.329781 |
| C | -2.478687 | -2.524847 | -0.446222 |
| C | -2.028265 | 3.615607 | -0.537688 |
| C | -3.801347 | 1.659267 | -1.523696 |
| C | -3.300678 | 3.989019 | -0.887897 |
| C | -4.207168 | 3.029026 | -1.409532 |
| H | -1.085158 | -3.932309 | -1.319022 |
| H | -3.620538 | 5.021862 | -0.799958 |
| C | -5.504709 | 3.418671 | -1.842025 |
| C | -6.367205 | 2.500452 | -2.395639 |
| C | -5.956277 | 1.154388 | -2.549177 |
| C | -4.710890 | 0.744185 | -2.125020 |
| H | -5.795858 | 4.460284 | -1.736181 |
| H | -7.354955 | 2.806594 | -2.727439 |
| H | -6.628354 | 0.437149 | -3.011475 |
| H | -4.414133 | -0.288388 | -2.262664 |
| C | -3.239537 | -3.515798 | 0.233603 |
| C | -4.301796 | -3.159613 | 1.032665 |
| C | -4.638211 | -1.792984 | 1.188460 |
| C | -3.934004 | -0.812687 | 0.523511 |
| H | -2.953183 | -4.558049 | 0.121268 |
| H | -4.872889 | -3.920559 | 1.556271 |
| H | -5.457980 | -1.512888 | 1.843596 |
| H | -4.200038 | 0.227469 | 0.665002 |
| C | 2.014481 | 1.708547 | -1.213528 |

| | | | |
|---|---|---|---|
| C | 2.937167 | 1.078477 | -1.962663 |
| H | 2.345453 | 2.485614 | -0.523493 |
| H | 2.609100 | 0.291856 | -2.641474 |
| C | 4.417453 | 1.290602 | -1.892533 |
| C | 5.119301 | 0.046585 | -1.304773 |
| H | 4.649568 | 2.171254 | -1.281398 |
| H | 4.815556 | 1.474508 | -2.900810 |
| C | 6.642269 | 0.196722 | -1.230068 |
| H | 4.712429 | -0.149266 | -0.304940 |
| H | 4.866524 | -0.831490 | -1.914761 |
| H | 7.038125 | 0.390247 | -2.237284 |
| H | 6.891543 | 1.081467 | -0.627218 |
| C | 7.338007 | -1.034308 | -0.637503 |
| C | 8.863682 | -0.897326 | -0.564836 |
| H | 7.082431 | -1.919852 | -1.237262 |
| H | 6.942523 | -1.224652 | 0.370616 |
| C | 9.548917 | -2.133984 | 0.023555 |
| H | 9.257235 | -0.704210 | -1.572386 |
| H | 9.119003 | -0.014474 | 0.037398 |
| H | 10.637087 | -2.010813 | 0.063265 |
| H | 9.198853 | -2.332491 | 1.043752 |
| H | 9.337363 | -3.026908 | -0.577111 |
| C | 0.318132 | -0.956742 | 1.475535 |
| H | -0.044934 | -1.895488 | 1.082313 |
| C | 1.764642 | -0.672707 | 1.616847 |
| N | -0.548369 | -0.093154 | 1.903251 |
| N | -1.332546 | 0.656712 | 2.250714 |
| I | -0.642185 | 5.089382 | 0.162897 |
| I | 1.218810 | -2.488679 | -2.829674 |
| F | 2.442520 | -1.119512 | 0.532159 |

| | | | |
|---|---|---|---|
| F | 2.337749 | -1.287328 | 2.687573 |
| F | 2.007592 | 0.649788 | 1.757260 |

Vibrational frequencies

| | | |
|---|---|---|
| 10.5020 | 13.3475 | 16.1575 |
| 25.2344 | 28.9036 | 31.4948 |
| 38.6689 | 47.0333 | 53.2457 |
| 55.2925 | 58.2590 | 64.7084 |
| 69.3273 | 83.4654 | 89.1316 |
| 92.2671 | 96.2281 | 102.0097 |
| 110.4831 | 112.0193 | 134.6865 |
| 135.5650 | 154.0966 | 157.4370 |
| 159.4549 | 160.8013 | 169.0018 |
| 179.2085 | 198.4194 | 203.3201 |
| 222.8129 | 231.2946 | 264.0039 |
| 277.9179 | 284.1923 | 295.2667 |
| 317.7577 | 328.3964 | 333.1779 |
| 341.8758 | 354.3378 | 364.8530 |
| 389.0356 | 396.4290 | 431.1786 |
| 446.3688 | 454.7503 | 458.6834 |
| 467.7684 | 478.1802 | 481.3094 |
| 506.8640 | 518.5092 | 521.8468 |
| 537.3282 | 547.3800 | 554.4996 |
| 560.3701 | 566.6628 | 584.2368 |
| 590.6908 | 595.4611 | 609.2163 |
| 634.9512 | 648.3001 | 658.4243 |
| 677.6920 | 694.5379 | 715.9844 |
| 736.4713 | 746.5838 | 747.1796 |
| 750.5148 | 760.1635 | 767.4827 |
| 768.9832 | 783.2456 | 801.7568 |

| | | |
|---|---|---|
| 811.6923 | 827.3655 | 846.6714 |
| 863.8999 | 869.5409 | 874.5081 |
| 875.5091 | 883.3029 | 905.8656 |
| 908.5427 | 909.3595 | 910.6371 |
| 951.7601 | 971.7513 | 974.3760 |
| 976.4914 | 996.7558 | 1002.2681 |
| 1004.0618 | 1013.0083 | 1020.5391 |
| 1023.8338 | 1044.7720 | 1057.8591 |
| 1060.9254 | 1063.3595 | 1068.2395 |
| 1075.0111 | 1107.4350 | 1112.3038 |
| 1133.0919 | 1141.6644 | 1152.9417 |
| 1165.1584 | 1185.0506 | 1190.2794 |
| 1198.3797 | 1207.5082 | 1209.8334 |
| 1229.5049 | 1239.5015 | 1242.6813 |
| 1253.1707 | 1254.1396 | 1255.0696 |
| 1259.9583 | 1275.6207 | 1285.0232 |
| 1286.5973 | 1301.2817 | 1307.0997 |
| 1321.4219 | 1338.2543 | 1339.4673 |
| 1344.2217 | 1349.7338 | 1352.2081 |
| 1363.6150 | 1370.5061 | 1399.8722 |
| 1401.4322 | 1404.5483 | 1407.3273 |
| 1418.4169 | 1418.7622 | 1427.7304 |
| 1448.9589 | 1453.5270 | 1454.7433 |
| 1474.6638 | 1479.9914 | 1482.6289 |
| 1482.8375 | 1487.7808 | 1497.7129 |
| 1498.2510 | 1508.1386 | 1514.1893 |
| 1539.8373 | 1543.0588 | 1602.5995 |
| 1613.9762 | 1619.0826 | 1622.7535 |
| 1667.0121 | 1668.4026 | 1699.1964 |
| 2234.0775 | 3011.6406 | 3015.2371 |

| | | |
|---|---|---|
| 3019.7456 | 3022.7020 | 3031.8650 |
| 3032.6840 | 3036.2420 | 3049.8638 |
| 3064.5096 | 3071.5312 | 3089.0574 |
| 3100.2781 | 3103.7062 | 3141.9463 |
| 3168.3423 | 3187.5158 | 3188.6332 |
| 3196.0279 | 3198.4122 | 3210.8908 |
| 3211.1851 | 3213.3842 | 3215.2621 |
| 3231.2422 | 3236.1747 | 3267.1136 |

**TS3R**

Zero-point correction= 0.498711

Thermal correction to Energy= 0.536086

Thermal correction to Enthalpy= 0.537030

Thermal correction to Gibbs Free Energy= 0.424426

Sum of electronic and zero-point Energies= -1765.584607

Sum of electronic and thermal Energies= -1765.547233

Sum of electronic and thermal Enthalpies= -1765.546288

Sum of electronic and thermal Free Energies= -1765.658892

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.171219 | -1.257274 | -0.164115 |
| B | 0.287963 | -0.124036 | 0.644116 |
| C | -1.460484 | -1.661981 | -0.144499 |
| O | -0.790468 | 0.780067 | 1.061024 |
| C | -2.512000 | -0.790090 | -0.446650 |
| C | -1.755897 | -3.027774 | 0.149184 |
| C | -1.419570 | 1.377998 | 0.018167 |
| C | -2.211114 | 0.616358 | -0.838390 |
| C | -3.044117 | -3.498428 | 0.185386 |
| C | -3.871438 | -1.237006 | -0.311725 |
| C | -4.133293 | -2.614058 | -0.018004 |

| | | | |
|---|---|---|---|
| C | -1.266255 | 2.773382 | -0.209553 |
| C | -2.718149 | 1.206428 | -2.043913 |
| C | -1.819813 | 3.381962 | -1.308250 |
| C | -2.525955 | 2.609236 | -2.268254 |
| H | -3.247900 | -4.541416 | 0.402936 |
| H | -1.704495 | 4.448181 | -1.472468 |
| C | -3.037240 | 3.208738 | -3.452487 |
| C | -3.691768 | 2.452984 | -4.398584 |
| C | -3.853572 | 1.060067 | -4.198074 |
| C | -3.382657 | 0.454038 | -3.053757 |
| H | -2.889604 | 4.275499 | -3.599613 |
| H | -4.074483 | 2.917632 | -5.302647 |
| H | -4.349785 | 0.462269 | -4.957441 |
| H | -3.506493 | -0.614391 | -2.921182 |
| C | -5.474604 | -3.074172 | 0.093775 |
| C | -6.531221 | -2.203823 | -0.046247 |
| C | -6.280068 | -0.831887 | -0.292029 |
| C | -4.991154 | -0.361915 | -0.421290 |
| H | -5.645792 | -4.126416 | 0.305637 |
| H | -7.553002 | -2.560438 | 0.045590 |
| H | -7.113111 | -0.139255 | -0.373250 |
| H | -4.824888 | 0.693911 | -0.595393 |
| C | 1.589229 | 0.608590 | 0.022780 |
| C | 2.368385 | 0.029310 | -0.909913 |
| H | 1.845435 | 1.603789 | 0.384586 |
| H | 2.127604 | -0.984391 | -1.231063 |
| C | 3.597247 | 0.624814 | -1.524071 |
| C | 4.845001 | -0.191454 | -1.115831 |
| H | 3.715156 | 1.670083 | -1.213966 |
| H | 3.514009 | 0.612933 | -2.619986 |

| | | | |
|---|---|---|---|
| C | 6.142256 | 0.350256 | -1.725077 |
| H | 4.919634 | -0.199654 | -0.020874 |
| H | 4.703721 | -1.237256 | -1.421114 |
| H | 6.049185 | 0.367269 | -2.820196 |
| H | 6.283408 | 1.394534 | -1.412374 |
| C | 7.376077 | -0.471071 | -1.332435 |
| C | 8.681679 | 0.060921 | -1.935457 |
| H | 7.231878 | -1.514990 | -1.646326 |
| H | 7.465228 | -0.491903 | -0.236680 |
| C | 9.903770 | -0.775416 | -1.546111 |
| H | 8.589538 | 0.088080 | -3.030075 |
| H | 8.831444 | 1.101158 | -1.614889 |
| H | 10.823417 | -0.374726 | -1.987306 |
| H | 10.038807 | -0.795950 | -0.457901 |
| H | 9.797561 | -1.813185 | -1.884819 |
| C | 1.079319 | -0.539718 | 2.005351 |
| H | 1.234070 | 0.295254 | 2.691753 |
| C | 2.302417 | -1.460870 | 2.074749 |
| N | -0.156791 | -1.361532 | 2.968894 |
| N | -1.249150 | -1.538346 | 3.057740 |
| I | -0.171976 | 3.949725 | 1.214773 |
| I | -0.161550 | -4.397163 | 0.570895 |
| F | 2.447766 | -2.251192 | 1.004333 |
| F | 2.269912 | -2.251927 | 3.166710 |
| F | 3.410834 | -0.691860 | 2.164413 |

Vibrational frequencies

| | | |
|---|---|---|
| -440.5784 | 12.8525 | 14.6804 |
| 21.1052 | 30.0795 | 34.7314 |
| 40.2141 | 51.0940 | 53.6277 |

| | | |
|---|---|---|
| 63.2017 | 71.8351 | 79.9518 |
| 82.9266 | 87.4681 | 93.7097 |
| 98.5501 | 100.5967 | 103.4547 |
| 108.1254 | 112.8366 | 145.3763 |
| 151.3449 | 156.5261 | 160.5845 |
| 165.2946 | 176.9157 | 192.8247 |
| 199.9904 | 214.2186 | 216.6411 |
| 228.6627 | 252.7300 | 268.5858 |
| 272.2198 | 275.8119 | 287.0369 |
| 290.7462 | 293.4460 | 315.0820 |
| 337.5667 | 342.5156 | 357.0671 |
| 366.4648 | 392.3119 | 416.0268 |
| 431.1390 | 444.3162 | 452.4289 |
| 459.9119 | 462.2392 | 475.0070 |
| 501.8148 | 512.1447 | 519.3737 |
| 526.4861 | 558.7085 | 565.1497 |
| 567.4812 | 573.9985 | 583.6171 |
| 588.7675 | 598.8846 | 633.0185 |
| 642.7372 | 656.5339 | 664.9891 |
| 672.2522 | 717.7183 | 735.1051 |
| 741.9190 | 749.8053 | 751.2601 |
| 764.2936 | 766.1585 | 769.2469 |
| 780.6680 | 782.7002 | 798.0151 |
| 813.0835 | 824.7326 | 833.7269 |
| 861.1359 | 874.4512 | 876.7688 |
| 882.2181 | 897.7090 | 906.0446 |
| 906.2357 | 909.3757 | 916.1359 |
| 949.3347 | 970.4249 | 972.2187 |
| 978.3704 | 990.8931 | 999.1837 |
| 1002.0683 | 1003.1293 | 1011.4972 |

| | | |
|---|---|---|
| 1020.2730 | 1030.6882 | 1040.6790 |
| 1058.1961 | 1059.2683 | 1063.9021 |
| 1066.7642 | 1071.8508 | 1077.0043 |
| 1107.7978 | 1120.3227 | 1135.5009 |
| 1148.6535 | 1160.4019 | 1164.8415 |
| 1183.1722 | 1189.0150 | 1191.5367 |
| 1193.3743 | 1218.5872 | 1240.0173 |
| 1241.6494 | 1250.1701 | 1264.7783 |
| 1269.3286 | 1276.7732 | 1283.7938 |
| 1288.3002 | 1291.6597 | 1303.3092 |
| 1310.9849 | 1314.8711 | 1329.2616 |
| 1342.1381 | 1344.5301 | 1345.7151 |
| 1354.0152 | 1365.3381 | 1368.7035 |
| 1392.3501 | 1402.9792 | 1403.3593 |
| 1406.2411 | 1419.1374 | 1421.8727 |
| 1424.2559 | 1449.7013 | 1453.3844 |
| 1474.6160 | 1479.3933 | 1482.1259 |
| 1483.9270 | 1489.6123 | 1498.2172 |
| 1500.3060 | 1509.5679 | 1515.4499 |
| 1537.0023 | 1540.2870 | 1590.5586 |
| 1604.1177 | 1619.3334 | 1621.5224 |
| 1648.9959 | 1666.4642 | 1667.3624 |
| 2361.1681 | 3013.2364 | 3017.5182 |
| 3023.1749 | 3023.9215 | 3032.7326 |
| 3033.3902 | 3037.4673 | 3050.9217 |
| 3064.3065 | 3072.5817 | 3088.0082 |
| 3100.2891 | 3103.8568 | 3154.9461 |
| 3161.6071 | 3168.7147 | 3183.4775 |
| 3183.7241 | 3192.1764 | 3193.2381 |
| 3207.3978 | 3207.7529 | 3210.4556 |

3213.0786 3225.2301 3231.4757

**TS3S**

Zero-point correction= 0.498500

Thermal correction to Energy= 0.535951

Thermal correction to Enthalpy= 0.536895

Thermal correction to Gibbs Free Energy= 0.423809

Sum of electronic and zero-point Energies= -1765.589398

Sum of electronic and thermal Energies= -1765.551948

Sum of electronic and thermal Enthalpies= -1765.551004

Sum of electronic and thermal Free Energies= -1765.664090

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.088434 | -0.806362 | -0.888847 |
| B | 0.447762 | 0.092658 | 0.140531 |
| C | -1.291832 | -1.389593 | -0.691656 |
| O | -0.571118 | 0.927655 | 0.770498 |
| C | -2.455643 | -0.622031 | -0.606059 |
| C | -1.371762 | -2.807556 | -0.583421 |
| C | -1.429169 | 1.569564 | -0.058075 |
| C | -2.354447 | 0.851001 | -0.817097 |
| C | -2.563104 | -3.447394 | -0.355091 |
| C | -3.699117 | -1.260225 | -0.273369 |
| C | -3.749466 | -2.689795 | -0.171460 |
| C | -1.400206 | 2.990321 | -0.136568 |
| C | -3.162496 | 1.540216 | -1.783532 |
| C | -2.224722 | 3.677604 | -0.990995 |
| C | -3.104221 | 2.970717 | -1.852426 |
| H | -2.610617 | -4.528738 | -0.280388 |
| H | -2.199082 | 4.761110 | -1.038800 |
| C | -3.914804 | 3.665709 | -2.792039 |

| | | | |
|---|---|---|---|
| C | -4.736730 | 2.979727 | -3.656988 |
| C | -4.769190 | 1.564261 | -3.620805 |
| C | -4.005351 | 0.864706 | -2.711981 |
| H | -3.862699 | 4.751060 | -2.818644 |
| H | -5.349199 | 3.517564 | -4.374816 |
| H | -5.398652 | 1.023360 | -4.321815 |
| H | -4.034756 | -0.218355 | -2.708993 |
| C | -4.979244 | -3.334284 | 0.136842 |
| C | -6.119889 | -2.600764 | 0.370465 |
| C | -6.067912 | -1.186683 | 0.313411 |
| C | -4.894261 | -0.535403 | 0.001742 |
| H | -4.995083 | -4.419467 | 0.196198 |
| H | -7.054155 | -3.100156 | 0.610009 |
| H | -6.962645 | -0.607659 | 0.524302 |
| H | -4.875210 | 0.547196 | -0.024732 |
| C | 1.785642 | 0.813262 | -0.386645 |
| C | 2.599257 | 0.256883 | -1.304528 |
| H | 2.073767 | 1.758734 | 0.072848 |
| H | 2.334521 | -0.721142 | -1.710203 |
| C | 3.886298 | 0.840299 | -1.803264 |
| C | 5.089184 | 0.005980 | -1.308756 |
| H | 3.992423 | 1.878373 | -1.466079 |
| H | 3.892729 | 0.847617 | -2.902359 |
| C | 6.433154 | 0.523161 | -1.832401 |
| H | 5.090243 | 0.006085 | -0.210653 |
| H | 4.953346 | -1.039358 | -1.618490 |
| H | 6.414462 | 0.529513 | -2.931471 |
| H | 6.567270 | 1.568749 | -1.521311 |
| C | 7.625972 | -0.309674 | -1.348743 |
| C | 8.975227 | 0.193647 | -1.875625 |

| | | | |
|---|---|---|---|
| H | 7.486060 | -1.356407 | -1.655277 |
| H | 7.644960 | -0.313706 | -0.249301 |
| C | 10.158261 | -0.647589 | -1.388478 |
| H | 8.954949 | 0.197918 | -2.974260 |
| H | 9.116549 | 1.238963 | -1.568189 |
| H | 11.110225 | -0.266148 | -1.774639 |
| H | 10.219477 | -0.647152 | -0.293431 |
| H | 10.062296 | -1.690909 | -1.712938 |
| C | 1.254905 | -0.742220 | 1.303714 |
| H | 1.786237 | -1.622949 | 0.944912 |
| C | 2.043950 | -0.069670 | 2.431640 |
| N | -0.003071 | -1.522586 | 2.231277 |
| N | -1.103092 | -1.589706 | 2.373691 |
| I | -0.048153 | 4.079315 | 1.124957 |
| I | 0.435614 | -3.956814 | -0.738811 |
| F | 3.273298 | 0.265838 | 1.999003 |
| F | 2.202221 | -0.901424 | 3.484114 |
| F | 1.438000 | 1.040838 | 2.880183 |

Vibrational frequencies

| | | |
|---|---|---|
| -441.8524 | 11.1488 | 14.4731 |
| 25.3079 | 35.3244 | 36.4472 |
| 39.8920 | 48.8998 | 50.4774 |
| 55.0808 | 58.8779 | 66.1921 |
| 81.5915 | 84.5042 | 89.2353 |
| 95.6963 | 100.4956 | 101.3091 |
| 117.8883 | 122.5657 | 138.4728 |
| 145.7085 | 147.0099 | 155.8600 |
| 158.6840 | 167.9678 | 192.5513 |
| 198.3401 | 213.4345 | 223.7570 |

| | | |
|---|---|---|
| 242.0265 | 262.5691 | 264.9587 |
| 268.2268 | 278.9773 | 285.3991 |
| 293.9105 | 301.2557 | 319.3844 |
| 335.5088 | 343.3175 | 364.4128 |
| 365.9376 | 402.2462 | 410.1593 |
| 421.0196 | 444.2682 | 452.2815 |
| 455.0300 | 460.1535 | 471.8796 |
| 500.9908 | 513.1168 | 519.2309 |
| 524.7114 | 559.8961 | 565.3146 |
| 567.0111 | 572.8479 | 583.2473 |
| 590.7102 | 600.7638 | 631.1717 |
| 640.6533 | 658.6037 | 671.9074 |
| 674.8468 | 713.9086 | 733.5812 |
| 751.2784 | 751.5629 | 758.9324 |
| 763.5151 | 766.6473 | 770.6872 |
| 779.1270 | 789.6006 | 799.0981 |
| 813.4441 | 824.5774 | 831.9298 |
| 867.1812 | 873.9445 | 875.7753 |
| 881.9038 | 899.6146 | 905.5300 |
| 905.8292 | 908.4299 | 911.7160 |
| 949.3477 | 969.3255 | 972.9972 |
| 977.4121 | 993.5540 | 997.7096 |
| 999.1052 | 1003.4929 | 1013.1673 |
| 1021.9388 | 1033.4282 | 1036.2013 |
| 1050.3441 | 1059.8432 | 1062.3622 |
| 1067.8241 | 1071.7042 | 1078.5698 |
| 1107.2388 | 1124.6096 | 1133.9576 |
| 1146.2452 | 1163.8406 | 1165.7978 |
| 1184.9275 | 1189.3945 | 1190.1682 |
| 1194.4238 | 1218.3666 | 1240.9541 |

| | | |
|---|---|---|
| 1242.4361 | 1249.5408 | 1261.7737 |
| 1268.2499 | 1273.8637 | 1284.6165 |
| 1288.2835 | 1291.4075 | 1297.8834 |
| 1307.4947 | 1309.4325 | 1323.2249 |
| 1336.0817 | 1337.1059 | 1345.2349 |
| 1346.3509 | 1363.5242 | 1367.7985 |
| 1394.2422 | 1397.1786 | 1403.2755 |
| 1405.3121 | 1417.3443 | 1419.7880 |
| 1421.5542 | 1452.4010 | 1455.4833 |
| 1475.5919 | 1479.1052 | 1481.5524 |
| 1484.3957 | 1488.5399 | 1497.4536 |
| 1498.5948 | 1508.5868 | 1515.3601 |
| 1538.4482 | 1540.8028 | 1589.8053 |
| 1602.9840 | 1620.3060 | 1621.9209 |
| 1651.3462 | 1667.1959 | 1667.8823 |
| 2346.8692 | 3011.3618 | 3016.0282 |
| 3021.9014 | 3023.5442 | 3029.2171 |
| 3032.1767 | 3036.6767 | 3048.9372 |
| 3061.5722 | 3070.6768 | 3085.2905 |
| 3099.4238 | 3104.2160 | 3141.3067 |
| 3154.2790 | 3183.9870 | 3184.6402 |
| 3192.8480 | 3193.7557 | 3194.9035 |
| 3207.5785 | 3208.7787 | 3210.2555 |
| 3213.3672 | 3227.5326 | 3233.1930 |

**TS3R-Br**

Zero-point correction= 0.499214

Thermal correction to Energy= 0.536367

Thermal correction to Enthalpy= 0.537311

Thermal correction to Gibbs Free Energy= 0.425886

Sum of electronic and zero-point Energies= -1769.147921

Sum of electronic and thermal Energies= -1769.110768

Sum of electronic and thermal Enthalpies= -1769.109824

Sum of electronic and thermal Free Energies= -1769.221249

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.173735 | -1.215343 | -0.236930 |
| B | 0.291936 | -0.105715 | 0.600872 |
| C | -1.457391 | -1.629733 | -0.194497 |
| O | -0.780158 | 0.808739 | 1.010875 |
| C | -2.525992 | -0.769056 | -0.465520 |
| C | -1.741262 | -2.996083 | 0.096895 |
| C | -1.420560 | 1.395510 | -0.028195 |
| C | -2.239860 | 0.638584 | -0.862552 |
| C | -3.016649 | -3.488852 | 0.166972 |
| C | -3.876860 | -1.231952 | -0.301017 |
| C | -4.118403 | -2.613134 | -0.005343 |
| C | -1.256573 | 2.783124 | -0.284413 |
| C | -2.773823 | 1.227653 | -2.057707 |
| C | -1.829272 | 3.398427 | -1.365784 |
| C | -2.575769 | 2.627765 | -2.296364 |
| H | -3.197761 | -4.535739 | 0.385289 |
| H | -1.697500 | 4.461165 | -1.538887 |
| C | -3.114387 | 3.225084 | -3.469235 |
| C | -3.800097 | 2.469170 | -4.392823 |
| C | -3.965941 | 1.078603 | -4.180951 |
| C | -3.469103 | 0.475046 | -3.046337 |
| H | -2.961701 | 4.289554 | -3.626852 |
| H | -4.203331 | 2.931971 | -5.288848 |
| H | -4.485505 | 0.480258 | -4.924044 |

| | | | |
|---|---|---|---|
| H | -3.595894 | -0.591947 | -2.905910 |
| C | -5.451858 | -3.086403 | 0.137688 |
| C | -6.519448 | -2.225392 | 0.026247 |
| C | -6.287781 | -0.850530 | -0.221755 |
| C | -5.007090 | -0.367685 | -0.381269 |
| H | -5.607897 | -4.140829 | 0.350020 |
| H | -7.535156 | -2.592043 | 0.142149 |
| H | -7.129282 | -0.166034 | -0.280808 |
| H | -4.854902 | 0.690123 | -0.556749 |
| C | 1.613246 | 0.609869 | 0.008951 |
| C | 2.412663 | 0.017697 | -0.898052 |
| H | 1.862160 | 1.608283 | 0.367235 |
| H | 2.177516 | -1.000024 | -1.211096 |
| C | 3.648467 | 0.609574 | -1.501928 |
| C | 4.895516 | -0.205374 | -1.090919 |
| H | 3.764647 | 1.655193 | -1.192126 |
| H | 3.569906 | 0.598451 | -2.598391 |
| C | 6.192489 | 0.340245 | -1.697407 |
| H | 4.968279 | -0.214779 | 0.004183 |
| H | 4.756883 | -1.251021 | -1.398022 |
| H | 6.100760 | 0.357894 | -2.792655 |
| H | 6.329868 | 1.384829 | -1.383931 |
| C | 7.428935 | -0.476704 | -1.304242 |
| C | 8.732384 | 0.060434 | -1.907452 |
| H | 7.288713 | -1.521199 | -1.618027 |
| H | 7.518082 | -0.496969 | -0.208478 |
| C | 9.958290 | -0.769831 | -1.517237 |
| H | 8.640277 | 0.086195 | -3.002116 |
| H | 8.877365 | 1.101675 | -1.587909 |
| H | 10.876059 | -0.365275 | -1.958847 |

| | | | |
|---|---|---|---|
| H | 10.093440 | -0.788681 | -0.429009 |
| H | 9.856906 | -1.808416 | -1.854966 |
| C | 1.044894 | -0.556152 | 1.974018 |
| H | 1.213894 | 0.266587 | 2.671890 |
| C | 2.234521 | -1.518021 | 2.056605 |
| N | -0.228187 | -1.349600 | 2.900751 |
| N | -1.329151 | -1.478083 | 2.970390 |
| F | 2.333564 | -2.346849 | 1.011661 |
| F | 2.183534 | -2.271390 | 3.175156 |
| F | 3.370673 | -0.788798 | 2.112150 |
| Br | -0.178707 | 3.858412 | 0.972732 |
| Br | -0.242577 | -4.234641 | 0.428159 |

Vibrational frequencies

| | | |
|---|---|---|
| -435.2148 | 12.7015 | 15.6739 |
| 20.7957 | 29.3824 | 36.5294 |
| 40.4507 | 49.8306 | 54.6426 |
| 65.0896 | 71.9178 | 78.3196 |
| 85.0484 | 91.0435 | 97.9018 |
| 99.5546 | 103.0583 | 110.0580 |
| 115.0948 | 125.8399 | 144.9790 |
| 151.4647 | 160.2725 | 170.3806 |
| 171.3769 | 182.2555 | 196.8574 |
| 199.7323 | 221.4798 | 238.3339 |
| 247.0682 | 256.6421 | 268.8388 |
| 271.0727 | 274.9029 | 287.8302 |
| 292.8420 | 297.6056 | 316.5733 |
| 338.4502 | 341.8599 | 358.0182 |
| 365.8542 | 391.9002 | 414.2634 |
| 429.3357 | 445.5855 | 452.6561 |

| | | |
|---|---|---|
| 459.0517 | 461.9413 | 474.7547 |
| 502.6776 | 513.6559 | 519.1590 |
| 528.0180 | 558.9640 | 567.2697 |
| 572.9694 | 575.1088 | 585.5910 |
| 589.2388 | 600.2708 | 634.0024 |
| 643.1957 | 658.1269 | 668.3571 |
| 671.9563 | 716.8452 | 736.2697 |
| 748.4233 | 750.5327 | 750.9867 |
| 763.4019 | 764.7476 | 768.0467 |
| 777.6243 | 782.8890 | 796.0457 |
| 810.4372 | 828.5812 | 834.4976 |
| 862.5162 | 872.3767 | 873.7920 |
| 883.1136 | 896.1698 | 897.0126 |
| 901.8568 | 909.7843 | 915.9964 |
| 950.5769 | 970.2364 | 972.1972 |
| 979.6544 | 991.4501 | 999.8980 |
| 1002.3226 | 1002.9030 | 1012.4788 |
| 1020.4009 | 1033.6689 | 1038.8592 |
| 1057.8612 | 1059.4503 | 1064.3332 |
| 1066.8612 | 1072.8071 | 1077.9963 |
| 1108.2786 | 1126.2038 | 1136.1897 |
| 1149.8512 | 1162.7451 | 1165.9557 |
| 1183.5844 | 1189.8954 | 1190.6775 |
| 1194.2146 | 1218.5323 | 1236.8473 |
| 1239.9897 | 1249.4422 | 1265.0198 |
| 1270.7273 | 1280.7760 | 1286.0044 |
| 1290.6113 | 1291.5629 | 1305.8272 |
| 1312.5568 | 1318.8689 | 1329.0911 |
| 1341.9587 | 1344.8012 | 1346.9389 |
| 1354.5970 | 1368.3024 | 1371.5512 |

| | | |
|---|---|---|
| 1396.4788 | 1402.1779 | 1403.0397 |
| 1405.3942 | 1419.1440 | 1423.9349 |
| 1424.2799 | 1452.8102 | 1455.9898 |
| 1479.3685 | 1480.3717 | 1483.8573 |
| 1484.6755 | 1489.2526 | 1498.2994 |
| 1499.9286 | 1509.1808 | 1515.2235 |
| 1539.6273 | 1542.7775 | 1591.8943 |
| 1605.3154 | 1625.4638 | 1627.8621 |
| 1650.0460 | 1667.2246 | 1668.0474 |
| 2355.6837 | 3013.1407 | 3017.1780 |
| 3022.6727 | 3023.0343 | 3032.5494 |
| 3032.8412 | 3037.2483 | 3050.4630 |
| 3063.8476 | 3071.8240 | 3087.0448 |
| 3100.2027 | 3103.8035 | 3154.5046 |
| 3161.7400 | 3174.1288 | 3184.4867 |
| 3184.9684 | 3193.1087 | 3194.0963 |
| 3208.3638 | 3208.7071 | 3215.6507 |
| 3216.3195 | 3226.9559 | 3230.0186 |

**TS3S-Br**

Zero-point correction= 0.498954

Thermal correction to Energy= 0.536230

Thermal correction to Enthalpy= 0.537174

Thermal correction to Gibbs Free Energy= 0.424831

Sum of electronic and zero-point Energies= -1769.151233

Sum of electronic and thermal Energies= -1769.113957

Sum of electronic and thermal Enthalpies= -1769.113013

Sum of electronic and thermal Free Energies= -1769.225356

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.089752 | -0.823470 | -0.855588 |

| | | | |
|---|---|---|---|
| B | 0.436896 | 0.079080 | 0.175478 |
| C | -1.297183 | -1.396861 | -0.669236 |
| O | -0.591200 | 0.907254 | 0.795988 |
| C | -2.464386 | -0.632253 | -0.601961 |
| C | -1.388289 | -2.810947 | -0.546440 |
| C | -1.431549 | 1.549936 | -0.047482 |
| C | -2.357364 | 0.840380 | -0.813689 |
| C | -2.573972 | -3.459627 | -0.332458 |
| C | -3.711519 | -1.271517 | -0.283712 |
| C | -3.763545 | -2.701193 | -0.175392 |
| C | -1.383811 | 2.966991 | -0.147145 |
| C | -3.151347 | 1.535912 | -1.787966 |
| C | -2.189511 | 3.667181 | -1.004498 |
| C | -3.076732 | 2.966019 | -1.862586 |
| H | -2.614836 | -4.540343 | -0.248887 |
| H | -2.140940 | 4.749434 | -1.058973 |
| C | -3.875109 | 3.666578 | -2.808180 |
| C | -4.699683 | 2.986220 | -3.674891 |
| C | -4.746459 | 1.571412 | -3.635125 |
| C | -3.994864 | 0.866707 | -2.720139 |
| H | -3.810973 | 4.751117 | -2.838395 |
| H | -5.302733 | 3.528227 | -4.397479 |
| H | -5.377184 | 1.034912 | -4.338291 |
| H | -4.035112 | -0.215914 | -2.714744 |
| C | -4.997419 | -3.344856 | 0.116938 |
| C | -6.141199 | -2.610249 | 0.330281 |
| C | -6.088350 | -1.196476 | 0.269224 |
| C | -4.910467 | -0.546173 | -0.027746 |
| H | -5.013985 | -4.429675 | 0.180743 |
| H | -7.078849 | -3.108822 | 0.557793 |

| | | | |
|---|---|---|---|
| H | -6.985935 | -0.616812 | 0.465488 |
| H | -4.891047 | 0.536296 | -0.057331 |
| C | 1.775151 | 0.807437 | -0.339960 |
| C | 2.595451 | 0.258437 | -1.256428 |
| H | 2.050935 | 1.753814 | 0.124851 |
| H | 2.337730 | -0.720881 | -1.663633 |
| C | 3.876431 | 0.852860 | -1.756433 |
| C | 5.086564 | 0.013516 | -1.288911 |
| H | 3.982946 | 1.885868 | -1.404159 |
| H | 3.871172 | 0.877533 | -2.855344 |
| C | 6.422467 | 0.540345 | -1.823410 |
| H | 5.102036 | -0.002014 | -0.191083 |
| H | 4.948243 | -1.027479 | -1.611916 |
| H | 6.387506 | 0.563912 | -2.921831 |
| H | 6.560457 | 1.581050 | -1.497960 |
| C | 7.622937 | -0.299159 | -1.371228 |
| C | 8.963250 | 0.211678 | -1.913453 |
| H | 7.477804 | -1.341388 | -1.690441 |
| H | 7.660104 | -0.318965 | -0.272447 |
| C | 10.153738 | -0.638956 | -1.462286 |
| H | 8.923362 | 0.234285 | -3.011347 |
| H | 9.111648 | 1.251509 | -1.591053 |
| H | 11.098830 | -0.252514 | -1.860223 |
| H | 10.235908 | -0.656182 | -0.368780 |
| H | 10.050001 | -1.676738 | -1.801778 |
| C | 1.238909 | -0.752448 | 1.344594 |
| H | 1.767361 | -1.637913 | 0.994413 |
| C | 2.043445 | -0.064369 | 2.454666 |
| N | -0.026452 | -1.517467 | 2.274893 |
| N | -1.127709 | -1.549530 | 2.422849 |

| | | | |
|---|---|---|---|
| F | 3.305066 | 0.150459 | 2.034777 |
| F | 2.114425 | -0.830933 | 3.564071 |
| F | 1.513445 | 1.115434 | 2.807499 |
| Br | -0.114069 | 3.953643 | 0.996146 |
| Br | 0.279497 | -3.868317 | -0.653927 |

Vibrational frequencies

| | | |
|---|---|---|
| -441.8336 | 9.9826 | 15.4692 |
| 26.1363 | 30.5639 | 37.3816 |
| 42.5478 | 47.5603 | 48.2958 |
| 51.3165 | 59.2336 | 64.6699 |
| 77.7614 | 87.8673 | 90.9953 |
| 96.0583 | 104.4228 | 112.5318 |
| 116.3218 | 122.5799 | 136.1351 |
| 146.5077 | 155.0594 | 161.2273 |
| 170.2588 | 173.1535 | 200.2307 |
| 206.6276 | 230.6291 | 244.0648 |
| 251.7365 | 263.0584 | 265.2450 |
| 270.8417 | 278.3809 | 287.6872 |
| 297.2499 | 302.5547 | 320.1228 |
| 336.2298 | 343.4819 | 361.6273 |
| 366.5114 | 401.0619 | 410.1129 |
| 420.8636 | 444.7451 | 452.3168 |
| 455.3698 | 461.6743 | 471.7492 |
| 501.4670 | 513.0978 | 518.9852 |
| 526.2071 | 560.2656 | 567.0311 |
| 571.2720 | 575.3479 | 586.9445 |
| 588.4320 | 602.2532 | 631.5238 |
| 640.4858 | 659.1188 | 672.0945 |
| 674.7607 | 711.4745 | 738.2338 |

| | | |
|---|---|---|
| 751.2139 | 754.3630 | 760.2345 |
| 762.8538 | 765.9918 | 770.3139 |
| 776.8579 | 787.2602 | 797.7095 |
| 811.1615 | 828.0074 | 833.5748 |
| 867.1404 | 871.9293 | 874.7590 |
| 882.6520 | 895.5579 | 898.0123 |
| 900.7777 | 908.1706 | 911.7280 |
| 950.6871 | 969.5027 | 974.1088 |
| 978.8714 | 994.3365 | 998.3859 |
| 999.7154 | 1004.8723 | 1013.9651 |
| 1022.2426 | 1035.3988 | 1037.2364 |
| 1051.4192 | 1060.4185 | 1062.8107 |
| 1068.4877 | 1072.4910 | 1081.8696 |
| 1107.1169 | 1126.4434 | 1134.2203 |
| 1148.8414 | 1161.6835 | 1165.7049 |
| 1184.8387 | 1186.7033 | 1190.7479 |
| 1195.0728 | 1218.7588 | 1237.0036 |
| 1239.9117 | 1249.6763 | 1262.6465 |
| 1268.3526 | 1275.1061 | 1286.6229 |
| 1289.4419 | 1292.4045 | 1299.3268 |
| 1307.7476 | 1311.3535 | 1324.2364 |
| 1337.5301 | 1338.5307 | 1347.0075 |
| 1348.1145 | 1364.8322 | 1372.8597 |
| 1397.8155 | 1398.0794 | 1403.2085 |
| 1404.6444 | 1418.0065 | 1420.0906 |
| 1423.1608 | 1455.3360 | 1457.8784 |
| 1479.5601 | 1480.7942 | 1483.9034 |
| 1484.2470 | 1488.2803 | 1497.3095 |
| 1498.6269 | 1508.3514 | 1514.9258 |
| 1540.9576 | 1543.2651 | 1591.0081 |

| | | |
|---|---|---|
| 1604.1853 | 1626.7502 | 1628.5183 |
| 1651.6568 | 1667.8942 | 1668.7819 |
| 2343.0004 | 3011.5300 | 3016.0304 |
| 3021.5883 | 3022.9019 | 3029.0325 |
| 3032.0477 | 3036.6259 | 3048.8046 |
| 3061.3816 | 3070.7329 | 3085.3460 |
| 3099.4470 | 3103.6152 | 3142.1772 |
| 3156.0789 | 3184.8366 | 3185.9420 |
| 3193.7237 | 3196.0126 | 3197.1913 |
| 3208.4471 | 3209.9333 | 3215.3372 |
| 3215.9625 | 3228.7796 | 3234.5052 |

**TS3R-H**

Zero-point correction= 0.519844

Thermal correction to Energy= 0.553554

Thermal correction to Enthalpy= 0.554498

Thermal correction to Gibbs Free Energy= 0.452834

Sum of electronic and zero-point Energies= -1744.007875

Sum of electronic and thermal Energies= -1743.974165

Sum of electronic and thermal Enthalpies= -1743.973221

Sum of electronic and thermal Free Energies= -1744.074885

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.049476 | -0.939871 | -0.672137 |
| B | 0.412640 | 0.052225 | 0.285836 |
| C | -1.294286 | -1.464558 | -0.480917 |
| O | -0.592213 | 1.052845 | 0.649628 |
| C | -2.433082 | -0.670472 | -0.609962 |
| C | -1.384388 | -2.841341 | -0.155281 |
| C | -1.367317 | 1.556058 | -0.352245 |

| | | | |
|---|---|---|---|
| C | -2.272118 | 0.747116 | -1.037270 |
| C | -2.606296 | -3.419433 | 0.084929 |
| C | -3.709121 | -1.243110 | -0.272838 |
| C | -3.793047 | -2.638922 | 0.058234 |
| C | -1.234535 | 2.935638 | -0.649015 |
| C | -2.985187 | 1.310156 | -2.152175 |
| C | -1.972829 | 3.503929 | -1.657129 |
| C | -2.847007 | 2.709432 | -2.447408 |
| H | -2.676667 | -4.476672 | 0.327461 |
| H | -1.877141 | 4.563297 | -1.880815 |
| C | -3.566367 | 3.270036 | -3.538111 |
| C | -4.372145 | 2.487894 | -4.334962 |
| C | -4.479140 | 1.100265 | -4.074381 |
| C | -3.806295 | 0.529010 | -3.015776 |
| H | -3.456899 | 4.333254 | -3.737934 |
| H | -4.913090 | 2.926999 | -5.168397 |
| H | -5.093359 | 0.477783 | -4.719298 |
| H | -3.892865 | -0.536755 | -2.840045 |
| C | -5.055882 | -3.211680 | 0.372966 |
| C | -6.197952 | -2.443150 | 0.396191 |
| C | -6.114793 | -1.057785 | 0.114631 |
| C | -4.908233 | -0.475491 | -0.208941 |
| H | -5.098058 | -4.272599 | 0.607472 |
| H | -7.156919 | -2.890298 | 0.642031 |
| H | -7.011310 | -0.445515 | 0.159936 |
| H | -4.865629 | 0.588221 | -0.410712 |
| C | 1.850857 | 0.665247 | -0.138887 |
| C | 2.706503 | 0.035986 | -0.964016 |
| H | 2.117417 | 1.646985 | 0.256382 |
| H | 2.453306 | -0.968265 | -1.307849 |

| | | | |
|---|---|---|---|
| C | 3.977418 | 0.612624 | -1.512757 |
| C | 3.960303 | 0.726254 | -3.049718 |
| H | 4.814190 | -0.040831 | -1.220884 |
| H | 4.168240 | 1.597272 | -1.068311 |
| C | 5.266256 | 1.292851 | -3.617661 |
| H | 3.767563 | -0.263807 | -3.484733 |
| H | 3.119423 | 1.364837 | -3.350798 |
| H | 5.455991 | 2.279982 | -3.172397 |
| H | 6.104878 | 0.651994 | -3.309731 |
| C | 5.257341 | 1.419435 | -5.145393 |
| C | 6.555688 | 2.004147 | -5.714866 |
| H | 4.411082 | 2.050623 | -5.452675 |
| H | 5.077817 | 0.430712 | -5.591748 |
| C | 6.538611 | 2.128903 | -7.240953 |
| H | 6.732393 | 2.992215 | -5.267810 |
| H | 7.401774 | 1.373994 | -5.407509 |
| H | 7.475373 | 2.552195 | -7.620831 |
| H | 6.398912 | 1.150599 | -7.716775 |
| H | 5.720332 | 2.778075 | -7.575458 |
| C | 0.986083 | -0.548264 | 1.703462 |
| H | 1.326465 | 0.205091 | 2.416903 |
| C | 1.900822 | -1.771505 | 1.797973 |
| N | -0.440969 | -1.018576 | 2.590944 |
| N | -1.530017 | -0.791781 | 2.623764 |
| F | 1.680596 | -2.672409 | 0.824713 |
| F | 1.749457 | -2.409584 | 2.978276 |
| F | 3.186886 | -1.382221 | 1.713573 |
| H | -0.536378 | 3.518079 | -0.055977 |
| H | -0.463457 | -3.410004 | -0.095726 |

Vibrational frequencies

| | | |
|---|---|---|
| -431.0787 | 11.1057 | 19.1869 |
| 30.5679 | 44.3774 | 50.9577 |
| 61.7799 | 65.3502 | 66.6436 |
| 68.0435 | 76.8600 | 79.8514 |
| 94.1132 | 101.9971 | 104.7003 |
| 122.0313 | 134.2504 | 146.4955 |
| 152.4539 | 164.6962 | 166.9859 |
| 177.0064 | 182.5278 | 190.5089 |
| 218.2886 | 235.1580 | 247.0310 |
| 253.9768 | 259.4839 | 262.7652 |
| 269.8103 | 304.2032 | 311.6331 |
| 325.1491 | 338.7539 | 357.0247 |
| 361.8745 | 387.9383 | 400.9216 |
| 428.2020 | 431.9462 | 438.4439 |
| 448.6766 | 465.4737 | 473.9849 |
| 478.1105 | 500.2802 | 501.6030 |
| 518.3009 | 531.5067 | 543.7516 |
| 550.8076 | 552.3906 | 568.6782 |
| 578.8233 | 587.4873 | 625.4345 |
| 640.9953 | 648.2936 | 667.7577 |
| 674.5305 | 691.8807 | 709.2928 |
| 721.1684 | 742.9285 | 747.8090 |
| 759.0549 | 765.6274 | 769.6189 |
| 778.7073 | 780.0929 | 800.8662 |
| 805.6622 | 809.5067 | 818.4103 |
| 837.2216 | 848.2523 | 855.3721 |
| 862.6179 | 882.0918 | 885.0381 |
| 885.4872 | 907.3322 | 910.8399 |
| 942.3231 | 960.4612 | 962.7076 |

| | | |
|---|---|---|
| 966.3255 | 972.5684 | 974.9496 |
| 988.8012 | 996.8505 | 998.5957 |
| 1003.2980 | 1014.5423 | 1024.4637 |
| 1028.7763 | 1033.4948 | 1057.0035 |
| 1059.0473 | 1064.6313 | 1066.2514 |
| 1073.5463 | 1076.2318 | 1099.1889 |
| 1119.8413 | 1134.7003 | 1147.7490 |
| 1154.3598 | 1171.5546 | 1172.1133 |
| 1173.5858 | 1186.8160 | 1189.4584 |
| 1197.9915 | 1217.1564 | 1218.9123 |
| 1238.6210 | 1240.7430 | 1243.2643 |
| 1260.8678 | 1263.9042 | 1271.9870 |
| 1287.2160 | 1288.8446 | 1292.8610 |
| 1303.8108 | 1309.0844 | 1314.1696 |
| 1326.2648 | 1333.9946 | 1339.7645 |
| 1342.7936 | 1367.3243 | 1367.9983 |
| 1373.8120 | 1397.9994 | 1400.5651 |
| 1401.7733 | 1406.1153 | 1419.4459 |
| 1420.9719 | 1432.3950 | 1464.9146 |
| 1466.4651 | 1474.8081 | 1483.8102 |
| 1487.8745 | 1495.1402 | 1497.9398 |
| 1500.3209 | 1502.7275 | 1507.8513 |
| 1514.7753 | 1553.1220 | 1554.0420 |
| 1606.2725 | 1615.0019 | 1641.1535 |
| 1643.8395 | 1652.8857 | 1668.8649 |
| 1670.7071 | 2327.9213 | 3006.5906 |
| 3012.2176 | 3014.4165 | 3022.3663 |
| 3029.5086 | 3032.8184 | 3035.6874 |
| 3047.1903 | 3059.9765 | 3067.1504 |
| 3080.9924 | 3100.3873 | 3103.7240 |

| | | |
|---|---|---|
| 3137.3298 | 3146.0057 | 3168.6766 |
| 3178.8444 | 3179.1904 | 3186.2839 |
| 3187.3413 | 3188.7304 | 3189.1376 |
| 3204.2198 | 3204.9650 | 3209.9435 |
| 3227.1438 | 3228.8360 | 3233.3021 |

**TS3S-H**

Zero-point correction= 0.519669

Thermal correction to Energy= 0.553549

Thermal correction to Enthalpy= 0.554493

Thermal correction to Gibbs Free Energy= 0.451481

Sum of electronic and zero-point Energies= -1744.007447

Sum of electronic and thermal Energies= -1743.973567

Sum of electronic and thermal Enthalpies= -1743.972623

Sum of electronic and thermal Free Energies= -1744.075635

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.098408 | -0.777583 | -0.944720 |
| B | 0.430857 | 0.100564 | 0.096845 |
| C | -1.310107 | -1.365082 | -0.738837 |
| O | -0.556557 | 0.980019 | 0.704941 |
| C | -2.473522 | -0.603620 | -0.631425 |
| C | -1.341244 | -2.780145 | -0.651967 |
| C | -1.440935 | 1.598901 | -0.127591 |
| C | -2.390413 | 0.869049 | -0.840169 |
| C | -2.519993 | -3.437069 | -0.400366 |
| C | -3.696646 | -1.273275 | -0.276062 |
| C | -3.718099 | -2.706717 | -0.177243 |
| C | -1.370954 | 3.011719 | -0.215404 |
| C | -3.223966 | 1.569110 | -1.781180 |

| | | | |
|---|---|---|---|
| C | -2.218847 | 3.698778 | -1.047895 |
| C | -3.147491 | 3.001069 | -1.866755 |
| H | -2.545301 | -4.522134 | -0.341130 |
| H | -2.171651 | 4.782799 | -1.111530 |
| C | -3.982693 | 3.695108 | -2.784524 |
| C | -4.845682 | 3.014856 | -3.614244 |
| C | -4.895516 | 1.600773 | -3.563684 |
| C | -4.108402 | 0.899556 | -2.675604 |
| H | -3.916459 | 4.779679 | -2.824405 |
| H | -5.476215 | 3.555296 | -4.314498 |
| H | -5.556508 | 1.061599 | -4.236790 |
| H | -4.153565 | -0.182945 | -2.662290 |
| C | -4.930196 | -3.370114 | 0.157885 |
| C | -6.079730 | -2.659288 | 0.420207 |
| C | -6.054514 | -1.244626 | 0.365840 |
| C | -4.899204 | -0.572473 | 0.029320 |
| H | -4.926282 | -4.456036 | 0.213786 |
| H | -6.999279 | -3.176478 | 0.678894 |
| H | -6.954445 | -0.681621 | 0.597951 |
| H | -4.899453 | 0.510695 | 0.005139 |
| C | 1.812365 | 0.782699 | -0.386003 |
| C | 2.630613 | 0.229982 | -1.300519 |
| H | 2.109700 | 1.717017 | 0.092725 |
| H | 2.358597 | -0.738191 | -1.724408 |
| C | 3.925139 | 0.813082 | -1.782003 |
| C | 5.126500 | -0.026055 | -1.293205 |
| H | 4.031300 | 1.846891 | -1.431676 |
| H | 3.937103 | 0.835339 | -2.880885 |
| C | 6.470269 | 0.502620 | -1.806203 |
| H | 5.124016 | -0.039664 | -0.195348 |

| | | | |
|---|---|---|---|
| H | 4.994717 | -1.067725 | -1.616720 |
| H | 6.456912 | 0.516649 | -2.905299 |
| H | 6.595901 | 1.547016 | -1.487454 |
| C | 7.667079 | -0.324265 | -1.322488 |
| C | 9.013995 | 0.192221 | -1.842762 |
| H | 7.535997 | -1.370531 | -1.634458 |
| H | 7.682447 | -0.333264 | -0.223021 |
| C | 10.202930 | -0.639213 | -1.353226 |
| H | 8.997820 | 0.199288 | -2.941450 |
| H | 9.144672 | 1.238013 | -1.532196 |
| H | 11.152595 | -0.248546 | -1.735829 |
| H | 10.260726 | -0.639906 | -0.257992 |
| H | 10.117423 | -1.682839 | -1.679654 |
| C | 1.181848 | -0.761964 | 1.283296 |
| H | 1.651150 | -1.687578 | 0.949737 |
| C | 2.038872 | -0.116274 | 2.379092 |
| N | -0.134589 | -1.404519 | 2.237732 |
| N | -1.230583 | -1.290465 | 2.392229 |
| F | 3.317204 | -0.020480 | 1.964617 |
| F | 2.040184 | -0.851462 | 3.511539 |
| F | 1.611181 | 1.116463 | 2.698058 |
| H | -0.630578 | 3.521456 | 0.393170 |
| H | -0.408110 | -3.317878 | -0.790573 |

Vibrational frequencies

| | | |
|---|---|---|
| -444.9649 | 11.0887 | 16.4914 |
| 28.3599 | 38.4174 | 42.8693 |
| 51.0485 | 53.9573 | 63.3322 |
| 69.8815 | 73.2540 | 79.5376 |
| 80.2298 | 93.4472 | 100.8312 |

| | | |
|---|---|---|
| 121.5100 | 125.5869 | 139.1837 |
| 145.4552 | 154.0298 | 160.7530 |
| 166.7258 | 180.8089 | 205.1201 |
| 221.7193 | 238.1788 | 247.7122 |
| 255.3821 | 266.0312 | 272.0982 |
| 281.0848 | 300.5510 | 315.6123 |
| 328.0571 | 341.2294 | 358.9972 |
| 360.4954 | 396.8821 | 400.9349 |
| 417.9155 | 427.9665 | 443.9262 |
| 446.8598 | 453.5532 | 468.8465 |
| 478.5146 | 498.1828 | 505.2762 |
| 520.5534 | 530.0584 | 543.4169 |
| 552.2101 | 554.0076 | 564.7043 |
| 579.4727 | 586.9581 | 623.6201 |
| 637.6679 | 649.4325 | 667.6397 |
| 673.0404 | 684.5615 | 704.6899 |
| 722.4362 | 750.7684 | 751.9936 |
| 762.1869 | 769.6272 | 770.9360 |
| 777.3056 | 783.7490 | 795.2704 |
| 804.5330 | 806.0414 | 827.8892 |
| 840.3483 | 849.0194 | 860.9967 |
| 867.9430 | 882.2790 | 885.6904 |
| 893.8495 | 907.6403 | 909.9474 |
| 943.6776 | 962.1775 | 963.7767 |
| 966.8187 | 972.5718 | 974.8063 |
| 991.7210 | 997.3063 | 999.7662 |
| 1005.5075 | 1016.2655 | 1022.4338 |
| 1035.0779 | 1036.5621 | 1048.6329 |
| 1059.0790 | 1061.1254 | 1066.4183 |
| 1070.9639 | 1076.0122 | 1099.4294 |

| | | |
|---|---|---|
| 1122.6092 | 1134.4299 | 1136.0241 |
| 1147.9593 | 1154.3382 | 1171.9857 |
| 1173.5575 | 1181.7623 | 1187.7233 |
| 1190.5292 | 1217.7878 | 1218.5931 |
| 1239.6098 | 1243.8498 | 1249.8057 |
| 1260.4934 | 1262.3983 | 1269.3873 |
| 1285.5447 | 1290.4717 | 1295.1911 |
| 1297.1281 | 1307.3047 | 1308.9734 |
| 1323.5973 | 1334.2641 | 1336.5211 |
| 1342.9888 | 1363.7299 | 1367.6991 |
| 1374.7955 | 1396.5768 | 1398.2659 |
| 1402.3262 | 1406.8044 | 1417.2533 |
| 1420.0062 | 1432.0342 | 1466.0027 |
| 1467.3359 | 1480.5647 | 1484.3044 |
| 1488.3011 | 1497.7569 | 1498.3946 |
| 1500.6977 | 1503.1865 | 1508.4476 |
| 1515.3018 | 1553.6721 | 1554.2447 |
| 1606.7702 | 1615.4708 | 1641.8075 |
| 1644.2584 | 1653.7818 | 1669.3729 |
| 1671.2237 | 2330.1074 | 3011.1757 |
| 3015.4823 | 3021.3548 | 3023.3241 |
| 3029.0638 | 3032.0907 | 3036.3194 |
| 3048.5584 | 3061.3625 | 3069.9353 |
| 3084.6125 | 3099.3704 | 3103.9430 |
| 3138.7615 | 3145.7181 | 3178.8324 |
| 3179.1839 | 3185.6649 | 3186.2947 |
| 3186.4266 | 3189.1885 | 3190.5664 |
| 3204.5168 | 3205.6714 | 3207.8923 |
| 3211.5984 | 3223.7634 | 3231.5737 |

**M3R**

Zero-point correction= 0.493764

Thermal correction to Energy= 0.528742

Thermal correction to Enthalpy= 0.529686

Thermal correction to Gibbs Free Energy= 0.421688

Sum of electronic and zero-point Energies= -1656.183454

Sum of electronic and thermal Energies= -1656.148477

Sum of electronic and thermal Enthalpies= -1656.147532

Sum of electronic and thermal Free Energies= -1656.255531

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.348180 | -1.258411 | 0.963916 |
| B | -0.106457 | -0.128298 | 1.698945 |
| C | -1.588326 | -1.551109 | 0.439863 |
| O | -0.967701 | 0.962155 | 1.650939 |
| C | -2.327539 | -0.614017 | -0.269697 |
| C | -2.080864 | -2.864830 | 0.657372 |
| C | -1.162818 | 1.481018 | 0.387666 |
| C | -1.729461 | 0.707147 | -0.615931 |
| C | -3.331208 | -3.222418 | 0.220996 |
| C | -3.680674 | -0.938859 | -0.639123 |
| C | -4.168817 | -2.265585 | -0.408761 |
| C | -0.724453 | 2.807512 | 0.134547 |
| C | -1.706842 | 1.200400 | -1.967058 |
| C | -0.794608 | 3.334235 | -1.130526 |
| C | -1.251320 | 2.536521 | -2.212156 |
| H | -3.706217 | -4.228118 | 0.378237 |
| H | -0.473062 | 4.351517 | -1.326132 |
| C | -1.243218 | 3.045817 | -3.539896 |
| C | -1.635663 | 2.257878 | -4.597579 |
| C | -2.044078 | 0.922194 | -4.365941 |

| | | | |
|---|---|---|---|
| C | -2.081570 | 0.407566 | -3.088134 |
| H | -0.907856 | 4.066636 | -3.701912 |
| H | -1.620267 | 2.651503 | -5.609549 |
| H | -2.326523 | 0.293816 | -5.205610 |
| H | -2.388009 | -0.619917 | -2.934604 |
| C | -5.496858 | -2.604688 | -0.788311 |
| C | -6.331362 | -1.662619 | -1.344440 |
| C | -5.869577 | -0.337510 | -1.531152 |
| C | -4.581421 | 0.015175 | -1.191240 |
| H | -5.842302 | -3.620454 | -0.616332 |
| H | -7.346291 | -1.927203 | -1.626051 |
| H | -6.539762 | 0.411957 | -1.942184 |
| H | -4.254287 | 1.037889 | -1.332521 |
| C | 2.173857 | 0.776722 | 1.579992 |
| C | 2.482901 | 0.366695 | 0.344136 |
| H | 2.566082 | 1.720529 | 1.949747 |
| H | 2.069980 | -0.572162 | -0.025639 |
| C | 3.397934 | 1.094819 | -0.596043 |
| C | 4.653561 | 0.273434 | -0.943916 |
| H | 3.693114 | 2.059408 | -0.164587 |
| H | 2.851293 | 1.314029 | -1.525145 |
| C | 5.559581 | 0.965698 | -1.968244 |
| H | 5.217908 | 0.078616 | -0.022039 |
| H | 4.347821 | -0.708524 | -1.330864 |
| H | 4.990526 | 1.144343 | -2.891907 |
| H | 5.846723 | 1.956956 | -1.589022 |
| C | 6.823603 | 0.162729 | -2.296199 |
| C | 7.725781 | 0.841084 | -3.334617 |
| H | 6.536907 | -0.833834 | -2.662208 |
| H | 7.396780 | -0.005321 | -1.372909 |

| | | | |
|---|---|---|---|
| C | 8.990687 | 0.036070 | -3.645042 |
| H | 7.155277 | 1.000109 | -4.260270 |
| H | 8.006206 | 1.840064 | -2.972697 |
| H | 9.615664 | 0.539264 | -4.391369 |
| H | 9.598897 | -0.107837 | -2.743880 |
| H | 8.740766 | -0.957732 | -4.035908 |
| C | 1.233391 | 0.021583 | 2.516712 |
| H | 1.030132 | 0.640122 | 3.395484 |
| C | 1.842492 | -1.256836 | 3.040052 |
| I | 0.045983 | 4.000400 | 1.735143 |
| I | -0.868284 | -4.304634 | 1.673930 |
| F | 2.166862 | -2.133466 | 2.062187 |
| F | 0.992939 | -1.898237 | 3.882826 |
| F | 2.981266 | -1.021721 | 3.740809 |

Vibrational frequencies

| | | |
|---|---|---|
| 9.1234 | 12.8409 | 24.5514 |
| 32.9888 | 38.2390 | 39.4049 |
| 49.5327 | 60.0407 | 63.7030 |
| 68.1191 | 79.9712 | 85.9810 |
| 92.4505 | 97.2234 | 101.3501 |
| 102.2169 | 109.2129 | 126.2544 |
| 143.1409 | 151.1070 | 157.4824 |
| 164.8808 | 171.6293 | 195.6983 |
| 200.5384 | 219.3460 | 231.2468 |
| 236.4420 | 253.5915 | 267.6233 |
| 270.0757 | 283.7054 | 293.3102 |
| 301.5518 | 316.3045 | 332.8024 |
| 342.3103 | 360.7368 | 379.5323 |
| 396.7748 | 438.2459 | 447.7155 |

| | | |
|---|---|---|
| 454.4587 | 459.2151 | 462.0760 |
| 474.5056 | 512.5260 | 519.5839 |
| 522.0571 | 532.4813 | 551.8533 |
| 560.1358 | 566.0538 | 581.6263 |
| 585.1489 | 596.5506 | 612.5826 |
| 649.4327 | 651.6087 | 657.3014 |
| 679.3081 | 713.4414 | 722.9492 |
| 731.8832 | 746.5783 | 752.1614 |
| 758.5108 | 762.1414 | 770.6576 |
| 772.1704 | 783.1554 | 800.4459 |
| 807.8905 | 825.0223 | 828.2452 |
| 831.8970 | 876.6467 | 879.7638 |
| 883.0611 | 895.6656 | 907.7746 |
| 911.1437 | 913.5230 | 913.8487 |
| 951.7235 | 974.6234 | 976.1193 |
| 978.0021 | 979.8111 | 1005.3580 |
| 1007.2955 | 1008.8491 | 1014.8124 |
| 1016.7340 | 1028.3641 | 1042.0823 |
| 1059.8599 | 1060.8756 | 1063.4604 |
| 1073.0469 | 1086.1061 | 1098.8185 |
| 1107.4940 | 1137.2920 | 1141.6335 |
| 1164.7726 | 1166.0549 | 1183.7323 |
| 1190.0089 | 1195.5531 | 1199.1698 |
| 1222.0791 | 1239.7102 | 1242.8408 |
| 1248.9780 | 1250.7632 | 1263.4358 |
| 1270.3694 | 1274.8398 | 1282.4082 |
| 1287.2095 | 1299.8557 | 1310.7008 |
| 1317.3838 | 1323.9041 | 1338.9342 |
| 1340.8588 | 1344.0778 | 1354.7974 |
| 1356.9155 | 1364.4881 | 1374.4216 |

| | | |
|---|---|---|
| 1385.7349 | 1402.5295 | 1404.5847 |
| 1405.0576 | 1408.2109 | 1420.2847 |
| 1423.2292 | 1427.2575 | 1447.8109 |
| 1455.1964 | 1474.5601 | 1478.9416 |
| 1480.5462 | 1484.0722 | 1488.7606 |
| 1498.2405 | 1498.5236 | 1508.2923 |
| 1514.7635 | 1541.5368 | 1543.1321 |
| 1604.5030 | 1614.7632 | 1619.9964 |
| 1623.1486 | 1667.5719 | 1668.4367 |
| 1722.1832 | 3011.1704 | 3013.6576 |
| 3014.8102 | 3021.8245 | 3026.1947 |
| 3033.7775 | 3034.6061 | 3045.6087 |
| 3057.7857 | 3066.4181 | 3079.1121 |
| 3101.0876 | 3105.0636 | 3105.3978 |
| 3153.9839 | 3184.5821 | 3187.4043 |
| 3188.6361 | 3197.0786 | 3197.1522 |
| 3210.5909 | 3211.8517 | 3214.1394 |
| 3215.2406 | 3230.1141 | 3231.6904 |

**M3S**

Zero-point correction= 0.493343

Thermal correction to Energy= 0.528600

Thermal correction to Enthalpy= 0.529544

Thermal correction to Gibbs Free Energy= 0.418655

Sum of electronic and zero-point Energies= -1656.182923

Sum of electronic and thermal Energies= -1656.147666

Sum of electronic and thermal Enthalpies= -1656.146722

Sum of electronic and thermal Free Energies= -1656.257611

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.468017 | -1.579823 | -0.099696 |

| | | | |
|---|---|---|---|
| B | 0.033581 | -0.692295 | 0.827071 |
| C | -1.821295 | -1.840032 | -0.114115 |
| O | -0.622402 | 0.473018 | 1.146217 |
| C | -2.754991 | -0.826924 | -0.273166 |
| C | -2.221741 | -3.188689 | 0.074182 |
| C | -1.322476 | 1.163746 | 0.177494 |
| C | -2.296544 | 0.553038 | -0.601432 |
| C | -3.551289 | -3.519635 | 0.138567 |
| C | -4.149186 | -1.137778 | -0.093903 |
| C | -4.541949 | -2.504821 | 0.081826 |
| C | -0.985253 | 2.530514 | -0.009421 |
| C | -2.834973 | 1.272924 | -1.725493 |
| C | -1.570577 | 3.263579 | -1.010842 |
| C | -2.479899 | 2.648258 | -1.909339 |
| H | -3.860668 | -4.551242 | 0.268220 |
| H | -1.322309 | 4.310519 | -1.148286 |
| C | -3.023578 | 3.378139 | -3.002142 |
| C | -3.862547 | 2.768293 | -3.906312 |
| C | -4.180297 | 1.396771 | -3.755780 |
| C | -3.684041 | 0.669591 | -2.695741 |
| H | -2.750806 | 4.423986 | -3.114111 |
| H | -4.269448 | 3.329775 | -4.742071 |
| H | -4.818676 | 0.909980 | -4.487385 |
| H | -3.931395 | -0.381181 | -2.606890 |
| C | -5.918485 | -2.830094 | 0.230804 |
| C | -6.876621 | -1.842638 | 0.241668 |
| C | -6.489816 | -0.486446 | 0.117854 |
| C | -5.165599 | -0.142413 | -0.046784 |
| H | -6.194856 | -3.874311 | 0.349486 |
| H | -7.925495 | -2.097729 | 0.360969 |

| | | | |
|---|---|---|---|
| H | -7.245050 | 0.293209 | 0.158460 |
| H | -4.892474 | 0.902278 | -0.128549 |
| C | 2.438713 | -0.136173 | 0.692746 |
| C | 3.186897 | -0.563857 | -0.329385 |
| H | 2.458927 | 0.912829 | 0.982291 |
| H | 3.143128 | -1.616811 | -0.613835 |
| C | 4.125841 | 0.299434 | -1.122579 |
| C | 5.595328 | -0.140588 | -0.982718 |
| H | 4.022901 | 1.347123 | -0.813219 |
| H | 3.846847 | 0.254509 | -2.185773 |
| C | 6.555992 | 0.709393 | -1.821588 |
| H | 5.884353 | -0.087693 | 0.075488 |
| H | 5.688218 | -1.195819 | -1.275111 |
| H | 6.266292 | 0.646259 | -2.880307 |
| H | 6.446866 | 1.765918 | -1.537691 |
| C | 8.023551 | 0.293805 | -1.669468 |
| C | 8.987645 | 1.143585 | -2.505935 |
| H | 8.134473 | -0.763257 | -1.951367 |
| H | 8.310865 | 0.358143 | -0.610028 |
| C | 10.452555 | 0.731681 | -2.334836 |
| H | 8.706542 | 1.071885 | -3.565808 |
| H | 8.869496 | 2.200499 | -2.229718 |
| H | 11.119063 | 1.352034 | -2.944661 |
| H | 10.770921 | 0.828501 | -1.289772 |
| H | 10.607444 | -0.313105 | -2.630339 |
| C | 1.456538 | -1.007748 | 1.448236 |
| H | 1.675992 | -2.066801 | 1.282538 |
| C | 1.531559 | -0.789117 | 2.939672 |
| I | 0.440957 | 3.471438 | 1.278426 |
| I | -0.733679 | -4.713582 | 0.277912 |

| | | | |
|---|---|---|---|
| F | 2.728680 | -1.170910 | 3.448536 |
| F | 0.580301 | -1.509243 | 3.590266 |
| F | 1.356368 | 0.505003 | 3.294254 |

Vibrational frequencies

| | | |
|---|---|---|
| 4.4665 | 8.9252 | 18.4096 |
| 28.4563 | 30.8720 | 38.1567 |
| 41.2811 | 54.9213 | 55.8883 |
| 59.7412 | 64.0304 | 75.3082 |
| 79.3780 | 91.9897 | 96.8439 |
| 102.0595 | 125.9414 | 130.2517 |
| 143.6548 | 148.0157 | 155.9392 |
| 158.3599 | 167.5173 | 196.4570 |
| 198.1673 | 212.0033 | 221.2549 |
| 235.5484 | 253.9000 | 264.6835 |
| 270.8742 | 276.2501 | 293.1030 |
| 305.6219 | 311.9547 | 332.0187 |
| 335.4076 | 367.5163 | 381.0626 |
| 392.8585 | 434.2529 | 445.4973 |
| 448.4985 | 456.9465 | 459.6597 |
| 485.4555 | 506.5084 | 515.5988 |
| 519.0300 | 538.5369 | 552.1465 |
| 558.6193 | 565.9713 | 571.8816 |
| 584.3982 | 595.0973 | 609.6363 |
| 638.8223 | 650.7655 | 663.2372 |
| 678.0984 | 695.1705 | 713.7640 |
| 736.7497 | 747.5383 | 749.7825 |
| 753.1571 | 761.0772 | 768.1410 |
| 769.9509 | 782.0959 | 801.1971 |
| 807.2533 | 827.9114 | 837.3646 |

| | | |
|---|---|---|
| 852.1941 | 876.3895 | 877.4302 |
| 882.9670 | 900.3575 | 907.6502 |
| 910.2657 | 912.3533 | 913.7413 |
| 951.4698 | 972.4731 | 976.3626 |
| 978.8128 | 988.7387 | 1002.8026 |
| 1004.8549 | 1012.4351 | 1015.6110 |
| 1018.8524 | 1031.9312 | 1054.8478 |
| 1060.5785 | 1062.6771 | 1064.2675 |
| 1073.2322 | 1089.9891 | 1102.3234 |
| 1110.5292 | 1136.5754 | 1140.7754 |
| 1164.4730 | 1174.5370 | 1182.3899 |
| 1188.3620 | 1191.6204 | 1198.5929 |
| 1223.5543 | 1237.7321 | 1241.7142 |
| 1246.5339 | 1251.6085 | 1262.2854 |
| 1266.8699 | 1279.0589 | 1282.1758 |
| 1298.6429 | 1300.2594 | 1304.4620 |
| 1313.5775 | 1319.7312 | 1334.9616 |
| 1338.5901 | 1339.7950 | 1344.8005 |
| 1346.2528 | 1361.5849 | 1368.5067 |
| 1395.1176 | 1403.1471 | 1404.0440 |
| 1406.1139 | 1407.7952 | 1419.2284 |
| 1423.5556 | 1427.4143 | 1447.5190 |
| 1455.4128 | 1474.5236 | 1480.3417 |
| 1481.2542 | 1483.6992 | 1488.0791 |
| 1497.6531 | 1500.2586 | 1507.3547 |
| 1514.2609 | 1541.2756 | 1542.4512 |
| 1605.4563 | 1615.1519 | 1620.1438 |
| 1622.6149 | 1667.3576 | 1668.3305 |
| 1733.6639 | 3011.0825 | 3013.6632 |
| 3014.6800 | 3021.9760 | 3025.4855 |

| | | |
|---|---|---|
| 3032.2638 | 3034.5948 | 3045.5561 |
| 3057.3938 | 3065.6223 | 3077.8428 |
| 3098.9916 | 3100.1500 | 3104.1401 |
| 3138.9299 | 3174.1605 | 3188.7427 |
| 3189.0930 | 3197.6244 | 3199.2746 |
| 3210.7990 | 3212.1027 | 3215.0522 |
| 3217.5367 | 3232.0708 | 3235.4810 |

**M04R**

Zero-point correction= 0.658845

Thermal correction to Energy= 0.703640

Thermal correction to Enthalpy= 0.704585

Thermal correction to Gibbs Free Energy= 0.574899

Sum of electronic and zero-point Energies= -1966.183112

Sum of electronic and thermal Energies= -1966.138317

Sum of electronic and thermal Enthalpies= -1966.137373

Sum of electronic and thermal Free Energies= -1966.267059

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.339979 | -1.261206 | 1.256236 |
| B | -0.319467 | -0.184746 | 2.219605 |
| C | -1.329689 | -1.487369 | 0.369892 |
| O | -1.220205 | 0.940249 | 1.917051 |
| C | -1.896620 | -0.476405 | -0.412239 |
| C | -1.754438 | -2.837103 | 0.169115 |
| C | -1.040019 | 1.563633 | 0.730335 |
| C | -1.279660 | 0.880101 | -0.457961 |
| C | -2.805709 | -3.150312 | -0.653405 |
| C | -3.066222 | -0.766893 | -1.197199 |
| C | -3.519354 | -2.119990 | -1.318713 |

| | | | |
|---|---|---|---|
| C | -0.598825 | 2.915016 | 0.694644 |
| C | -0.868094 | 1.472072 | -1.701328 |
| C | -0.305021 | 3.543830 | -0.487765 |
| C | -0.391913 | 2.824455 | -1.708831 |
| H | -3.111691 | -4.181200 | -0.796931 |
| H | 0.034842 | 4.573903 | -0.504753 |
| C | 0.022971 | 3.420963 | -2.931287 |
| C | 0.007140 | 2.704088 | -4.105843 |
| C | -0.425290 | 1.355561 | -4.099289 |
| C | -0.856114 | 0.758404 | -2.934267 |
| H | 0.370561 | 4.450656 | -2.914359 |
| H | 0.337573 | 3.162832 | -5.033160 |
| H | -0.412498 | 0.783189 | -5.022508 |
| H | -1.172409 | -0.277420 | -2.950187 |
| C | -4.666443 | -2.415962 | -2.104720 |
| C | -5.364477 | -1.412382 | -2.737644 |
| C | -4.940655 | -0.068527 | -2.597629 |
| C | -3.823413 | 0.245304 | -1.854000 |
| H | -4.984114 | -3.452024 | -2.189116 |
| H | -6.242617 | -1.645125 | -3.332955 |
| H | -5.504855 | 0.725516 | -3.078708 |
| H | -3.522388 | 1.281215 | -1.752909 |
| C | 1.898384 | 0.793871 | 1.255440 |
| C | 2.236063 | 0.045651 | 0.199962 |
| H | 2.060317 | 1.869271 | 1.203237 |
| H | 2.059753 | -1.028363 | 0.231276 |
| C | 2.834651 | 0.592242 | -1.065632 |
| C | 4.245879 | 0.054474 | -1.362776 |
| H | 2.863451 | 1.688798 | -1.018701 |
| H | 2.177978 | 0.336006 | -1.910520 |

| | | | |
|---|---|---|---|
| C | 4.828602 | 0.613923 | -2.665280 |
| H | 4.908986 | 0.305188 | -0.523466 |
| H | 4.215305 | -1.043046 | -1.413502 |
| H | 4.158739 | 0.360685 | -3.499811 |
| H | 4.843187 | 1.712208 | -2.610002 |
| C | 6.241014 | 0.104850 | -2.975460 |
| C | 6.825750 | 0.684580 | -4.269111 |
| H | 6.226608 | -0.992672 | -3.043705 |
| H | 6.908119 | 0.349178 | -2.136003 |
| C | 8.237130 | 0.173159 | -4.572702 |
| H | 6.158983 | 0.441139 | -5.107911 |
| H | 6.839691 | 1.781163 | -4.198527 |
| H | 8.631329 | 0.602858 | -5.500694 |
| H | 8.933139 | 0.430476 | -3.764962 |
| H | 8.247305 | -0.918278 | -4.680850 |
| C | 1.227181 | 0.291579 | 2.519919 |
| H | 1.177709 | 1.117251 | 3.238270 |
| C | 2.063179 | -0.754717 | 3.220109 |
| I | -0.333532 | 3.977600 | 2.541316 |
| I | -0.664247 | -4.435679 | 1.102833 |
| F | 2.061345 | -1.962001 | 2.594681 |
| F | 1.638561 | -0.984317 | 4.492494 |
| F | 3.372645 | -0.393650 | 3.333097 |
| C | -0.936906 | -2.872492 | 4.631614 |
| C | -1.727748 | -1.872458 | 3.815202 |
| H | -1.538747 | -3.774245 | 4.785551 |
| H | -0.018038 | -3.150473 | 4.111637 |
| H | -0.675999 | -2.454213 | 5.608405 |
| H | -2.018804 | -2.267212 | 2.844679 |
| H | -2.629996 | -1.542903 | 4.336207 |

| | | | |
|---|---|---|---|
| O | -0.915838 | -0.682065 | 3.582599 |
| H | -1.205745 | 0.110189 | 4.171553 |
| C | -3.933646 | 0.987061 | 5.561037 |
| C | -3.063062 | 1.610602 | 4.489583 |
| H | -4.989289 | 1.142961 | 5.316294 |
| H | -3.758421 | -0.091106 | 5.637158 |
| H | -3.731575 | 1.439032 | 6.537010 |
| H | -3.264302 | 1.185324 | 3.499784 |
| H | -3.225116 | 2.692040 | 4.433858 |
| O | -1.668854 | 1.372736 | 4.832988 |
| H | -1.139767 | 2.022387 | 4.335554 |

Vibrational frequencies

| | | |
|---|---|---|
| 9.2851 | 13.2263 | 21.2777 |
| 26.1950 | 32.5248 | 33.9646 |
| 38.9530 | 42.4213 | 47.4723 |
| 52.6864 | 54.3444 | 59.8108 |
| 68.7941 | 72.3192 | 83.5748 |
| 85.9128 | 89.0920 | 93.7458 |
| 94.7659 | 100.7670 | 102.6383 |
| 104.1881 | 118.8378 | 128.7828 |
| 131.8679 | 133.4481 | 144.8549 |
| 156.3487 | 160.2052 | 162.4942 |
| 188.6030 | 198.4679 | 208.8542 |
| 214.9971 | 224.9799 | 235.0373 |
| 237.9491 | 241.0112 | 252.0896 |
| 255.2814 | 266.6877 | 277.9848 |
| 288.6068 | 298.5157 | 304.8288 |
| 309.7700 | 310.4750 | 334.1278 |
| 340.7894 | 351.2685 | 364.7435 |

| | | |
|---|---|---|
| 381.4330 | 407.0375 | 416.2821 |
| 434.6121 | 441.0108 | 450.7599 |
| 455.2179 | 458.7004 | 478.4812 |
| 489.3453 | 503.7179 | 512.7609 |
| 519.3454 | 532.0283 | 536.8022 |
| 560.2192 | 563.7012 | 564.3556 |
| 570.2861 | 583.5128 | 594.8852 |
| 609.3678 | 625.0299 | 649.4937 |
| 659.8435 | 673.6798 | 705.3785 |
| 720.2895 | 734.3397 | 737.1860 |
| 745.4496 | 750.9578 | 760.3539 |
| 766.2640 | 770.0905 | 780.3702 |
| 783.6418 | 802.4389 | 807.4972 |
| 815.7737 | 820.4456 | 824.7474 |
| 828.7796 | 838.4251 | 872.4080 |
| 873.8404 | 875.9075 | 882.9303 |
| 885.8107 | 902.8050 | 903.6971 |
| 905.1997 | 906.4589 | 907.2904 |
| 948.5805 | 970.0438 | 973.6928 |
| 977.3366 | 981.3790 | 989.4521 |
| 999.2853 | 1002.6255 | 1004.5475 |
| 1011.6797 | 1018.4032 | 1030.2585 |
| 1032.5559 | 1041.1319 | 1046.7392 |
| 1054.8449 | 1059.5777 | 1061.0297 |
| 1069.5855 | 1071.0626 | 1079.2793 |
| 1087.8827 | 1096.2086 | 1110.2608 |
| 1115.7353 | 1121.3532 | 1137.2640 |
| 1143.0013 | 1164.3273 | 1165.3638 |
| 1182.2970 | 1184.4064 | 1190.0050 |
| 1192.0218 | 1195.6815 | 1223.0589 |

| | | |
|---|---|---|
| 1239.4541 | 1242.4660 | 1247.4394 |
| 1251.3993 | 1259.9901 | 1274.4668 |
| 1281.2502 | 1283.2391 | 1285.5166 |
| 1292.2772 | 1307.8186 | 1311.1912 |
| 1312.9909 | 1320.0375 | 1333.5723 |
| 1340.5219 | 1341.1315 | 1342.1400 |
| 1345.2944 | 1356.8668 | 1366.5789 |
| 1370.1602 | 1384.9367 | 1397.5804 |
| 1403.6581 | 1404.2127 | 1405.8265 |
| 1406.1792 | 1411.0648 | 1419.1861 |
| 1422.0715 | 1424.6234 | 1437.7922 |
| 1450.4945 | 1451.7786 | 1452.7171 |
| 1476.8935 | 1481.0214 | 1481.1789 |
| 1483.3512 | 1484.1537 | 1484.2891 |
| 1487.5986 | 1489.4873 | 1495.3773 |
| 1495.9161 | 1498.3215 | 1507.7239 |
| 1514.5310 | 1522.2081 | 1531.0059 |
| 1537.5798 | 1539.6406 | 1592.0158 |
| 1605.7225 | 1620.0476 | 1622.7239 |
| 1650.6697 | 1665.9238 | 1666.4523 |
| 1731.9550 | 2625.0382 | 3008.1290 |
| 3010.4244 | 3011.7027 | 3021.0016 |
| 3022.7504 | 3030.8676 | 3032.3556 |
| 3042.5991 | 3051.7559 | 3051.8219 |
| 3058.5462 | 3059.1809 | 3062.6156 |
| 3072.7157 | 3073.2969 | 3097.8681 |
| 3101.8871 | 3102.3659 | 3113.3534 |
| 3129.1466 | 3130.5394 | 3133.0548 |
| 3155.1987 | 3156.4422 | 3171.1757 |
| 3184.0905 | 3185.2057 | 3192.2171 |

| | | |
|---|---|---|
| 3194.2749 | 3202.6495 | 3208.1307 |
| 3208.3828 | 3211.7340 | 3212.0084 |
| 3230.7800 | 3232.1995 | 3685.9127 |

**M04S**

Zero-point correction= 0.659065

Thermal correction to Energy= 0.703658

Thermal correction to Enthalpy= 0.704603

Thermal correction to Gibbs Free Energy= 0.576881

Sum of electronic and zero-point Energies= -1966.185668

Sum of electronic and thermal Energies= -1966.141075

Sum of electronic and thermal Enthalpies= -1966.140131

Sum of electronic and thermal Free Energies= -1966.267853

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.607009 | -2.145158 | 0.774917 |
| B | -0.506246 | -1.168697 | 1.840124 |
| C | -1.678029 | -2.285436 | -0.033931 |
| O | -1.249033 | 0.087950 | 1.631568 |
| C | -2.255899 | -1.201845 | -0.697392 |
| C | -2.177169 | -3.599684 | -0.286955 |
| C | -1.185793 | 0.742318 | 0.452779 |
| C | -1.565184 | 0.118619 | -0.733291 |
| C | -3.316092 | -3.808922 | -1.021712 |
| C | -3.511042 | -1.383712 | -1.377268 |
| C | -4.041617 | -2.704358 | -1.538249 |
| C | -0.784435 | 2.109682 | 0.429019 |
| C | -1.280108 | 0.765718 | -1.986283 |
| C | -0.607185 | 2.786409 | -0.749692 |
| C | -0.801137 | 2.116088 | -1.986429 |
| H | -3.680598 | -4.813429 | -1.208805 |

| | | | |
|---|---|---|---|
| H | -0.300285 | 3.826955 | -0.755257 |
| C | -0.521370 | 2.767831 | -3.218411 |
| C | -0.682567 | 2.108973 | -4.416303 |
| C | -1.124474 | 0.763965 | -4.422551 |
| C | -1.418954 | 0.112452 | -3.244112 |
| H | -0.166219 | 3.794746 | -3.192979 |
| H | -0.460470 | 2.611638 | -5.353168 |
| H | -1.226594 | 0.236268 | -5.366697 |
| H | -1.742047 | -0.921201 | -3.271088 |
| C | -5.271665 | -2.896066 | -2.224662 |
| C | -5.977199 | -1.822129 | -2.718084 |
| C | -5.476884 | -0.510516 | -2.532367 |
| C | -4.278712 | -0.296807 | -1.885409 |
| H | -5.646152 | -3.909501 | -2.343586 |
| H | -6.918554 | -1.975266 | -3.237756 |
| H | -6.046530 | 0.338373 | -2.900054 |
| H | -3.920107 | 0.716079 | -1.745835 |
| C | 1.744099 | -0.082886 | 1.170962 |
| C | 2.296320 | -0.441789 | 0.008825 |
| H | 1.675054 | 0.974762 | 1.421587 |
| H | 2.351082 | -1.502322 | -0.244407 |
| C | 2.869055 | 0.509549 | -1.004517 |
| C | 4.381800 | 0.313991 | -1.214053 |
| H | 2.668179 | 1.544745 | -0.700154 |
| H | 2.361613 | 0.363912 | -1.969576 |
| C | 4.969863 | 1.249152 | -2.276658 |
| H | 4.898160 | 0.471840 | -0.257298 |
| H | 4.575071 | -0.730024 | -1.498548 |
| H | 4.448786 | 1.086763 | -3.231218 |
| H | 4.768558 | 2.292190 | -1.992645 |

| | | | |
|---|---|---|---|
| C | 6.477642 | 1.061301 | -2.480994 |
| C | 7.075214 | 1.998655 | -3.537427 |
| H | 6.678540 | 0.018746 | -2.767541 |
| H | 6.996010 | 1.218954 | -1.524029 |
| C | 8.582697 | 1.804626 | -3.724911 |
| H | 6.562036 | 1.838209 | -4.495865 |
| H | 6.872046 | 3.040338 | -3.252554 |
| H | 8.986343 | 2.485840 | -4.482566 |
| H | 9.124586 | 1.989087 | -2.789315 |
| H | 8.813327 | 0.780248 | -4.041714 |
| C | 1.105601 | -1.036959 | 2.147464 |
| H | 1.518500 | -2.041170 | 1.997591 |
| C | 1.467578 | -0.677973 | 3.565315 |
| I | -0.513931 | 3.149163 | 2.284769 |
| I | -1.060203 | -5.309115 | 0.381157 |
| F | 2.787208 | -0.379797 | 3.716950 |
| F | 1.215313 | -1.688668 | 4.440875 |
| F | 0.788067 | 0.406717 | 4.031761 |
| C | -0.826892 | -3.932562 | 3.945156 |
| C | -1.846470 | -2.971141 | 3.373869 |
| H | -1.298167 | -4.909958 | 4.090624 |
| H | 0.012618 | -4.057896 | 3.257592 |
| H | -0.448704 | -3.575395 | 4.905746 |
| H | -2.264799 | -3.325976 | 2.432774 |
| H | -2.668621 | -2.794122 | 4.071728 |
| O | -1.241065 | -1.666469 | 3.139009 |
| H | -1.744713 | -0.900795 | 3.614037 |
| C | -1.502794 | -0.334283 | 6.336785 |
| C | -1.929692 | 0.809188 | 5.437260 |
| H | -1.176697 | 0.059070 | 7.304913 |

| | | | |
|---|---|---|---|
| H | -2.335557 | -1.023658 | 6.511683 |
| H | -0.670125 | -0.885121 | 5.892209 |
| H | -2.719397 | 1.408037 | 5.905879 |
| H | -1.082955 | 1.464631 | 5.213791 |
| O | -2.455529 | 0.255458 | 4.202991 |
| H | -2.356791 | 0.908930 | 3.489296 |

Vibrational frequencies

| | | |
|---|---|---|
| 12.6156 | 14.5536 | 22.2846 |
| 31.4779 | 38.1548 | 40.6203 |
| 43.0570 | 44.9233 | 52.1347 |
| 55.5271 | 63.1018 | 71.6827 |
| 73.9893 | 78.2410 | 81.4392 |
| 83.9295 | 90.3369 | 95.2615 |
| 98.3008 | 101.5638 | 109.8972 |
| 115.2807 | 126.8853 | 131.2780 |
| 138.7270 | 145.3203 | 152.9628 |
| 160.7263 | 162.4590 | 169.4530 |
| 182.9963 | 195.1873 | 210.9257 |
| 213.3180 | 219.2405 | 234.9053 |
| 238.5463 | 247.7040 | 249.8549 |
| 255.8864 | 267.4762 | 276.6196 |
| 290.7337 | 295.2753 | 299.7716 |
| 303.4074 | 309.3446 | 330.7315 |
| 339.9480 | 350.1007 | 368.8789 |
| 380.4721 | 398.7841 | 413.9294 |
| 428.2092 | 446.2177 | 449.4688 |
| 457.3367 | 463.8576 | 477.9309 |
| 492.8308 | 501.6468 | 510.2093 |
| 517.4714 | 530.9756 | 536.3553 |

| | | |
|---|---|---|
| 540.8901 | 559.9303 | 564.0381 |
| 565.2800 | 582.8427 | 590.8996 |
| 593.0187 | 618.1210 | 655.6080 |
| 657.6152 | 670.5522 | 693.3792 |
| 718.9548 | 729.8909 | 735.3256 |
| 743.1079 | 748.2300 | 758.3144 |
| 761.2644 | 767.8684 | 773.8005 |
| 780.0291 | 804.6199 | 812.1436 |
| 822.4624 | 825.2461 | 830.2751 |
| 834.7069 | 844.3037 | 870.9569 |
| 876.1047 | 882.8343 | 885.6385 |
| 891.8270 | 898.8746 | 904.2830 |
| 905.3721 | 907.5967 | 908.9180 |
| 949.0737 | 966.6869 | 969.9580 |
| 973.5605 | 991.0536 | 998.6881 |
| 1002.7172 | 1005.2587 | 1010.0948 |
| 1013.9721 | 1026.0368 | 1032.6785 |
| 1038.6117 | 1044.1161 | 1051.3667 |
| 1053.7402 | 1062.0024 | 1065.2620 |
| 1068.5968 | 1073.3302 | 1074.8911 |
| 1099.3879 | 1104.1973 | 1111.7092 |
| 1115.2221 | 1121.1728 | 1137.2334 |
| 1141.7017 | 1164.0615 | 1179.3410 |
| 1184.2928 | 1187.2629 | 1188.6756 |
| 1193.3542 | 1197.1897 | 1205.8183 |
| 1226.7690 | 1240.4562 | 1241.8747 |
| 1254.0006 | 1262.7074 | 1270.5474 |
| 1274.3919 | 1280.5856 | 1286.2757 |
| 1290.3926 | 1305.7079 | 1310.9786 |
| 1314.5506 | 1322.8354 | 1328.8740 |

| | | |
|---|---|---|
| 1339.3196 | 1339.5393 | 1340.7590 |
| 1343.9070 | 1348.8526 | 1365.4786 |
| 1368.4616 | 1395.8651 | 1398.0038 |
| 1403.1821 | 1405.5288 | 1407.3416 |
| 1408.5643 | 1410.2904 | 1419.5671 |
| 1424.7586 | 1425.9949 | 1439.2048 |
| 1448.2112 | 1450.9378 | 1451.8837 |
| 1476.8053 | 1480.7276 | 1483.6546 |
| 1484.9165 | 1485.6974 | 1488.7069 |
| 1491.4944 | 1493.7575 | 1496.5736 |
| 1498.7281 | 1503.8104 | 1508.1328 |
| 1515.0459 | 1523.6013 | 1532.9411 |
| 1536.9630 | 1539.7556 | 1593.9861 |
| 1604.7664 | 1614.2661 | 1621.0155 |
| 1626.6646 | 1666.1007 | 1666.5433 |
| 1745.1509 | 2565.0942 | 3010.8190 |
| 3013.2062 | 3014.6004 | 3021.4486 |
| 3023.5777 | 3033.1246 | 3034.1052 |
| 3044.2782 | 3054.6096 | 3055.1328 |
| 3056.7940 | 3063.2584 | 3064.8918 |
| 3070.6360 | 3075.3109 | 3100.8294 |
| 3103.4928 | 3103.6955 | 3109.6868 |
| 3129.5598 | 3133.4832 | 3139.3138 |
| 3150.3886 | 3152.4090 | 3164.3860 |
| 3182.5467 | 3184.1247 | 3185.0623 |
| 3192.5010 | 3194.3994 | 3208.4981 |
| 3208.6749 | 3210.2348 | 3210.5322 |
| 3225.2884 | 3232.1566 | 3737.5644 |

**TS4R**

Zero-point correction= 0.655853

Thermal correction to Energy= 0.699516

Thermal correction to Enthalpy= 0.700460

Thermal correction to Gibbs Free Energy= 0.574747

Sum of electronic and zero-point Energies= -1966.170982

Sum of electronic and thermal Energies= -1966.127319

Sum of electronic and thermal Enthalpies= -1966.126375

Sum of electronic and thermal Free Energies= -1966.252088

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.145727 | -1.034905 | 1.281507 |
| B | -0.038986 | -0.085028 | 2.383620 |
| C | -1.255727 | -1.248303 | 0.554058 |
| O | -0.880199 | 1.219591 | 2.033568 |
| C | -1.920561 | -0.218839 | -0.122708 |
| C | -1.731358 | -2.587985 | 0.385462 |
| C | -0.812183 | 1.810230 | 0.799820 |
| C | -1.259395 | 1.104848 | -0.303384 |
| C | -2.927871 | -2.858228 | -0.227440 |
| C | -3.223432 | -0.461405 | -0.678737 |
| C | -3.737031 | -1.797543 | -0.713138 |
| C | -0.292809 | 3.124486 | 0.680887 |
| C | -1.026528 | 1.655280 | -1.611755 |
| C | -0.139755 | 3.703978 | -0.552347 |
| C | -0.469788 | 2.972239 | -1.724535 |
| H | -3.275518 | -3.879756 | -0.339810 |
| H | 0.257037 | 4.708581 | -0.651784 |
| C | -0.235152 | 3.529328 | -3.011622 |
| C | -0.511958 | 2.809320 | -4.151407 |
| C | -1.029575 | 1.495798 | -4.045396 |
| C | -1.282842 | 0.935103 | -2.812093 |

| | | | |
|---|---|---|---|
| H | 0.179567 | 4.531777 | -3.075087 |
| H | -0.323243 | 3.239469 | -5.130642 |
| H | -1.223783 | 0.920803 | -4.946243 |
| H | -1.665936 | -0.076225 | -2.752191 |
| C | -5.027676 | -2.045675 | -1.253308 |
| C | -5.803682 | -1.010924 | -1.726131 |
| C | -5.311399 | 0.315670 | -1.674889 |
| C | -4.056223 | 0.583635 | -1.171508 |
| H | -5.392108 | -3.069365 | -1.277733 |
| H | -6.792147 | -1.206954 | -2.131135 |
| H | -5.931749 | 1.132826 | -2.032137 |
| H | -3.701519 | 1.607240 | -1.132658 |
| C | 2.135189 | 0.920131 | 1.265096 |
| C | 2.411602 | 0.165031 | 0.197259 |
| H | 2.354193 | 1.985802 | 1.221580 |
| H | 2.185967 | -0.899462 | 0.229780 |
| C | 3.041423 | 0.672331 | -1.069554 |
| C | 4.433615 | 0.062400 | -1.315572 |
| H | 3.116452 | 1.767518 | -1.041037 |
| H | 2.394216 | 0.423952 | -1.924080 |
| C | 5.078022 | 0.520883 | -2.628625 |
| H | 5.088291 | 0.321138 | -0.472051 |
| H | 4.351256 | -1.033664 | -1.313039 |
| H | 4.415624 | 0.263093 | -3.467671 |
| H | 5.160128 | 1.617471 | -2.630158 |
| C | 6.462238 | -0.092855 | -2.867487 |
| C | 7.117296 | 0.359273 | -4.178547 |
| H | 6.377622 | -1.189352 | -2.865294 |
| H | 7.122743 | 0.162685 | -2.026177 |
| C | 8.495674 | -0.267864 | -4.406146 |

| | | | |
|---|---|---|---|
| H | 6.456120 | 0.106637 | -5.019134 |
| H | 7.207332 | 1.454515 | -4.179025 |
| H | 8.942338 | 0.070405 | -5.347903 |
| H | 9.187617 | -0.006009 | -3.596432 |
| H | 8.430928 | -1.362155 | -4.442322 |
| C | 1.516247 | 0.422022 | 2.557983 |
| H | 1.476754 | 1.253137 | 3.269753 |
| C | 2.414125 | -0.588830 | 3.225373 |
| I | 0.255314 | 4.198863 | 2.450262 |
| I | -0.489635 | -4.231698 | 0.988791 |
| F | 2.409056 | -1.804759 | 2.608878 |
| F | 2.067891 | -0.810235 | 4.519674 |
| F | 3.720808 | -0.199441 | 3.259812 |
| C | -0.185984 | -2.747569 | 4.511053 |
| C | -1.205475 | -1.799360 | 3.901681 |
| H | -0.670153 | -3.705314 | 4.733375 |
| H | 0.640194 | -2.930073 | 3.823136 |
| H | 0.219243 | -2.335270 | 5.439157 |
| H | -1.627258 | -2.225112 | 2.989133 |
| H | -2.036996 | -1.662363 | 4.604911 |
| O | -0.672595 | -0.490370 | 3.643158 |
| H | -1.944342 | 0.538196 | 4.062991 |
| C | -4.631422 | 0.145636 | 4.329289 |
| C | -3.775823 | 0.632920 | 3.182293 |
| H | -5.551453 | -0.293601 | 3.930722 |
| H | -4.111163 | -0.623798 | 4.909073 |
| H | -4.898354 | 0.970744 | 4.995896 |
| H | -3.489461 | -0.176677 | 2.503686 |
| H | -4.269163 | 1.416680 | 2.604342 |
| O | -2.548989 | 1.258997 | 3.702557 |

| | | | |
|---|---|---|---|
| H | -1.820543 | 1.427522 | 2.817559 |

Vibrational frequencies

| | | |
|---|---|---|
| -383.7891 | 11.1536 | 16.7494 |
| 17.4831 | 24.6980 | 33.4598 |
| 36.4026 | 43.9640 | 46.1847 |
| 55.2581 | 63.4621 | 70.9836 |
| 74.7705 | 79.7214 | 86.7540 |
| 90.1135 | 92.6668 | 95.1521 |
| 100.5648 | 103.4173 | 106.2396 |
| 114.0298 | 123.6443 | 132.0946 |
| 137.0594 | 142.5231 | 151.1518 |
| 157.6372 | 160.6984 | 164.2272 |
| 173.2026 | 190.1868 | 207.0979 |
| 214.3591 | 229.2969 | 238.5153 |
| 247.1668 | 248.2593 | 262.9225 |
| 266.7704 | 270.4569 | 283.3430 |
| 292.6599 | 298.1898 | 306.5976 |
| 313.3968 | 327.5032 | 334.1427 |
| 342.6197 | 351.6477 | 358.9758 |
| 365.9719 | 396.9666 | 417.4667 |
| 436.1677 | 444.3241 | 454.1981 |
| 457.9023 | 461.4674 | 480.0275 |
| 488.4189 | 510.0358 | 517.3371 |
| 527.0588 | 532.8538 | 539.3309 |
| 559.9984 | 565.4922 | 566.7196 |
| 579.9801 | 585.6989 | 593.0140 |
| 622.1980 | 629.2685 | 645.1754 |
| 653.9463 | 672.0587 | 700.2715 |
| 725.8293 | 727.8550 | 738.1375 |

| | | |
|---|---|---|
| 746.3764 | 760.0963 | 763.7014 |
| 768.5004 | 771.2175 | 778.6411 |
| 787.3465 | 795.7905 | 807.8895 |
| 811.3102 | 823.3784 | 825.1367 |
| 831.1927 | 832.5999 | 862.1021 |
| 874.9802 | 876.7421 | 879.1086 |
| 886.1520 | 899.3275 | 905.1756 |
| 905.6700 | 907.2747 | 909.3037 |
| 922.4282 | 955.1878 | 970.1956 |
| 972.2956 | 980.7597 | 984.6515 |
| 1000.0354 | 1004.0125 | 1007.9868 |
| 1012.8652 | 1016.7976 | 1025.8601 |
| 1036.4207 | 1042.2438 | 1051.1343 |
| 1057.2268 | 1059.5585 | 1062.5051 |
| 1069.5200 | 1070.5274 | 1087.4077 |
| 1094.0663 | 1101.1857 | 1104.2058 |
| 1113.1007 | 1127.9011 | 1136.7769 |
| 1140.7692 | 1163.5291 | 1164.7895 |
| 1166.7625 | 1183.7404 | 1189.5434 |
| 1193.5514 | 1195.4306 | 1220.9816 |
| 1237.9915 | 1238.3741 | 1242.8854 |
| 1250.7180 | 1257.2979 | 1276.5341 |
| 1280.5792 | 1287.3851 | 1293.5118 |
| 1298.9188 | 1311.0936 | 1311.4263 |
| 1322.5790 | 1329.6671 | 1333.3016 |
| 1340.3369 | 1341.9555 | 1345.1343 |
| 1352.6939 | 1356.0398 | 1365.9365 |
| 1368.7627 | 1384.0010 | 1398.5995 |
| 1402.9130 | 1404.4862 | 1408.3739 |
| 1412.4416 | 1418.4254 | 1418.7115 |

| | | |
|---|---|---|
| 1423.9504 | 1427.2737 | 1445.6996 |
| 1448.4218 | 1449.8232 | 1453.0944 |
| 1465.1031 | 1477.5071 | 1481.4039 |
| 1483.4342 | 1485.7248 | 1488.2699 |
| 1490.0577 | 1494.5445 | 1497.0209 |
| 1497.0887 | 1499.6817 | 1503.2730 |
| 1508.6541 | 1514.9738 | 1523.8777 |
| 1531.3488 | 1536.8233 | 1543.3688 |
| 1591.9403 | 1615.2488 | 1621.0794 |
| 1624.3667 | 1665.6094 | 1668.0056 |
| 1734.7153 | 1861.2235 | 3007.0949 |
| 3010.1905 | 3011.9393 | 3020.5538 |
| 3022.3054 | 3031.7317 | 3032.8075 |
| 3042.6758 | 3043.5323 | 3051.7011 |
| 3056.2045 | 3058.6924 | 3062.5132 |
| 3072.4366 | 3080.9059 | 3081.2709 |
| 3099.1660 | 3102.7842 | 3121.5412 |
| 3128.0783 | 3132.5649 | 3137.7733 |
| 3143.6860 | 3152.8597 | 3158.9762 |
| 3172.5892 | 3173.8357 | 3183.8776 |
| 3185.3011 | 3192.8923 | 3196.5222 |
| 3206.2846 | 3208.5648 | 3211.6110 |
| 3213.5802 | 3221.9945 | 3231.7559 |

**TS4S**

Zero-point correction= 0.656402

Thermal correction to Energy= 0.700090

Thermal correction to Enthalpy= 0.701034

Thermal correction to Gibbs Free Energy= 0.575923

Sum of electronic and zero-point Energies= -1966.172793

Sum of electronic and thermal Energies= -1966.129105

Sum of electronic and thermal Enthalpies= -1966.128161

Sum of electronic and thermal Free Energies= -1966.253272

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.410230 | -2.074761 | 0.679914 |
| B | -0.383295 | -1.355500 | 1.937828 |
| C | -1.544373 | -2.232181 | -0.032724 |
| O | -1.056568 | 0.139768 | 1.717640 |
| C | -2.217981 | -1.132372 | -0.560012 |
| C | -2.018360 | -3.543587 | -0.339096 |
| C | -1.051038 | 0.817724 | 0.513556 |
| C | -1.530513 | 0.188924 | -0.624742 |
| C | -3.226004 | -3.741059 | -0.959044 |
| C | -3.525503 | -1.305366 | -1.128105 |
| C | -4.037317 | -2.630294 | -1.312695 |
| C | -0.564910 | 2.153398 | 0.459454 |
| C | -1.316137 | 0.817486 | -1.903701 |
| C | -0.451728 | 2.807436 | -0.741395 |
| C | -0.778508 | 2.143228 | -1.950894 |
| H | -3.576660 | -4.742417 | -1.185722 |
| H | -0.088976 | 3.828673 | -0.784343 |
| C | -0.568455 | 2.778278 | -3.205515 |
| C | -0.852180 | 2.121318 | -4.380832 |
| C | -1.350859 | 0.797066 | -4.342660 |
| C | -1.580491 | 0.163680 | -3.140346 |
| H | -0.168314 | 3.788482 | -3.215259 |
| H | -0.683579 | 2.609839 | -5.336067 |
| H | -1.548683 | 0.270323 | -5.271761 |
| H | -1.946663 | -0.855317 | -3.136408 |

| | | | |
|---|---|---|---|
| C | -5.328503 | -2.814920 | -1.877527 |
| C | -6.100649 | -1.732871 | -2.236680 |
| C | -5.606345 | -0.420384 | -2.041217 |
| C | -4.352626 | -0.211148 | -1.507982 |
| H | -5.694977 | -3.828806 | -2.015275 |
| H | -7.088322 | -1.881356 | -2.663293 |
| H | -6.223731 | 0.431736 | -2.311141 |
| H | -3.993961 | 0.801029 | -1.359681 |
| C | 1.870902 | -0.202941 | 1.362698 |
| C | 2.410864 | -0.547711 | 0.190822 |
| H | 1.828049 | 0.851203 | 1.629803 |
| H | 2.445510 | -1.601638 | -0.089855 |
| C | 2.961919 | 0.425646 | -0.813844 |
| C | 4.464452 | 0.235733 | -1.088485 |
| H | 2.775880 | 1.453384 | -0.476159 |
| H | 2.416829 | 0.308114 | -1.762655 |
| C | 5.001345 | 1.193182 | -2.158535 |
| H | 5.020209 | 0.378848 | -0.151653 |
| H | 4.648342 | -0.802264 | -1.399882 |
| H | 4.441993 | 1.040844 | -3.092997 |
| H | 4.801608 | 2.229463 | -1.849487 |
| C | 6.500741 | 1.026962 | -2.431371 |
| C | 7.034986 | 1.985633 | -3.502791 |
| H | 6.702143 | -0.009171 | -2.739974 |
| H | 7.059842 | 1.180716 | -1.496974 |
| C | 8.533487 | 1.814615 | -3.768129 |
| H | 6.476320 | 1.830805 | -4.436364 |
| H | 6.833140 | 3.020834 | -3.194194 |
| H | 8.889331 | 2.511228 | -4.535672 |
| H | 9.119169 | 1.995097 | -2.858500 |

| | | | |
|---|---|---|---|
| H | 8.761802 | 0.797826 | -4.109941 |
| C | 1.197050 | -1.151968 | 2.320978 |
| H | 1.645119 | -2.148850 | 2.236470 |
| C | 1.430749 | -0.724271 | 3.746502 |
| I | -0.063175 | 3.225961 | 2.240343 |
| I | -0.755957 | -5.236848 | 0.043786 |
| F | 2.739288 | -0.445417 | 4.004134 |
| F | 1.067022 | -1.665824 | 4.654549 |
| F | 0.741575 | 0.403582 | 4.078876 |
| C | -0.465218 | -4.086253 | 3.665590 |
| C | -1.614019 | -3.205444 | 3.197992 |
| H | -0.822875 | -5.116092 | 3.774001 |
| H | 0.348790 | -4.089647 | 2.936110 |
| H | -0.073794 | -3.747693 | 4.626849 |
| H | -2.058448 | -3.609261 | 2.284056 |
| H | -2.401971 | -3.190380 | 3.959587 |
| O | -1.248011 | -1.835804 | 2.995339 |
| H | -2.350521 | -0.692680 | 3.560878 |
| C | -1.992112 | -0.050489 | 5.852468 |
| C | -2.269912 | 0.942721 | 4.739621 |
| H | -1.755550 | 0.490399 | 6.774573 |
| H | -2.865353 | -0.684009 | 6.042073 |
| H | -1.138281 | -0.685555 | 5.600295 |
| H | -3.105234 | 1.603282 | 4.987412 |
| H | -1.390029 | 1.556228 | 4.536482 |
| O | -2.645576 | 0.257965 | 3.503806 |
| H | -1.818275 | 0.393845 | 2.490184 |

Vibrational frequencies

| | | |
|---|---|---|
| -71.0763 | 12.4134 | 16.9695 |

| | | |
|---|---|---|
| 22.2091 | 27.1917 | 37.6849 |
| 44.0423 | 50.1810 | 52.2657 |
| 57.2836 | 63.3828 | 68.1035 |
| 74.1961 | 74.6070 | 85.2151 |
| 88.9876 | 91.0786 | 91.3806 |
| 97.0779 | 101.6072 | 103.8801 |
| 118.9959 | 129.3102 | 130.3450 |
| 135.8552 | 144.7102 | 151.9670 |
| 160.7419 | 165.0279 | 167.7113 |
| 174.6337 | 192.3412 | 203.2193 |
| 208.4470 | 217.4662 | 223.2856 |
| 237.3252 | 250.6622 | 251.7292 |
| 254.9933 | 273.0355 | 282.0788 |
| 291.6609 | 295.7885 | 300.5077 |
| 309.3539 | 324.3538 | 331.6864 |
| 342.1316 | 352.1916 | 361.1664 |
| 374.5945 | 398.2335 | 423.5048 |
| 432.5387 | 443.1002 | 450.7519 |
| 456.8751 | 465.7610 | 469.3444 |
| 487.3972 | 496.6981 | 508.0487 |
| 522.0660 | 534.7627 | 546.3153 |
| 557.1447 | 565.5444 | 574.9833 |
| 582.0369 | 589.0929 | 599.4518 |
| 609.0052 | 621.0708 | 649.1591 |
| 655.4981 | 668.4174 | 701.0318 |
| 711.2602 | 726.6013 | 738.7552 |
| 747.0969 | 748.7743 | 761.2697 |
| 765.4528 | 770.2989 | 771.5957 |
| 786.4559 | 802.8692 | 812.2035 |
| 821.2350 | 827.3110 | 829.1883 |

| | | |
|---|---|---|
| 834.5289 | 841.9145 | 863.1386 |
| 875.0827 | 876.5853 | 882.5436 |
| 884.2754 | 904.1455 | 905.1953 |
| 906.4535 | 908.2097 | 925.1080 |
| 949.7862 | 969.7325 | 972.3767 |
| 976.9421 | 988.4281 | 1000.6419 |
| 1004.4653 | 1006.9665 | 1012.6696 |
| 1016.3368 | 1019.1759 | 1034.2049 |
| 1038.5336 | 1043.0528 | 1053.0960 |
| 1062.4434 | 1065.9534 | 1068.5026 |
| 1073.9810 | 1079.9650 | 1097.5974 |
| 1100.7445 | 1107.2181 | 1116.8504 |
| 1134.9869 | 1138.9175 | 1146.3219 |
| 1165.1118 | 1173.4213 | 1182.6511 |
| 1185.4026 | 1189.9372 | 1194.9985 |
| 1196.1073 | 1198.9273 | 1218.6901 |
| 1226.0772 | 1240.8263 | 1242.5384 |
| 1252.0381 | 1258.7887 | 1267.0615 |
| 1279.6121 | 1282.6460 | 1290.4821 |
| 1301.2805 | 1305.8069 | 1314.3985 |
| 1322.5925 | 1326.1114 | 1333.6544 |
| 1338.6901 | 1339.9884 | 1345.9687 |
| 1347.1924 | 1348.8729 | 1363.9113 |
| 1366.9649 | 1390.5656 | 1394.2085 |
| 1400.5689 | 1405.2489 | 1406.2209 |
| 1408.2846 | 1408.6088 | 1417.9687 |
| 1421.2098 | 1423.5459 | 1429.0555 |
| 1440.4105 | 1450.0642 | 1452.5250 |
| 1469.8555 | 1479.9729 | 1481.1181 |
| 1483.7211 | 1488.3250 | 1489.4040 |

| | | |
|---|---|---|
| 1490.2350 | 1490.7366 | 1494.6706 |
| 1499.0111 | 1500.9148 | 1506.9900 |
| 1508.2685 | 1515.2200 | 1535.6209 |
| 1538.0584 | 1541.1296 | 1548.7137 |
| 1598.8947 | 1615.2259 | 1620.7887 |
| 1624.1777 | 1666.3124 | 1668.8396 |
| 1745.2507 | 1772.2373 | 3008.9595 |
| 3011.2325 | 3012.2469 | 3020.4311 |
| 3022.6765 | 3032.7317 | 3033.2357 |
| 3043.0999 | 3052.4880 | 3053.1328 |
| 3056.4268 | 3059.4390 | 3063.4000 |
| 3067.6494 | 3073.5807 | 3087.9026 |
| 3099.9489 | 3103.6984 | 3114.4340 |
| 3122.4412 | 3130.9526 | 3138.3662 |
| 3139.5642 | 3153.7686 | 3158.7869 |
| 3172.3196 | 3184.3161 | 3187.8870 |
| 3193.2790 | 3197.2565 | 3207.1165 |
| 3210.0568 | 3210.7191 | 3213.6212 |
| 3221.8023 | 3237.7804 | 3275.1325 |

**M4R**

Zero-point correction= 0.658056

Thermal correction to Energy= 0.702758

Thermal correction to Enthalpy= 0.703702

Thermal correction to Gibbs Free Energy= 0.575401

Sum of electronic and zero-point Energies= -1966.171116

Sum of electronic and thermal Energies= -1966.126414

Sum of electronic and thermal Enthalpies= -1966.125470

Sum of electronic and thermal Free Energies= -1966.253771

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.080868 | -1.104814 | 1.356647 |
| B | 0.114593 | -0.217683 | 2.488760 |
| C | -1.228017 | -1.286723 | 0.681646 |
| O | -0.718898 | 1.200064 | 2.128517 |
| C | -1.869139 | -0.244456 | 0.004252 |
| C | -1.767643 | -2.607277 | 0.573505 |
| C | -0.685411 | 1.774676 | 0.869767 |
| C | -1.169399 | 1.055397 | -0.206348 |
| C | -2.990662 | -2.841161 | 0.000158 |
| C | -3.192824 | -0.446483 | -0.518048 |
| C | -3.762144 | -1.759831 | -0.502474 |
| C | -0.114420 | 3.062022 | 0.723086 |
| C | -0.941491 | 1.575132 | -1.528986 |
| C | 0.037173 | 3.611200 | -0.524429 |
| C | -0.340482 | 2.868957 | -1.675458 |
| H | -3.388684 | -3.848154 | -0.067155 |
| H | 0.470332 | 4.597417 | -0.650989 |
| C | -0.103849 | 3.390345 | -2.977165 |
| C | -0.419937 | 2.655686 | -4.097019 |
| C | -0.982226 | 1.363877 | -3.957246 |
| C | -1.239443 | 0.838791 | -2.709367 |
| H | 0.345766 | 4.375403 | -3.068018 |
| H | -0.228184 | 3.057571 | -5.087559 |
| H | -1.207685 | 0.777698 | -4.843349 |
| H | -1.658535 | -0.156083 | -2.622563 |
| C | -5.076455 | -1.966918 | -1.001174 |
| C | -5.822156 | -0.912954 | -1.480217 |
| C | -5.274438 | 0.392417 | -1.477082 |
| C | -3.995020 | 0.619816 | -1.015722 |

| | | | |
|---|---|---|---|
| H | -5.483880 | -2.974443 | -0.987751 |
| H | -6.829204 | -1.077189 | -1.852076 |
| H | -5.870017 | 1.225862 | -1.838591 |
| H | -3.598243 | 1.628531 | -1.014510 |
| C | 2.264488 | 0.750281 | 1.289820 |
| C | 2.543182 | 0.003647 | 0.216366 |
| H | 2.435046 | 1.824051 | 1.233220 |
| H | 2.366899 | -1.070025 | 0.254845 |
| C | 3.103904 | 0.545435 | -1.068635 |
| C | 4.513740 | 0.013428 | -1.386162 |
| H | 3.128602 | 1.642630 | -1.029907 |
| H | 2.434747 | 0.277048 | -1.900073 |
| C | 5.076693 | 0.564733 | -2.700505 |
| H | 5.187120 | 0.273504 | -0.558101 |
| H | 4.488165 | -1.084611 | -1.428003 |
| H | 4.397336 | 0.302563 | -3.524512 |
| H | 5.089408 | 1.663433 | -2.654052 |
| C | 6.486483 | 0.055944 | -3.023568 |
| C | 7.055775 | 0.626204 | -4.328138 |
| H | 6.473055 | -1.042098 | -3.083031 |
| H | 7.162643 | 0.307752 | -2.193678 |
| C | 8.464521 | 0.114160 | -4.642854 |
| H | 6.380276 | 0.374895 | -5.157560 |
| H | 7.068840 | 1.723333 | -4.266544 |
| H | 8.847432 | 0.535480 | -5.579368 |
| H | 9.169217 | 0.380267 | -3.845568 |
| H | 8.475215 | -0.978259 | -4.740495 |
| C | 1.681793 | 0.248832 | 2.595179 |
| H | 1.708335 | 1.060318 | 3.329683 |
| C | 2.536185 | -0.836945 | 3.207086 |

| | | | |
|---|---|---|---|
| I | 0.506877 | 4.144343 | 2.460258 |
| I | -0.587271 | -4.272941 | 1.229301 |
| F | 2.425936 | -2.034459 | 2.564386 |
| F | 2.219719 | -1.072925 | 4.506055 |
| F | 3.865105 | -0.534723 | 3.201513 |
| C | -0.393330 | -2.733184 | 4.757214 |
| C | -1.239253 | -1.686669 | 4.044544 |
| H | -1.003185 | -3.610746 | 5.000616 |
| H | 0.437482 | -3.051071 | 4.123766 |
| H | 0.019648 | -2.324814 | 5.684804 |
| H | -1.698646 | -2.113817 | 3.148778 |
| H | -2.062698 | -1.375170 | 4.703464 |
| O | -0.477366 | -0.527090 | 3.735143 |
| H | -2.526881 | 0.828416 | 4.240021 |
| C | -5.066233 | 0.346628 | 3.736411 |
| C | -3.874922 | 0.496998 | 2.812093 |
| H | -5.856778 | -0.215252 | 3.228004 |
| H | -4.793265 | -0.201823 | 4.645506 |
| H | -5.462792 | 1.325028 | 4.024215 |
| H | -3.468742 | -0.475191 | 2.514493 |
| H | -4.138234 | 1.045207 | 1.905427 |
| O | -2.824221 | 1.289591 | 3.436489 |
| H | -1.625911 | 1.280490 | 2.650315 |

Vibrational frequencies

| | | |
|---|---|---|
| 9.6972 | 17.2023 | 22.4101 |
| 28.0912 | 33.0827 | 37.4604 |
| 45.2661 | 46.3606 | 47.1764 |
| 50.5394 | 57.7733 | 61.7628 |
| 70.8617 | 85.4682 | 90.7218 |

| | | |
|---|---|---|
| 95.1739 | 96.1163 | 98.7282 |
| 100.1035 | 104.3221 | 108.4945 |
| 116.9015 | 128.7520 | 131.0832 |
| 138.5894 | 148.4219 | 153.2945 |
| 158.5839 | 160.9195 | 163.4047 |
| 170.3413 | 183.1128 | 193.0428 |
| 209.1020 | 215.0075 | 230.5303 |
| 237.7774 | 246.1237 | 247.2144 |
| 254.7654 | 278.3590 | 279.7091 |
| 282.7259 | 295.1427 | 305.4491 |
| 308.2530 | 310.7093 | 319.3871 |
| 341.2194 | 350.7907 | 365.4267 |
| 368.6277 | 401.9155 | 416.7895 |
| 433.9489 | 450.6486 | 454.5826 |
| 456.5597 | 468.3092 | 469.9376 |
| 484.4692 | 505.6720 | 511.7227 |
| 519.1425 | 530.3907 | 532.2403 |
| 548.0903 | 560.3037 | 565.8821 |
| 572.3874 | 583.7931 | 588.5116 |
| 608.0311 | 614.6484 | 634.1403 |
| 651.3182 | 662.6595 | 670.1082 |
| 711.2269 | 728.6907 | 734.7343 |
| 743.8736 | 745.2994 | 759.5412 |
| 760.9486 | 768.7094 | 769.3798 |
| 783.2464 | 793.4467 | 806.1231 |
| 810.7676 | 826.4244 | 827.1919 |
| 829.7745 | 835.4276 | 862.6887 |
| 874.4250 | 877.8517 | 881.4016 |
| 882.4491 | 903.6141 | 904.5955 |
| 907.3397 | 908.1554 | 909.5226 |

| | | |
|---|---|---|
| 951.6814 | 971.5735 | 973.2105 |
| 978.0683 | 983.7039 | 1000.9292 |
| 1005.5529 | 1010.0678 | 1012.3680 |
| 1024.0096 | 1026.7326 | 1032.4139 |
| 1041.1471 | 1046.4974 | 1055.6298 |
| 1059.2367 | 1060.1598 | 1063.4989 |
| 1071.2108 | 1076.7266 | 1088.7078 |
| 1096.9243 | 1109.3886 | 1117.9470 |
| 1127.4451 | 1136.4627 | 1141.1817 |
| 1150.1582 | 1161.5203 | 1163.9108 |
| 1173.4973 | 1183.2349 | 1189.2544 |
| 1193.9265 | 1204.6213 | 1223.6750 |
| 1237.3320 | 1238.0442 | 1242.3850 |
| 1248.1812 | 1257.7528 | 1269.9286 |
| 1282.3552 | 1284.0434 | 1286.3838 |
| 1289.5024 | 1304.5830 | 1311.2873 |
| 1320.4097 | 1334.5772 | 1339.2694 |
| 1340.5626 | 1343.6380 | 1351.9239 |
| 1354.5738 | 1363.0408 | 1369.8075 |
| 1373.8922 | 1384.4025 | 1400.1373 |
| 1403.1638 | 1403.8748 | 1409.0181 |
| 1410.2492 | 1412.8077 | 1419.0171 |
| 1421.4845 | 1427.8162 | 1441.3010 |
| 1447.9696 | 1451.8043 | 1454.4766 |
| 1476.6257 | 1481.6029 | 1482.2579 |
| 1482.9887 | 1484.5832 | 1485.6641 |
| 1487.3405 | 1492.0580 | 1494.7120 |
| 1495.3594 | 1497.6642 | 1507.3110 |
| 1514.2215 | 1522.7775 | 1526.3864 |
| 1537.1986 | 1542.3572 | 1587.8666 |

| | | |
|---|---|---|
| 1593.3323 | 1617.8507 | 1620.6638 |
| 1622.7993 | 1665.1894 | 1668.1432 |
| 1734.5106 | 2305.3160 | 3005.5152 |
| 3009.8189 | 3011.5321 | 3014.8233 |
| 3020.9897 | 3022.8304 | 3030.9406 |
| 3032.5236 | 3042.4784 | 3046.2210 |
| 3050.1941 | 3050.7241 | 3062.2271 |
| 3072.5286 | 3080.7249 | 3083.6755 |
| 3097.9914 | 3101.9155 | 3103.9843 |
| 3114.5539 | 3123.2039 | 3132.3627 |
| 3148.6497 | 3152.1000 | 3156.5645 |
| 3173.1064 | 3183.9476 | 3186.6935 |
| 3193.6641 | 3197.6441 | 3207.3082 |
| 3209.7330 | 3211.4327 | 3215.1489 |
| 3222.4454 | 3231.5933 | 3744.7250 |

**M4S**

Zero-point correction= 0.658026

Thermal correction to Energy= 0.702465

Thermal correction to Enthalpy= 0.703409

Thermal correction to Gibbs Free Energy= 0.576632

Sum of electronic and zero-point Energies= -1966.171437

Sum of electronic and thermal Energies= -1966.126997

Sum of electronic and thermal Enthalpies= -1966.126053

Sum of electronic and thermal Free Energies= -1966.252830

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.406068 | -2.086418 | 0.671996 |
| B | -0.372951 | -1.400484 | 1.938830 |
| C | -1.543142 | -2.242184 | -0.039488 |

| | | | |
|---|---|---|---|
| O | -1.048574 | 0.137548 | 1.699765 |
| C | -2.209639 | -1.140563 | -0.571454 |
| C | -2.022487 | -3.553061 | -0.337713 |
| C | -1.050836 | 0.820383 | 0.496037 |
| C | -1.521570 | 0.181346 | -0.638941 |
| C | -3.229525 | -3.747695 | -0.959548 |
| C | -3.517480 | -1.310972 | -1.140854 |
| C | -4.034393 | -2.634668 | -1.320379 |
| C | -0.563063 | 2.154353 | 0.442668 |
| C | -1.304314 | 0.806732 | -1.919107 |
| C | -0.448125 | 2.804294 | -0.760228 |
| C | -0.770833 | 2.134383 | -1.968110 |
| H | -3.585205 | -4.748425 | -1.181029 |
| H | -0.085162 | 3.825311 | -0.806395 |
| C | -0.558715 | 2.765821 | -3.224247 |
| C | -0.837133 | 2.104264 | -4.398268 |
| C | -1.332093 | 0.778753 | -4.357723 |
| C | -1.563252 | 0.148291 | -3.154171 |
| H | -0.161437 | 3.777081 | -3.236165 |
| H | -0.667103 | 2.590346 | -5.354476 |
| H | -1.526143 | 0.248907 | -5.285824 |
| H | -1.927133 | -0.871547 | -3.147939 |
| C | -5.325397 | -2.816759 | -1.886465 |
| C | -6.093128 | -1.733316 | -2.250514 |
| C | -5.594420 | -0.421998 | -2.058972 |
| C | -4.340493 | -0.215253 | -1.525241 |
| H | -5.695482 | -3.829806 | -2.020448 |
| H | -7.080859 | -1.879816 | -2.677645 |
| H | -6.208596 | 0.431347 | -2.332227 |
| H | -3.979206 | 0.796301 | -1.379672 |

| | | | |
|---|---|---|---|
| C | 1.869215 | -0.221899 | 1.362215 |
| C | 2.415470 | -0.559255 | 0.191202 |
| H | 1.813911 | 0.831018 | 1.631662 |
| H | 2.461556 | -1.612365 | -0.090947 |
| C | 2.959072 | 0.421066 | -0.810732 |
| C | 4.462877 | 0.242930 | -1.086165 |
| H | 2.765449 | 1.446426 | -0.470225 |
| H | 2.415044 | 0.301868 | -1.759918 |
| C | 4.991304 | 1.205852 | -2.155579 |
| H | 5.018232 | 0.388954 | -0.149558 |
| H | 4.654383 | -0.793181 | -1.399173 |
| H | 4.432580 | 1.049746 | -3.089791 |
| H | 4.783328 | 2.240184 | -1.845468 |
| C | 6.491756 | 1.052042 | -2.429848 |
| C | 7.016871 | 2.014935 | -3.502018 |
| H | 6.701404 | 0.017588 | -2.738582 |
| H | 7.050584 | 1.210454 | -1.496070 |
| C | 8.516552 | 1.856662 | -3.768493 |
| H | 6.458887 | 1.855038 | -4.435161 |
| H | 6.806389 | 3.048482 | -3.193639 |
| H | 8.865793 | 2.556177 | -4.536434 |
| H | 9.101515 | 2.042201 | -2.859420 |
| H | 8.753189 | 0.841807 | -4.110452 |
| C | 1.202952 | -1.179972 | 2.316756 |
| H | 1.658369 | -2.173475 | 2.225099 |
| C | 1.436870 | -0.759048 | 3.744166 |
| I | -0.057646 | 3.220188 | 2.226115 |
| I | -0.771153 | -5.250149 | 0.062092 |
| F | 2.745375 | -0.482561 | 4.002087 |
| F | 1.072711 | -1.705425 | 4.646413 |

| | | | |
|---|---|---|---|
| F | 0.748343 | 0.368407 | 4.079051 |
| C | -0.561035 | -4.102938 | 3.714720 |
| C | -1.666873 | -3.197725 | 3.193993 |
| H | -0.951387 | -5.119498 | 3.835444 |
| H | 0.274745 | -4.145786 | 3.011092 |
| H | -0.188618 | -3.752784 | 4.679690 |
| H | -2.091791 | -3.601508 | 2.271021 |
| H | -2.480026 | -3.146110 | 3.926757 |
| O | -1.246069 | -1.844810 | 2.987376 |
| H | -2.343369 | -0.634838 | 3.608844 |
| C | -1.945693 | -0.047874 | 5.903282 |
| C | -2.224592 | 0.963917 | 4.805390 |
| H | -1.688277 | 0.473763 | 6.830951 |
| H | -2.825640 | -0.671822 | 6.094543 |
| H | -1.105831 | -0.693098 | 5.630354 |
| H | -3.045769 | 1.632953 | 5.080839 |
| H | -1.338710 | 1.572910 | 4.607782 |
| O | -2.623551 | 0.311421 | 3.568211 |
| H | -1.742833 | 0.423688 | 2.446960 |

Vibrational frequencies

| | | |
|---|---|---|
| 12.4915 | 16.5836 | 22.8165 |
| 27.4014 | 37.2834 | 42.8278 |
| 48.6414 | 51.4459 | 54.8549 |
| 62.2893 | 67.0594 | 68.3023 |
| 75.2634 | 85.3491 | 88.3699 |
| 90.6307 | 93.1814 | 100.0705 |
| 101.1455 | 102.3423 | 114.5748 |
| 122.5805 | 129.5215 | 134.1842 |
| 142.9486 | 150.8028 | 156.0349 |

| | | |
|---|---|---|
| 159.7616 | 162.9823 | 174.0841 |
| 179.4859 | 191.9034 | 195.9255 |
| 206.1657 | 217.7907 | 222.5489 |
| 233.1972 | 245.9854 | 249.5394 |
| 256.4955 | 269.9330 | 280.6223 |
| 290.1630 | 296.5733 | 302.8458 |
| 309.6882 | 319.4539 | 326.2878 |
| 340.0889 | 354.6069 | 359.2922 |
| 375.1425 | 396.4156 | 420.7669 |
| 428.6290 | 443.6146 | 450.1016 |
| 452.9626 | 463.3209 | 467.2988 |
| 485.9361 | 495.8899 | 502.8246 |
| 522.4779 | 532.7896 | 545.2652 |
| 557.9720 | 563.9346 | 567.3535 |
| 576.2808 | 588.9907 | 592.9532 |
| 608.2365 | 617.8311 | 648.0030 |
| 655.4128 | 671.8715 | 695.3349 |
| 717.3329 | 733.8796 | 738.9814 |
| 745.7695 | 748.9339 | 760.9129 |
| 764.8459 | 769.9437 | 770.9184 |
| 786.9931 | 793.6981 | 808.3868 |
| 813.5082 | 824.1694 | 828.4213 |
| 832.7182 | 842.9438 | 875.4140 |
| 877.2183 | 877.6431 | 882.9470 |
| 884.4019 | 904.7209 | 905.1083 |
| 906.8241 | 909.2599 | 922.2307 |
| 950.9018 | 970.3705 | 973.1547 |
| 977.6705 | 988.8344 | 1001.0223 |
| 1006.8534 | 1007.7168 | 1013.1652 |
| 1020.8924 | 1033.6179 | 1037.9604 |

| | | |
|---|---|---|
| 1044.1622 | 1047.2224 | 1051.4929 |
| 1054.6451 | 1063.6038 | 1066.6361 |
| 1069.8005 | 1074.2466 | 1101.3375 |
| 1106.3899 | 1108.7289 | 1118.8728 |
| 1132.5376 | 1136.6922 | 1142.5269 |
| 1149.9882 | 1165.4736 | 1183.9449 |
| 1185.6655 | 1190.1459 | 1193.9335 |
| 1195.1845 | 1196.5153 | 1205.8437 |
| 1226.4622 | 1240.3877 | 1242.1561 |
| 1251.9570 | 1258.8133 | 1267.2012 |
| 1279.6764 | 1284.0816 | 1290.1409 |
| 1301.3651 | 1306.4653 | 1313.0255 |
| 1322.3782 | 1326.7683 | 1338.4635 |
| 1339.9168 | 1342.6932 | 1345.0329 |
| 1348.4099 | 1358.1811 | 1365.9541 |
| 1373.0489 | 1390.8892 | 1400.3125 |
| 1405.2216 | 1406.0872 | 1408.3845 |
| 1408.9763 | 1416.9822 | 1417.9793 |
| 1420.8815 | 1428.4980 | 1437.8829 |
| 1441.1152 | 1448.9106 | 1453.0246 |
| 1477.3566 | 1481.1793 | 1483.7583 |
| 1484.0567 | 1488.3155 | 1489.4703 |
| 1490.5796 | 1494.8532 | 1498.2703 |
| 1499.1130 | 1506.9481 | 1508.3324 |
| 1515.2413 | 1533.6224 | 1537.1646 |
| 1538.2612 | 1541.8793 | 1597.5733 |
| 1604.7822 | 1617.4510 | 1621.0881 |
| 1630.1169 | 1666.4075 | 1668.8613 |
| 1745.7092 | 2161.9426 | 3009.2305 |
| 3011.4876 | 3012.3901 | 3020.5488 |

| | | |
|---|---|---|
| 3022.9985 | 3032.7596 | 3033.4022 |
| 3043.3459 | 3051.1330 | 3053.5481 |
| 3055.7135 | 3059.0330 | 3062.8373 |
| 3063.7298 | 3074.0120 | 3075.6552 |
| 3100.0165 | 3103.6825 | 3116.0605 |
| 3116.9551 | 3127.8299 | 3130.1790 |
| 3138.1520 | 3145.6827 | 3155.1793 |
| 3172.5719 | 3184.6869 | 3188.4109 |
| 3193.6084 | 3197.7546 | 3207.4800 |
| 3210.1805 | 3211.0147 | 3214.1352 |
| 3222.5017 | 3237.7537 | 3426.2108 |

**TS5R**

Zero-point correction= 0.738915

Thermal correction to Energy= 0.787377

Thermal correction to Enthalpy= 0.788321

Thermal correction to Gibbs Free Energy= 0.654709

Sum of electronic and zero-point Energies= -2121.166828

Sum of electronic and thermal Energies= -2121.118366

Sum of electronic and thermal Enthalpies= -2121.117422

Sum of electronic and thermal Free Energies= -2121.251034

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | 0.262233 | -2.085424 | 0.946316 |
| B | 0.185525 | -2.044937 | 2.548670 |
| C | -0.860931 | -2.303204 | 0.190523 |
| O | -2.415059 | 0.363447 | 2.040789 |
| C | -1.609233 | -1.206482 | -0.221267 |
| C | -1.286400 | -3.614000 | -0.189124 |
| C | -1.634710 | 0.922994 | 1.092368 |

| | | | |
|---|---|---|---|
| C | -1.137176 | 0.190877 | 0.017118 |
| C | -2.439977 | -3.806919 | -0.911007 |
| C | -2.818999 | -1.385570 | -0.967794 |
| C | -3.243152 | -2.708420 | -1.305019 |
| C | -1.347239 | 2.319017 | 1.165919 |
| C | -0.302022 | 0.811610 | -0.962634 |
| C | -0.551445 | 2.942167 | 0.237098 |
| C | 0.001894 | 2.205934 | -0.843610 |
| H | -2.753115 | -4.806595 | -1.192425 |
| H | -0.336138 | 4.002811 | 0.313961 |
| C | 0.821813 | 2.832290 | -1.821786 |
| C | 1.314769 | 2.115998 | -2.890081 |
| C | 1.009838 | 0.738046 | -3.016520 |
| C | 0.225861 | 0.101724 | -2.078184 |
| H | 1.046250 | 3.890198 | -1.713339 |
| H | 1.934933 | 2.602487 | -3.636885 |
| H | 1.400038 | 0.178660 | -3.861883 |
| H | 0.000874 | -0.953833 | -2.185591 |
| C | -4.446515 | -2.899826 | -2.037553 |
| C | -5.207591 | -1.820524 | -2.425276 |
| C | -4.790574 | -0.506726 | -2.096535 |
| C | -3.627856 | -0.292370 | -1.388996 |
| H | -4.751441 | -3.913443 | -2.283873 |
| H | -6.127232 | -1.971520 | -2.983078 |
| H | -5.396203 | 0.340568 | -2.405278 |
| H | -3.321525 | 0.717856 | -1.143011 |
| C | 1.722977 | 0.133224 | 2.045524 |
| C | 2.978969 | 0.123459 | 1.589780 |
| H | 1.011665 | 0.847989 | 1.642025 |
| H | 3.675098 | -0.612373 | 1.997183 |

| | | | |
|---|---|---|---|
| C | 3.523582 | 0.985692 | 0.487967 |
| C | 3.934702 | 0.152051 | -0.740771 |
| H | 4.405183 | 1.537895 | 0.847281 |
| H | 2.779232 | 1.731525 | 0.184921 |
| C | 4.610230 | 0.982220 | -1.836285 |
| H | 4.611856 | -0.655049 | -0.424734 |
| H | 3.037515 | -0.333396 | -1.145282 |
| H | 3.969106 | 1.838423 | -2.083505 |
| H | 5.549225 | 1.401937 | -1.447557 |
| C | 4.894315 | 0.183060 | -3.112029 |
| C | 5.575844 | 1.008112 | -4.209742 |
| H | 3.948144 | -0.221678 | -3.499292 |
| H | 5.521777 | -0.687240 | -2.868708 |
| C | 5.828920 | 0.208815 | -5.490597 |
| H | 4.953236 | 1.883738 | -4.441049 |
| H | 6.527398 | 1.402935 | -3.827596 |
| H | 6.318464 | 0.819359 | -6.257683 |
| H | 6.471693 | -0.658235 | -5.295158 |
| H | 4.889298 | -0.166454 | -5.914020 |
| C | 1.209074 | -0.835050 | 3.078230 |
| H | 2.082277 | -1.357331 | 3.486619 |
| C | 0.655383 | -0.090505 | 4.265119 |
| I | -2.197070 | 3.478416 | 2.757788 |
| I | -0.160907 | -5.383357 | 0.276163 |
| F | 1.582574 | 0.727405 | 4.846000 |
| F | 0.235852 | -0.926285 | 5.255828 |
| F | -0.394456 | 0.706570 | 3.954217 |
| C | -3.467257 | -2.657659 | 2.666906 |
| C | -2.062312 | -2.968276 | 3.158070 |
| H | -4.128393 | -3.504057 | 2.882646 |

| | | | |
|---|---|---|---|
| H | -3.873931 | -1.773326 | 3.168216 |
| H | -3.477313 | -2.477685 | 1.589561 |
| H | -2.084410 | -3.174586 | 4.236442 |
| H | -1.670441 | -3.859807 | 2.659672 |
| O | -1.188742 | -1.850162 | 2.930093 |
| H | -2.002201 | -0.486795 | 2.350434 |
| C | 1.499625 | -5.165657 | 4.266069 |
| C | 0.972436 | -3.740721 | 4.242542 |
| H | 1.686555 | -5.489464 | 5.295435 |
| H | 0.779797 | -5.851942 | 3.809220 |
| H | 2.441817 | -5.236701 | 3.709759 |
| H | 0.034552 | -3.669145 | 4.805031 |
| H | 1.687945 | -3.062129 | 4.727758 |
| O | 0.756680 | -3.361751 | 2.883882 |
| H | 2.095057 | -3.474651 | 1.832883 |
| C | 4.511827 | -4.252858 | 0.848070 |
| C | 3.304022 | -3.729275 | 0.102895 |
| H | 5.167972 | -4.779221 | 0.147991 |
| H | 5.074416 | -3.433648 | 1.305112 |
| H | 4.214203 | -4.959069 | 1.630825 |
| H | 3.575382 | -3.006070 | -0.668251 |
| H | 2.709381 | -4.529829 | -0.342075 |
| O | 2.463427 | -2.977068 | 1.034869 |
| H | 1.498090 | -2.553559 | 0.706466 |

Vibrational frequencies

| | | |
|---|---|---|
| -203.4195 | 13.7076 | 21.6537 |
| 24.2634 | 35.2962 | 42.0274 |
| 47.5467 | 53.4177 | 55.3473 |
| 58.9356 | 65.4102 | 65.8280 |

| | | |
|---|---|---|
| 70.8943 | 72.9576 | 79.2568 |
| 83.3738 | 85.1313 | 89.1696 |
| 94.0562 | 95.8775 | 100.9551 |
| 106.6178 | 108.5788 | 113.0274 |
| 116.0508 | 122.5339 | 133.4529 |
| 146.9702 | 156.8867 | 162.6039 |
| 163.7644 | 166.8761 | 168.3896 |
| 170.5249 | 173.8100 | 181.9123 |
| 187.7975 | 194.2961 | 204.9294 |
| 223.5679 | 227.2513 | 235.9033 |
| 247.7338 | 252.4958 | 267.2912 |
| 272.5909 | 278.7139 | 284.9277 |
| 288.1691 | 288.5015 | 295.5365 |
| 299.5672 | 315.7018 | 319.1903 |
| 330.2530 | 342.6986 | 352.6174 |
| 364.9864 | 375.8467 | 383.5636 |
| 401.4394 | 416.7693 | 442.9897 |
| 444.4365 | 451.8469 | 458.1932 |
| 463.4134 | 487.4430 | 499.5910 |
| 504.1145 | 516.7764 | 535.9880 |
| 540.7808 | 548.6290 | 561.1515 |
| 566.4532 | 570.0358 | 581.1955 |
| 584.7380 | 612.5288 | 631.2845 |
| 638.6796 | 646.1881 | 658.4409 |
| 685.2779 | 696.4134 | 708.6322 |
| 721.1754 | 736.3858 | 745.6204 |
| 745.8871 | 757.1709 | 759.9026 |
| 765.2686 | 766.5014 | 771.6406 |
| 778.8802 | 791.2494 | 798.9711 |
| 809.8977 | 825.9616 | 827.2342 |

| | | |
|---|---|---|
| 828.9230 | 831.3278 | 837.9613 |
| 873.1627 | 877.1623 | 878.8156 |
| 883.4379 | 893.6504 | 906.3936 |
| 908.9583 | 909.8999 | 911.1844 |
| 914.8075 | 932.7418 | 944.3935 |
| 948.0515 | 966.2346 | 975.2781 |
| 984.3737 | 993.0321 | 998.3536 |
| 1003.5794 | 1006.4452 | 1007.1078 |
| 1016.0215 | 1025.4809 | 1034.0151 |
| 1046.1334 | 1054.2619 | 1057.1702 |
| 1058.2965 | 1059.9435 | 1066.2715 |
| 1075.6044 | 1091.2099 | 1100.7016 |
| 1104.8870 | 1108.7322 | 1112.6150 |
| 1120.8666 | 1132.6615 | 1134.2478 |
| 1139.3083 | 1149.9090 | 1163.3641 |
| 1170.8691 | 1174.9959 | 1184.3550 |
| 1185.7455 | 1187.6285 | 1188.2198 |
| 1195.2405 | 1221.3444 | 1240.1058 |
| 1242.3186 | 1246.2664 | 1247.8001 |
| 1258.6210 | 1267.9481 | 1272.4818 |
| 1280.3165 | 1281.1744 | 1297.1432 |
| 1304.6834 | 1309.8796 | 1316.4171 |
| 1318.0974 | 1322.8832 | 1328.8321 |
| 1332.2110 | 1339.9829 | 1340.7377 |
| 1341.4024 | 1348.7382 | 1359.3810 |
| 1365.3001 | 1388.7670 | 1395.0451 |
| 1398.5184 | 1401.2865 | 1406.5363 |
| 1408.0924 | 1411.3038 | 1412.0156 |
| 1418.7290 | 1421.9823 | 1424.0434 |
| 1424.4136 | 1432.5586 | 1437.3946 |

| | | |
|---|---|---|
| 1439.1012 | 1445.9647 | 1467.3530 |
| 1478.9788 | 1480.8344 | 1481.9578 |
| 1484.1378 | 1484.8401 | 1488.5062 |
| 1488.7337 | 1493.0386 | 1496.1537 |
| 1497.5365 | 1498.0786 | 1499.6320 |
| 1504.8515 | 1507.2768 | 1512.0497 |
| 1514.5720 | 1526.6396 | 1533.7964 |
| 1536.7284 | 1548.7617 | 1554.3689 |
| 1601.9143 | 1610.3113 | 1622.5718 |
| 1623.8082 | 1664.5916 | 1669.0665 |
| 1741.4021 | 1996.2579 | 3005.4238 |
| 3008.4547 | 3013.6983 | 3018.0663 |
| 3020.9362 | 3021.7426 | 3028.6158 |
| 3032.3623 | 3036.7620 | 3041.6600 |
| 3052.7701 | 3053.4295 | 3053.6726 |
| 3059.0164 | 3061.6506 | 3070.6792 |
| 3073.7777 | 3082.8401 | 3087.6372 |
| 3099.1372 | 3099.1731 | 3103.9874 |
| 3110.5681 | 3116.0350 | 3121.5948 |
| 3125.1561 | 3127.4515 | 3129.6215 |
| 3140.4083 | 3153.0428 | 3164.4048 |
| 3183.8653 | 3187.7828 | 3191.8596 |
| 3195.2823 | 3206.9037 | 3207.5163 |
| 3209.9771 | 3210.2925 | 3212.3384 |
| 3216.0528 | 3223.2351 | 3238.3538 |

**TS5S**

Zero-point correction= 0.737782

Thermal correction to Energy= 0.786921

Thermal correction to Enthalpy= 0.787865

Thermal correction to Gibbs Free Energy= 0.650723

Sum of electronic and zero-point Energies= -2121.156819

Sum of electronic and thermal Energies= -2121.107680

Sum of electronic and thermal Enthalpies= -2121.106736

Sum of electronic and thermal Free Energies= -2121.243878

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.090108 | 0.251134 | -1.029075 |
| B | 0.366892 | -1.298568 | -0.819929 |
| C | -0.047671 | 1.316725 | -0.183103 |
| O | -2.972994 | 1.045074 | -0.977059 |
| C | -0.971619 | 1.432132 | 0.852495 |
| C | 0.905382 | 2.361110 | -0.390107 |
| C | -2.998877 | 0.217407 | 0.102561 |
| C | -1.990525 | 0.361808 | 1.050317 |
| C | 0.951019 | 3.459988 | 0.432554 |
| C | -0.962963 | 2.586044 | 1.701445 |
| C | 0.026820 | 3.600176 | 1.498686 |
| C | -3.998603 | -0.777897 | 0.289743 |
| C | -1.949561 | -0.497375 | 2.190638 |
| C | -3.979883 | -1.615913 | 1.376871 |
| C | -2.954935 | -1.504176 | 2.349527 |
| H | 1.685123 | 4.242170 | 0.270304 |
| H | -4.744160 | -2.375351 | 1.501686 |
| C | -2.907486 | -2.379795 | 3.468811 |
| C | -1.907699 | -2.266218 | 4.407779 |
| C | -0.915971 | -1.265064 | 4.262019 |
| C | -0.936980 | -0.403039 | 3.188328 |
| H | -3.676103 | -3.142289 | 3.565216 |
| H | -1.874133 | -2.941527 | 5.257657 |

| | | | |
|---|---|---|---|
| H | -0.126859 | -1.179312 | 5.003642 |
| H | -0.167882 | 0.355064 | 3.094932 |
| C | 0.051114 | 4.741094 | 2.347442 |
| C | -0.878064 | 4.888844 | 3.352116 |
| C | -1.875555 | 3.900451 | 3.541278 |
| C | -1.918723 | 2.781068 | 2.739236 |
| H | 0.814702 | 5.496642 | 2.182271 |
| H | -0.854280 | 5.763138 | 3.996042 |
| H | -2.615476 | 4.027941 | 4.326309 |
| H | -2.690233 | 2.035879 | 2.894613 |
| C | 2.703420 | -0.824903 | 0.284765 |
| C | 3.864086 | -1.482654 | 0.191695 |
| H | 2.724015 | 0.253448 | 0.148788 |
| H | 3.893979 | -2.562418 | 0.331170 |
| C | 5.192146 | -0.814574 | -0.045346 |
| C | 6.127629 | -0.913412 | 1.174184 |
| H | 5.037740 | 0.241626 | -0.301886 |
| H | 5.693570 | -1.277339 | -0.908742 |
| C | 7.495445 | -0.259451 | 0.947374 |
| H | 5.634369 | -0.444095 | 2.036406 |
| H | 6.266642 | -1.971035 | 1.439768 |
| H | 7.990304 | -0.736926 | 0.089317 |
| H | 7.351144 | 0.794539 | 0.669009 |
| C | 8.413318 | -0.338187 | 2.172835 |
| C | 9.779988 | 0.324536 | 1.960277 |
| H | 8.561407 | -1.392197 | 2.449337 |
| H | 7.912880 | 0.133889 | 3.030726 |
| C | 10.681763 | 0.244333 | 3.195249 |
| H | 10.283657 | -0.149433 | 1.106346 |
| H | 9.631874 | 1.377312 | 1.682183 |

| | | | |
|---|---|---|---|
| H | 11.649193 | 0.728650 | 3.020211 |
| H | 10.215214 | 0.735581 | 4.057784 |
| H | 10.877527 | -0.797768 | 3.475609 |
| C | 1.319910 | -1.369811 | 0.527735 |
| H | 0.834774 | -0.716414 | 1.261190 |
| C | 1.316995 | -2.716596 | 1.211119 |
| I | -5.565010 | -1.010016 | -1.168797 |
| I | 2.288368 | 2.285367 | -2.033480 |
| F | 1.739036 | -3.735605 | 0.402977 |
| F | 0.101329 | -3.076326 | 1.677859 |
| F | 2.144970 | -2.751176 | 2.298344 |
| C | -2.483923 | -3.630359 | -1.370768 |
| C | -1.667199 | -2.393976 | -1.713353 |
| H | -3.208130 | -3.849917 | -2.162810 |
| H | -1.826226 | -4.497669 | -1.248536 |
| H | -3.027079 | -3.481894 | -0.433367 |
| H | -1.132588 | -2.563960 | -2.659074 |
| H | -2.334336 | -1.534042 | -1.868731 |
| O | -0.765427 | -2.131534 | -0.659441 |
| H | 0.347686 | -0.620934 | -3.211389 |
| C | 2.033070 | -2.743149 | -3.908286 |
| C | 1.631890 | -2.739451 | -2.443371 |
| H | 2.510682 | -3.691953 | -4.174296 |
| H | 1.158220 | -2.609590 | -4.555778 |
| H | 2.738837 | -1.931161 | -4.113061 |
| H | 0.917647 | -3.545515 | -2.231620 |
| H | 2.506698 | -2.900848 | -1.805361 |
| O | 1.055389 | -1.470687 | -2.128054 |
| H | -3.778573 | 0.925015 | -1.506816 |
| C | -1.314032 | 0.665593 | -5.515461 |

| | | | |
|---|---|---|---|
| C | -1.456391 | 0.027569 | -4.150841 |
| H | -2.247196 | 0.541287 | -6.074992 |
| H | -1.101798 | 1.734912 | -5.424592 |
| H | -0.505866 | 0.193303 | -6.082614 |
| H | -2.246920 | 0.492804 | -3.558283 |
| H | -1.655802 | -1.043521 | -4.221577 |
| O | -0.213806 | 0.225356 | -3.401265 |
| H | -0.309854 | 0.441181 | -2.316471 |

Vibrational frequencies

| | | |
|---|---|---|
| -324.7830 | 11.2218 | 15.9804 |
| 25.9437 | 30.4576 | 34.4654 |
| 36.7866 | 41.8268 | 43.3169 |
| 49.8253 | 50.4613 | 53.2118 |
| 57.5821 | 61.1723 | 74.5867 |
| 75.6916 | 79.6254 | 88.9800 |
| 95.0602 | 99.7124 | 106.2487 |
| 107.9307 | 110.8343 | 114.2644 |
| 120.8782 | 126.2038 | 128.3684 |
| 134.1492 | 142.4412 | 145.1876 |
| 153.7002 | 156.6216 | 159.8892 |
| 170.8185 | 179.0024 | 184.4939 |
| 188.2405 | 190.9035 | 202.3930 |
| 223.7074 | 228.1907 | 238.6841 |
| 249.9529 | 256.6740 | 261.0279 |
| 268.0683 | 275.9927 | 282.9118 |
| 283.4350 | 286.5724 | 294.8672 |
| 299.0354 | 304.7976 | 312.3842 |
| 318.8563 | 325.5961 | 351.3742 |
| 358.5595 | 367.3921 | 369.7244 |

| | | |
|---|---|---|
| 381.5242 | 388.6564 | 424.2640 |
| 442.6654 | 453.0824 | 454.1238 |
| 464.4084 | 469.0070 | 485.2941 |
| 497.1968 | 502.3777 | 526.3749 |
| 529.4846 | 531.5215 | 547.5024 |
| 553.6769 | 560.7048 | 570.2752 |
| 581.0159 | 591.2778 | 621.5867 |
| 625.8803 | 627.9131 | 644.5108 |
| 651.7978 | 691.7712 | 710.1553 |
| 720.1023 | 732.0549 | 735.9708 |
| 744.9065 | 749.6847 | 758.1594 |
| 759.1075 | 765.6594 | 768.6309 |
| 774.9338 | 783.2091 | 802.6658 |
| 806.0044 | 825.3128 | 827.7210 |
| 830.0576 | 841.3159 | 852.2714 |
| 861.4947 | 872.9067 | 876.8008 |
| 883.1422 | 900.4358 | 906.4639 |
| 907.6953 | 907.9063 | 911.0889 |
| 913.6183 | 939.9511 | 949.3030 |
| 969.5851 | 971.0210 | 980.7805 |
| 984.8540 | 994.1816 | 1002.1469 |
| 1009.7772 | 1013.7522 | 1023.4698 |
| 1031.3989 | 1033.0992 | 1042.3623 |
| 1046.9531 | 1053.0103 | 1060.1462 |
| 1060.9497 | 1063.7197 | 1065.9193 |
| 1074.0846 | 1080.2882 | 1097.5052 |
| 1103.9832 | 1109.4294 | 1119.3370 |
| 1132.6930 | 1136.3217 | 1140.7830 |
| 1142.3414 | 1163.6553 | 1166.1374 |
| 1180.4885 | 1182.3665 | 1184.4569 |

| | | |
|---|---|---|
| 1188.6163 | 1191.5687 | 1193.4982 |
| 1205.3660 | 1215.5161 | 1223.8950 |
| 1237.9747 | 1245.1662 | 1251.2145 |
| 1253.7807 | 1259.1618 | 1274.0943 |
| 1280.2366 | 1282.9890 | 1299.2704 |
| 1303.4921 | 1306.1523 | 1311.5617 |
| 1313.3998 | 1319.5425 | 1336.0428 |
| 1336.5493 | 1340.4841 | 1350.3490 |
| 1355.6792 | 1359.8148 | 1364.2262 |
| 1367.8141 | 1373.5840 | 1383.4562 |
| 1396.2804 | 1401.0801 | 1403.3130 |
| 1404.2483 | 1406.7327 | 1411.6234 |
| 1416.8115 | 1418.4437 | 1420.5557 |
| 1423.2164 | 1430.0021 | 1436.1357 |
| 1436.9703 | 1447.4078 | 1462.6791 |
| 1472.3764 | 1480.8378 | 1482.6614 |
| 1483.0897 | 1483.5213 | 1486.6923 |
| 1487.4317 | 1491.8158 | 1494.6024 |
| 1495.0097 | 1497.1056 | 1497.6444 |
| 1502.5228 | 1507.5531 | 1511.6358 |
| 1514.3878 | 1528.8663 | 1537.0865 |
| 1547.7494 | 1554.1997 | 1564.1840 |
| 1605.0526 | 1618.4450 | 1624.6038 |
| 1627.7705 | 1668.6782 | 1669.9037 |
| 1739.0577 | 1933.7111 | 2744.4433 |
| 3003.4776 | 3005.1357 | 3010.1812 |
| 3012.0280 | 3020.0873 | 3021.8116 |
| 3031.5308 | 3032.7230 | 3037.1429 |
| 3039.2080 | 3040.7324 | 3042.8533 |
| 3047.2110 | 3053.0297 | 3054.0253 |

| | | |
|---|---|---|
| 3063.1314 | 3072.4426 | 3085.9906 |
| 3090.9720 | 3099.2748 | 3101.9546 |
| 3102.2649 | 3114.9889 | 3117.0916 |
| 3124.1150 | 3129.6584 | 3133.8539 |
| 3134.4375 | 3159.5956 | 3165.8430 |
| 3183.0422 | 3184.6775 | 3188.8952 |
| 3193.4584 | 3193.6713 | 3206.0947 |
| 3206.5831 | 3208.4371 | 3213.9446 |
| 3218.9449 | 3225.9467 | 3721.8474 |

**PR/S**

Zero-point correction= 0.394622

Thermal correction to Energy= 0.418817

Thermal correction to Enthalpy= 0.419761

Thermal correction to Gibbs Free Energy= 0.337427

Sum of electronic and zero-point Energies= -1023.771718

Sum of electronic and thermal Energies= -1023.747523

Sum of electronic and thermal Enthalpies= -1023.746579

Sum of electronic and thermal Free Energies= -1023.828913

Cartesian coordinates

| | | | |
|---|---|---|---|
| B | 0.126792 | -2.304840 | 3.777707 |
| C | 1.392499 | -0.201544 | 3.130003 |
| C | 2.600095 | -0.028178 | 2.583594 |
| H | 0.530248 | 0.318112 | 2.713903 |
| H | 3.452781 | -0.561045 | 3.009255 |
| C | 2.893075 | 0.820523 | 1.379009 |
| C | 3.385917 | -0.014840 | 0.181450 |
| H | 3.668904 | 1.557785 | 1.632302 |
| H | 1.999134 | 1.387212 | 1.089216 |

| | | | |
|---|---|---|---|
| C | 3.765809 | 0.840723 | -1.032072 |
| H | 4.253421 | -0.614721 | 0.490673 |
| H | 2.601639 | -0.730403 | -0.100527 |
| H | 2.901259 | 1.449803 | -1.332585 |
| H | 4.553909 | 1.550182 | -0.741698 |
| C | 4.244920 | 0.013289 | -2.230349 |
| C | 4.643742 | 0.867572 | -3.439795 |
| H | 3.452268 | -0.688373 | -2.527809 |
| H | 5.101750 | -0.605347 | -1.926154 |
| C | 5.115621 | 0.032143 | -4.633261 |
| H | 3.788749 | 1.488668 | -3.740802 |
| H | 5.438706 | 1.565388 | -3.142186 |
| H | 5.392775 | 0.664937 | -5.483998 |
| H | 5.990827 | -0.574577 | -4.370499 |
| H | 4.329023 | -0.653344 | -4.971101 |
| C | 1.101310 | -1.132596 | 4.285019 |
| H | 2.039150 | -1.546453 | 4.667286 |
| C | 0.496017 | -0.384791 | 5.451289 |
| F | 1.370562 | 0.494268 | 6.006379 |
| F | 0.123968 | -1.236927 | 6.445531 |
| F | -0.602515 | 0.330919 | 5.116800 |
| C | -3.407727 | -2.178342 | 2.715694 |
| C | -2.085422 | -2.887550 | 2.938778 |
| H | -4.150774 | -2.880024 | 2.322052 |
| H | -3.786566 | -1.763050 | 3.655265 |
| H | -3.291614 | -1.358748 | 1.998913 |
| H | -2.197122 | -3.712769 | 3.652294 |
| H | -1.703017 | -3.313240 | 2.002965 |
| O | -1.140381 | -1.932278 | 3.450848 |
| C | 2.694611 | -3.934908 | 2.643108 |

| | | | |
|---|---|---|---|
| C | 1.798519 | -4.137902 | 3.854423 |
| H | 3.677606 | -4.385328 | 2.818290 |
| H | 2.252202 | -4.401776 | 1.757122 |
| H | 2.832285 | -2.869084 | 2.436595 |
| H | 1.661800 | -5.204702 | 4.058677 |
| H | 2.239782 | -3.687243 | 4.751399 |
| O | 0.488952 | -3.606581 | 3.615933 |

Vibrational frequencies

| | | |
|---|---|---|
| 15.6805 | 26.9290 | 34.4127 |
| 49.2253 | 51.2231 | 56.5835 |
| 68.5870 | 80.4159 | 85.3346 |
| 92.8004 | 105.3144 | 115.2388 |
| 135.3229 | 139.4011 | 155.0736 |
| 164.3922 | 172.3648 | 214.6594 |
| 232.1149 | 253.3065 | 258.8189 |
| 260.5944 | 283.6465 | 295.1780 |
| 308.3817 | 315.3556 | 339.8798 |
| 373.4376 | 412.2656 | 442.2268 |
| 458.1734 | 488.4425 | 504.1133 |
| 538.0591 | 568.3153 | 618.8479 |
| 646.8109 | 693.4763 | 746.6503 |
| 758.8542 | 770.3001 | 809.3706 |
| 827.6355 | 829.4465 | 840.2748 |
| 889.0273 | 904.5015 | 907.9976 |
| 909.6980 | 955.9929 | 989.8637 |
| 1013.4932 | 1015.6789 | 1031.3832 |
| 1051.4137 | 1055.4358 | 1064.8693 |
| 1072.3216 | 1077.6189 | 1098.9933 |
| 1111.2238 | 1122.8958 | 1130.9421 |

| | | |
|---|---|---|
| 1136.9205 | 1140.5621 | 1172.3877 |
| 1184.3225 | 1184.9651 | 1213.3283 |
| 1228.0440 | 1253.5267 | 1259.7448 |
| 1278.5448 | 1300.9802 | 1310.4273 |
| 1314.8117 | 1318.1218 | 1329.8104 |
| 1333.9003 | 1341.3435 | 1341.4285 |
| 1347.5031 | 1362.2920 | 1368.4477 |
| 1388.4920 | 1403.4178 | 1406.8256 |
| 1419.6547 | 1419.7729 | 1420.0290 |
| 1435.3386 | 1460.9124 | 1479.7293 |
| 1482.8037 | 1483.6102 | 1483.7914 |
| 1488.7339 | 1496.5909 | 1497.0335 |
| 1497.7270 | 1498.3693 | 1507.4151 |
| 1514.6637 | 1527.2121 | 1537.2062 |
| 1736.0867 | 3010.9003 | 3012.9392 |
| 3014.5426 | 3021.6311 | 3023.5170 |
| 3032.5889 | 3034.7473 | 3041.4281 |
| 3045.2734 | 3048.2797 | 3049.5428 |
| 3053.2020 | 3056.5072 | 3065.9244 |
| 3076.3649 | 3080.6356 | 3094.3870 |
| 3096.6063 | 3099.7748 | 3104.0003 |
| 3124.1931 | 3125.1517 | 3126.6306 |
| 3132.4596 | 3137.4417 | 3163.4356 |

**Pre-TS6**

Zero-point correction= 0.709666

Thermal correction to Energy= 0.754581

Thermal correction to Enthalpy= 0.755525

Thermal correction to Gibbs Free Energy= 0.622026

Sum of electronic and zero-point Energies= -1727.433668

Sum of electronic and thermal Energies= -1727.388753

Sum of electronic and thermal Enthalpies= -1727.387809

Sum of electronic and thermal Free Energies= -1727.521308

Cartesian coordinates

| | | | |
|---|---|---|---|
| B | -1.349472 | -2.348452 | -0.110725 |
| B | -3.076490 | -1.180685 | 1.103193 |
| B | -0.964859 | -0.097930 | 0.662366 |
| O | -2.614177 | -2.313886 | 0.448217 |
| O | -0.547478 | -1.220850 | -0.032198 |
| O | -2.225913 | -0.098254 | 1.241210 |
| C | -0.040688 | 1.130048 | 0.789525 |
| C | -0.354903 | 2.193291 | 1.550538 |
| H | 0.924785 | 1.123045 | 0.280429 |
| H | -1.309961 | 2.187692 | 2.079259 |
| C | 0.517125 | 3.384671 | 1.810078 |
| C | 1.015778 | 3.425962 | 3.270469 |
| H | -0.053853 | 4.303336 | 1.610009 |
| H | 1.376686 | 3.381864 | 1.128206 |
| C | 1.828429 | 4.685651 | 3.586977 |
| H | 0.155231 | 3.361948 | 3.950192 |
| H | 1.622496 | 2.533278 | 3.460962 |
| H | 2.680239 | 4.752122 | 2.895009 |
| H | 1.210270 | 5.574846 | 3.397303 |
| C | 2.344103 | 4.723772 | 5.030406 |
| C | 3.157694 | 5.982806 | 5.353423 |
| H | 2.962145 | 3.834076 | 5.219070 |
| H | 1.492380 | 4.654966 | 5.722550 |
| C | 3.669673 | 6.013870 | 6.796342 |
| H | 4.008350 | 6.050449 | 4.661148 |

| | | | |
|---|---|---|---|
| H | 2.539088 | 6.871067 | 5.164211 |
| H | 4.251509 | 6.920523 | 6.997291 |
| H | 2.839463 | 5.986244 | 7.512521 |
| H | 4.314467 | 5.151798 | 7.006137 |
| C | -4.516203 | -1.123627 | 1.657993 |
| C | -5.373650 | -2.154300 | 1.550716 |
| H | -4.855047 | -0.215503 | 2.160466 |
| H | -5.028566 | -3.065362 | 1.056882 |
| C | -6.775908 | -2.203050 | 2.078594 |
| C | -6.950785 | -3.283353 | 3.165214 |
| H | -7.462799 | -2.431004 | 1.249623 |
| H | -7.066281 | -1.223332 | 2.477547 |
| C | -8.394182 | -3.395025 | 3.669124 |
| H | -6.625786 | -4.254171 | 2.766436 |
| H | -6.282080 | -3.055515 | 4.005843 |
| H | -8.721371 | -2.418681 | 4.053977 |
| H | -9.055886 | -3.627956 | 2.822594 |
| C | -8.571886 | -4.456550 | 4.760836 |
| C | -10.014955 | -4.577895 | 5.265657 |
| H | -7.911211 | -4.221665 | 5.607754 |
| H | -8.239999 | -5.432105 | 4.376973 |
| C | -10.179084 | -5.642335 | 6.353834 |
| H | -10.346558 | -3.604138 | 5.651952 |
| H | -10.675549 | -4.812524 | 4.419433 |
| H | -11.216709 | -5.708286 | 6.700117 |
| H | -9.887280 | -6.633280 | 5.985424 |
| H | -9.551618 | -5.417483 | 7.224844 |
| C | -0.836264 | -3.631040 | -0.802343 |
| C | 0.382899 | -3.710439 | -1.366207 |
| H | -1.485058 | -4.508239 | -0.842694 |

| | | | |
|---|---|---|---|
| H | 1.031863 | -2.832875 | -1.322825 |
| C | 0.967318 | -4.906277 | -2.055625 |
| C | 2.295020 | -5.367580 | -1.422947 |
| H | 1.160769 | -4.646146 | -3.107607 |
| H | 0.245741 | -5.732670 | -2.058138 |
| C | 2.927716 | -6.547816 | -2.168540 |
| H | 2.999863 | -4.524851 | -1.406333 |
| H | 2.118441 | -5.644338 | -0.374759 |
| H | 2.220289 | -7.389095 | -2.183018 |
| H | 3.089754 | -6.266092 | -3.218815 |
| C | 4.255418 | -7.010654 | -1.557785 |
| C | 4.892063 | -8.186394 | -2.308785 |
| H | 4.094408 | -7.295250 | -0.507933 |
| H | 4.961291 | -6.167678 | -1.540782 |
| C | 6.221178 | -8.639016 | -1.697817 |
| H | 4.187941 | -9.029767 | -2.322720 |
| H | 5.048681 | -7.901760 | -3.358531 |
| H | 6.653252 | -9.479755 | -2.252253 |
| H | 6.956481 | -7.825160 | -1.702015 |
| H | 6.089706 | -8.959035 | -0.657078 |
| C | 0.262847 | -1.715951 | 3.264362 |
| H | 0.864370 | -2.387488 | 2.668116 |
| C | 0.842224 | -0.528900 | 3.942144 |
| N | -0.964410 | -2.046023 | 3.522273 |
| N | -2.051409 | -2.327831 | 3.721384 |
| F | 1.799679 | 0.024696 | 3.166361 |
| F | 1.440357 | -0.816637 | 5.129816 |
| F | -0.097361 | 0.406927 | 4.207598 |

Vibrational frequencies

| | | |
|---|---|---|
| 9.8043 | 12.9774 | 15.6499 |
| 18.8871 | 25.6690 | 29.1819 |
| 30.7643 | 33.4724 | 37.8106 |
| 50.1954 | 51.1752 | 59.0448 |
| 61.3691 | 63.6915 | 66.8263 |
| 69.6258 | 74.3612 | 80.0223 |
| 88.7866 | 94.4459 | 95.3448 |
| 99.6936 | 101.5544 | 107.7656 |
| 110.6655 | 133.4108 | 134.7902 |
| 141.9386 | 151.9500 | 154.6948 |
| 158.0246 | 161.2054 | 165.0129 |
| 167.1808 | 170.2926 | 176.1346 |
| 181.4545 | 198.4603 | 217.8878 |
| 222.7758 | 229.9997 | 263.7336 |
| 275.2260 | 275.6893 | 279.5820 |
| 284.7430 | 295.7423 | 316.6801 |
| 334.5648 | 336.6879 | 360.0784 |
| 366.8132 | 373.9702 | 376.6205 |
| 430.2472 | 445.7018 | 448.2376 |
| 451.7933 | 473.2986 | 477.4053 |
| 487.2830 | 489.0149 | 512.4905 |
| 538.3573 | 548.8744 | 567.4156 |
| 569.0900 | 592.3870 | 632.0271 |
| 633.1668 | 694.5081 | 699.6393 |
| 712.5174 | 746.6989 | 750.1145 |
| 751.5132 | 760.0738 | 763.6116 |
| 765.4066 | 801.4635 | 803.2881 |
| 808.9000 | 815.1602 | 842.9966 |
| 846.5420 | 850.7596 | 864.3604 |
| 879.1666 | 879.8942 | 906.4556 |

| | | |
|---|---|---|
| 908.0153 | 908.6562 | 910.8937 |
| 917.1286 | 918.9040 | 991.2244 |
| 993.5835 | 994.8768 | 1014.2791 |
| 1014.4409 | 1016.2075 | 1028.3067 |
| 1029.2456 | 1030.3605 | 1041.9314 |
| 1043.1212 | 1047.0877 | 1058.7478 |
| 1058.7816 | 1058.9629 | 1068.0891 |
| 1068.2945 | 1071.5334 | 1075.0799 |
| 1076.5154 | 1077.9045 | 1114.4650 |
| 1133.3932 | 1134.2925 | 1135.5115 |
| 1140.1090 | 1140.5775 | 1141.6331 |
| 1162.5505 | 1184.5077 | 1201.4109 |
| 1212.3629 | 1213.4510 | 1219.1052 |
| 1233.3411 | 1234.8583 | 1240.6056 |
| 1243.9310 | 1254.8310 | 1256.2949 |
| 1257.8864 | 1279.5623 | 1280.9553 |
| 1284.6330 | 1306.6376 | 1310.1410 |
| 1311.7493 | 1315.2326 | 1317.3828 |
| 1323.0729 | 1328.3811 | 1330.3784 |
| 1336.6974 | 1338.7837 | 1339.9489 |
| 1340.8744 | 1342.2308 | 1343.9094 |
| 1345.3550 | 1350.6499 | 1350.9588 |
| 1360.0983 | 1367.0109 | 1368.7286 |
| 1376.8820 | 1379.6948 | 1381.3812 |
| 1402.6533 | 1403.1166 | 1404.0871 |
| 1418.4028 | 1419.3718 | 1419.9444 |
| 1420.5135 | 1421.5199 | 1423.1781 |
| 1438.1395 | 1476.6422 | 1477.9666 |
| 1480.7934 | 1483.4747 | 1485.2240 |
| 1485.5733 | 1488.1215 | 1489.8827 |

| | | |
|---|---|---|
| 1490.6231 | 1495.5624 | 1497.9975 |
| 1498.6712 | 1500.1524 | 1500.2316 |
| 1501.3223 | 1507.8558 | 1509.3406 |
| 1509.5647 | 1514.3258 | 1515.5875 |
| 1516.4022 | 1697.0122 | 1699.2243 |
| 1702.0130 | 2224.2067 | 3008.0107 |
| 3011.4370 | 3011.7733 | 3013.1020 |
| 3013.2187 | 3014.6454 | 3015.6388 |
| 3015.8595 | 3016.7760 | 3022.6524 |
| 3023.2809 | 3024.5091 | 3025.3945 |
| 3027.8047 | 3032.8094 | 3033.6411 |
| 3033.7563 | 3035.0022 | 3035.0196 |
| 3036.3982 | 3038.5033 | 3046.4640 |
| 3048.3446 | 3051.2423 | 3058.7653 |
| 3060.4756 | 3065.8130 | 3067.1637 |
| 3068.1178 | 3068.4189 | 3079.0213 |
| 3080.8479 | 3096.1033 | 3100.1960 |
| 3100.8459 | 3101.1974 | 3104.2244 |
| 3104.6964 | 3105.9103 | 3128.5321 |
| 3129.0859 | 3133.6345 | 3135.3998 |
| 3136.1399 | 3142.2204 | 3263.9325 |

**TS6**

Zero-point correction= 0.707856

Thermal correction to Energy= 0.751841

Thermal correction to Enthalpy= 0.752785

Thermal correction to Gibbs Free Energy= 0.622670

Sum of electronic and zero-point Energies= -1727.398715

Sum of electronic and thermal Energies= -1727.354730

Sum of electronic and thermal Enthalpies= -1727.353786

Sum of electronic and thermal Free Energies= -1727.483901

Cartesian coordinates

| | | | |
|---|---|---|---|
| B | -0.828021 | -2.425539 | 0.620028 |
| B | -2.429352 | -1.452746 | 2.135663 |
| B | -0.081767 | -0.742942 | 2.252581 |
| O | -2.137450 | -2.297010 | 1.065910 |
| O | 0.171583 | -1.688915 | 1.186378 |
| O | -1.450244 | -0.707660 | 2.715815 |
| C | 0.594311 | 0.716304 | 2.005158 |
| C | 0.086139 | 1.849739 | 2.522149 |
| H | 1.494104 | 0.767651 | 1.389667 |
| H | -0.774190 | 1.772848 | 3.188707 |
| C | 0.611753 | 3.235661 | 2.301007 |
| C | 1.152329 | 3.842089 | 3.614950 |
| H | -0.196885 | 3.880234 | 1.927464 |
| H | 1.402411 | 3.229669 | 1.540908 |
| C | 1.632094 | 5.288403 | 3.452533 |
| H | 0.366368 | 3.800013 | 4.381292 |
| H | 1.974279 | 3.215980 | 3.983560 |
| H | 2.413134 | 5.329036 | 2.680037 |
| H | 0.801800 | 5.906861 | 3.083204 |
| C | 2.173384 | 5.887948 | 4.755578 |
| C | 2.649317 | 7.338421 | 4.609811 |
| H | 3.004973 | 5.268922 | 5.122110 |
| H | 1.392994 | 5.839451 | 5.528728 |
| C | 3.188065 | 7.923928 | 5.918294 |
| H | 3.428401 | 7.387490 | 3.836471 |
| H | 1.817302 | 7.957039 | 4.246012 |
| H | 3.519611 | 8.960527 | 5.789993 |

| | | | |
|---|---|---|---|
| H | 2.419672 | 7.914272 | 6.700851 |
| H | 4.042730 | 7.344593 | 6.288027 |
| C | -3.886332 | -1.379107 | 2.674744 |
| C | -4.898516 | -2.108025 | 2.174321 |
| H | -4.101370 | -0.707511 | 3.509695 |
| H | -4.687525 | -2.785831 | 1.343941 |
| C | -6.318054 | -2.108934 | 2.661877 |
| C | -6.772646 | -3.497620 | 3.152550 |
| H | -6.981568 | -1.799564 | 1.839792 |
| H | -6.440700 | -1.371874 | 3.465722 |
| C | -8.230740 | -3.516625 | 3.624692 |
| H | -6.639248 | -4.228725 | 2.343079 |
| H | -6.116340 | -3.821279 | 3.971628 |
| H | -8.358713 | -2.783932 | 4.434368 |
| H | -8.881871 | -3.182459 | 2.804129 |
| C | -8.693579 | -4.894915 | 4.110859 |
| C | -10.148632 | -4.913468 | 4.594661 |
| H | -8.037249 | -5.232626 | 4.926052 |
| H | -8.572459 | -5.626558 | 3.298887 |
| C | -10.602719 | -6.294316 | 5.076054 |
| H | -10.267714 | -4.184253 | 5.408023 |
| H | -10.804684 | -4.573908 | 3.781117 |
| H | -11.642657 | -6.278581 | 5.421345 |
| H | -10.530658 | -7.037665 | 4.272798 |
| H | -9.981342 | -6.646889 | 5.908221 |
| C | -0.515151 | -3.437850 | -0.520440 |
| C | 0.729025 | -3.649970 | -0.981675 |
| H | -1.333275 | -4.014947 | -0.958179 |
| H | 1.546440 | -3.077075 | -0.537136 |
| C | 1.138720 | -4.634602 | -2.037694 |

| | | | |
|---|---|---|---|
| C | 2.097290 | -5.708779 | -1.486626 |
| H | 1.650396 | -4.099271 | -2.851932 |
| H | 0.253972 | -5.114229 | -2.475037 |
| C | 2.593016 | -6.684575 | -2.559980 |
| H | 2.959545 | -5.215567 | -1.016309 |
| H | 1.588476 | -6.266049 | -0.688539 |
| H | 1.730286 | -7.171768 | -3.036435 |
| H | 3.103447 | -6.120733 | -3.353914 |
| C | 3.539826 | -7.755794 | -2.007300 |
| C | 4.050302 | -8.732010 | -3.074364 |
| H | 3.026234 | -8.321347 | -1.216395 |
| H | 4.398187 | -7.266865 | -1.523880 |
| C | 4.993335 | -9.796754 | -2.507304 |
| H | 3.192653 | -9.220785 | -3.556985 |
| H | 4.565126 | -8.167680 | -3.864228 |
| H | 5.343146 | -10.482388 | -3.287306 |
| H | 5.876740 | -9.337964 | -2.046547 |
| H | 4.493875 | -10.396429 | -1.736685 |
| C | 0.969595 | -1.050469 | 3.492255 |
| H | 2.011372 | -1.187096 | 3.194802 |
| C | 0.925060 | -0.343659 | 4.851477 |
| N | 0.630801 | -2.713703 | 3.885830 |
| N | 0.122242 | -3.608411 | 3.459995 |
| F | 1.736825 | 0.733607 | 4.833616 |
| F | 1.363414 | -1.153033 | 5.840694 |
| F | -0.305660 | 0.070584 | 5.187232 |

Vibrational frequencies

| | | |
|---|---|---|
| -463.8130 | 10.1112 | 10.8842 |
| 13.6510 | 21.6128 | 26.4039 |

| | | |
|---|---|---|
| 29.5446 | 36.8234 | 41.0064 |
| 45.0881 | 54.7498 | 57.2451 |
| 59.3170 | 64.8233 | 69.9696 |
| 73.7221 | 77.7572 | 78.5747 |
| 90.6284 | 94.1718 | 98.8737 |
| 103.8123 | 118.3405 | 127.8514 |
| 134.2929 | 136.0969 | 139.9303 |
| 149.6827 | 152.9271 | 155.0932 |
| 160.8043 | 163.6891 | 167.7258 |
| 171.9184 | 179.9909 | 191.2853 |
| 206.8460 | 216.3096 | 224.8158 |
| 240.7226 | 259.5750 | 262.5257 |
| 265.8649 | 267.6807 | 270.5017 |
| 274.2407 | 278.5661 | 290.0384 |
| 296.9992 | 332.0552 | 338.0845 |
| 357.5909 | 365.4274 | 371.8675 |
| 377.2191 | 422.5764 | 438.3454 |
| 444.7733 | 454.5481 | 469.4334 |
| 483.5345 | 485.4305 | 503.5362 |
| 514.6285 | 556.7388 | 568.5958 |
| 579.5951 | 630.2191 | 641.0820 |
| 664.0592 | 680.9320 | 708.6652 |
| 746.7955 | 748.1226 | 748.3476 |
| 753.0762 | 759.1198 | 759.6694 |
| 764.9159 | 770.9083 | 802.2711 |
| 803.3396 | 815.1444 | 833.6901 |
| 842.7082 | 848.0284 | 862.6797 |
| 872.6660 | 890.1520 | 906.0085 |
| 906.6141 | 908.9861 | 910.1821 |
| 912.8516 | 915.9178 | 990.3599 |

| | | |
|---|---|---|
| 992.4396 | 993.8483 | 1009.1865 |
| 1014.2160 | 1014.8117 | 1019.8771 |
| 1029.8232 | 1032.1637 | 1033.5894 |
| 1042.0245 | 1046.2265 | 1049.3165 |
| 1055.2815 | 1058.1938 | 1059.9293 |
| 1066.4518 | 1067.5925 | 1070.2049 |
| 1073.7574 | 1074.7353 | 1076.6397 |
| 1095.3962 | 1114.9241 | 1133.8710 |
| 1135.4556 | 1137.3935 | 1139.9593 |
| 1144.1070 | 1148.4847 | 1160.4336 |
| 1184.5811 | 1212.3296 | 1216.6740 |
| 1217.8105 | 1232.3877 | 1243.1902 |
| 1247.7093 | 1253.3190 | 1257.1764 |
| 1259.4646 | 1273.4323 | 1277.6336 |
| 1280.2011 | 1287.9381 | 1288.4814 |
| 1303.0367 | 1307.7288 | 1308.3961 |
| 1311.2077 | 1318.6864 | 1321.6601 |
| 1323.7709 | 1332.7908 | 1334.8135 |
| 1336.2877 | 1337.1302 | 1337.7950 |
| 1339.6242 | 1339.7992 | 1341.6084 |
| 1345.9709 | 1346.8427 | 1353.5095 |
| 1361.6264 | 1369.9031 | 1373.3724 |
| 1394.6568 | 1400.9235 | 1402.6317 |
| 1412.1171 | 1416.1392 | 1418.9607 |
| 1420.3793 | 1421.5609 | 1421.7096 |
| 1425.6393 | 1478.6023 | 1478.9431 |
| 1479.7031 | 1483.1843 | 1483.5310 |
| 1483.6011 | 1487.4517 | 1487.9988 |
| 1488.0623 | 1495.8969 | 1496.8010 |
| 1497.8678 | 1497.9764 | 1498.8157 |

| | | |
|---|---|---|
| 1499.6963 | 1506.9785 | 1507.7664 |
| 1507.9207 | 1514.1558 | 1514.2219 |
| 1514.7622 | 1650.6108 | 1703.4328 |
| 1704.8474 | 2319.2996 | 3008.1860 |
| 3009.3559 | 3011.1827 | 3011.8573 |
| 3012.0088 | 3013.6663 | 3014.7275 |
| 3015.5168 | 3020.6049 | 3021.3363 |
| 3023.0237 | 3023.3802 | 3023.8066 |
| 3025.9530 | 3032.6821 | 3032.6826 |
| 3033.2875 | 3033.2922 | 3034.8082 |
| 3034.9354 | 3036.7597 | 3045.5071 |
| 3046.3823 | 3049.6754 | 3056.7333 |
| 3057.7194 | 3063.8758 | 3065.7465 |
| 3066.0340 | 3070.9562 | 3077.3050 |
| 3077.4631 | 3088.0890 | 3099.5795 |
| 3100.5681 | 3100.9125 | 3103.5750 |
| 3104.5711 | 3104.9353 | 3118.2704 |
| 3120.5960 | 3127.6215 | 3131.1296 |
| 3136.6414 | 3148.8923 | 3167.6035 |

**M6**

Zero-point correction= 0.703599

Thermal correction to Energy= 0.745165

Thermal correction to Enthalpy= 0.746109

Thermal correction to Gibbs Free Energy= 0.620775

Sum of electronic and zero-point Energies= -1618.005682

Sum of electronic and thermal Energies= -1617.964116

Sum of electronic and thermal Enthalpies= -1617.963172

Sum of electronic and thermal Free Energies= -1618.088506

Cartesian coordinates

| | | | |
|---|---|---|---|
| B | -0.531607 | -2.964643 | 1.182078 |
| B | -2.059291 | -1.998045 | 2.783456 |
| B | 0.308565 | -1.705187 | 3.046337 |
| O | -1.816973 | -2.738275 | 1.638081 |
| O | 0.534297 | -2.427936 | 1.899810 |
| O | -0.974154 | -1.496209 | 3.494162 |
| C | 1.733775 | 0.344009 | 3.194647 |
| C | 0.842927 | 1.338102 | 3.292920 |
| H | 2.656401 | 0.505614 | 2.640361 |
| H | -0.081510 | 1.169727 | 3.844062 |
| C | 1.043260 | 2.720269 | 2.740859 |
| C | 1.197610 | 3.775161 | 3.853856 |
| H | 0.178859 | 2.991942 | 2.117635 |
| H | 1.926379 | 2.742375 | 2.089577 |
| C | 1.333037 | 5.203436 | 3.314142 |
| H | 0.332790 | 3.719902 | 4.529479 |
| H | 2.077846 | 3.523207 | 4.460529 |
| H | 2.181720 | 5.249864 | 2.616733 |
| H | 0.439106 | 5.454447 | 2.725293 |
| C | 1.526109 | 6.249194 | 4.418278 |
| C | 1.644016 | 7.684257 | 3.890435 |
| H | 2.427025 | 6.001905 | 4.998243 |
| H | 0.684928 | 6.192223 | 5.124230 |
| C | 1.848345 | 8.714955 | 5.004319 |
| H | 2.479994 | 7.741690 | 3.179534 |
| H | 0.739196 | 7.935074 | 3.319465 |
| H | 1.923287 | 9.732174 | 4.603649 |
| H | 1.014648 | 8.698499 | 5.716756 |
| H | 2.766693 | 8.511439 | 5.568389 |

| | | | |
|---|---|---|---|
| C | -3.495946 | -1.720300 | 3.266884 |
| C | -4.582425 | -2.164541 | 2.608417 |
| H | -3.642232 | -1.131948 | 4.174641 |
| H | -4.435482 | -2.757507 | 1.702929 |
| C | -6.010404 | -1.944060 | 3.006195 |
| C | -6.751605 | -3.264995 | 3.295318 |
| H | -6.531508 | -1.428639 | 2.185318 |
| H | -6.062773 | -1.287236 | 3.883185 |
| C | -8.228355 | -3.050531 | 3.645313 |
| H | -6.673278 | -3.924502 | 2.420114 |
| H | -6.248047 | -3.785205 | 4.120804 |
| H | -8.301793 | -2.374680 | 4.509229 |
| H | -8.726421 | -2.535960 | 2.811189 |
| C | -8.973762 | -4.353057 | 3.957252 |
| C | -10.452935 | -4.138931 | 4.300759 |
| H | -8.477809 | -4.864087 | 4.795041 |
| H | -8.896174 | -5.033007 | 3.096521 |
| C | -11.187433 | -5.441509 | 4.629446 |
| H | -10.529418 | -3.450060 | 5.153361 |
| H | -10.950570 | -3.638698 | 3.458444 |
| H | -12.241308 | -5.259654 | 4.868366 |
| H | -11.153579 | -6.140121 | 3.784586 |
| H | -10.732853 | -5.945115 | 5.491163 |
| C | -0.281290 | -3.797825 | -0.090538 |
| C | 0.949889 | -3.997159 | -0.596194 |
| H | -1.133856 | -4.242070 | -0.607536 |
| H | 1.802498 | -3.552161 | -0.078354 |
| C | 1.289635 | -4.798874 | -1.816211 |
| C | 2.294378 | -5.928337 | -1.515155 |
| H | 1.737834 | -4.129500 | -2.566479 |

| | | | |
|---|---|---|---|
| H | 0.377853 | -5.214950 | -2.262145 |
| C | 2.673129 | -6.736842 | -2.761019 |
| H | 3.200511 | -5.495819 | -1.068983 |
| H | 1.866323 | -6.598551 | -0.757884 |
| H | 1.765051 | -7.175402 | -3.198583 |
| H | 3.083124 | -6.058075 | -3.522600 |
| C | 3.687734 | -7.849376 | -2.473581 |
| C | 4.063050 | -8.668220 | -3.714617 |
| H | 3.281692 | -8.522957 | -1.705103 |
| H | 4.598048 | -7.408398 | -2.042276 |
| C | 5.084241 | -9.770092 | -3.418454 |
| H | 3.154314 | -9.114528 | -4.141666 |
| H | 4.463441 | -7.994213 | -4.484588 |
| H | 5.334379 | -10.340132 | -4.320345 |
| H | 6.016166 | -9.349533 | -3.021522 |
| H | 4.698875 | -10.477712 | -2.674267 |
| C | 1.547147 | -1.048620 | 3.786950 |
| H | 2.434087 | -1.650940 | 3.571911 |
| C | 1.427589 | -1.038465 | 5.292426 |
| F | 2.535476 | -0.532553 | 5.891226 |
| F | 1.268411 | -2.301071 | 5.773108 |
| F | 0.379651 | -0.314346 | 5.750917 |

Vibrational frequencies

| | | |
|---|---|---|
| 9.2826 | 10.3356 | 16.6764 |
| 22.0348 | 26.3969 | 30.0487 |
| 35.7696 | 38.5158 | 47.3062 |
| 55.4656 | 59.8020 | 62.3820 |
| 64.9934 | 72.2136 | 74.4698 |
| 80.9386 | 89.3087 | 93.9389 |

| | | |
|---|---|---|
| 102.3102 | 105.2860 | 109.1208 |
| 117.8883 | 129.6217 | 132.1245 |
| 141.1872 | 150.3817 | 152.2969 |
| 161.7326 | 163.5731 | 167.5697 |
| 172.8577 | 174.5844 | 184.4287 |
| 202.6937 | 219.0972 | 226.4745 |
| 242.8151 | 261.6866 | 264.1654 |
| 266.0004 | 268.8490 | 270.2750 |
| 286.4251 | 291.5975 | 303.3302 |
| 317.7495 | 341.0585 | 361.6347 |
| 365.3764 | 371.8690 | 416.3489 |
| 449.4856 | 454.8359 | 465.8745 |
| 470.8465 | 489.4751 | 502.5573 |
| 505.6850 | 531.4684 | 567.1235 |
| 577.0590 | 590.5960 | 628.5784 |
| 653.6952 | 694.9109 | 707.5379 |
| 743.3789 | 746.7186 | 749.5837 |
| 753.3510 | 758.1355 | 760.7878 |
| 763.9979 | 802.9845 | 803.9963 |
| 804.6367 | 811.5538 | 819.8570 |
| 838.7693 | 846.2165 | 849.5340 |
| 881.6245 | 901.0629 | 908.3601 |
| 909.3505 | 910.4353 | 912.6733 |
| 918.3672 | 930.9320 | 979.0440 |
| 992.9229 | 997.2909 | 1013.7920 |
| 1013.9516 | 1015.4008 | 1015.7426 |
| 1028.5806 | 1030.7213 | 1030.8274 |
| 1041.7414 | 1045.6038 | 1046.6090 |
| 1059.4692 | 1059.8711 | 1061.7805 |
| 1070.5524 | 1073.2691 | 1073.5370 |

| | | |
|---|---|---|
| 1077.8366 | 1079.6228 | 1085.4730 |
| 1106.8451 | 1133.3201 | 1136.3597 |
| 1138.0637 | 1139.7431 | 1141.3005 |
| 1142.3058 | 1165.1487 | 1183.2559 |
| 1208.0221 | 1213.9888 | 1218.8551 |
| 1225.7544 | 1233.1572 | 1241.4163 |
| 1253.9031 | 1256.2014 | 1258.1663 |
| 1263.1859 | 1275.9029 | 1280.3792 |
| 1283.0255 | 1292.1866 | 1309.6870 |
| 1310.8120 | 1314.3373 | 1318.8462 |
| 1320.9171 | 1323.0634 | 1330.9784 |
| 1336.5063 | 1338.3508 | 1339.3054 |
| 1340.9384 | 1341.8849 | 1342.8446 |
| 1344.8385 | 1347.8801 | 1351.1395 |
| 1353.0132 | 1358.8653 | 1366.9167 |
| 1371.6024 | 1378.0023 | 1380.0617 |
| 1384.9261 | 1397.7432 | 1402.0318 |
| 1404.5876 | 1405.1347 | 1419.9006 |
| 1420.9319 | 1421.4603 | 1424.4825 |
| 1425.6571 | 1430.2607 | 1475.8762 |
| 1476.3931 | 1479.9680 | 1482.5552 |
| 1484.4234 | 1484.4757 | 1487.0647 |
| 1488.9499 | 1489.4150 | 1496.1638 |
| 1498.0464 | 1498.2781 | 1499.9206 |
| 1500.0932 | 1500.1661 | 1506.4582 |
| 1508.0323 | 1508.8546 | 1513.2215 |
| 1515.0429 | 1515.3383 | 1696.5206 |
| 1699.0247 | 1723.4773 | 3008.4002 |
| 3011.1990 | 3011.4008 | 3012.0119 |
| 3013.1530 | 3013.4987 | 3014.8687 |

| | | |
|---|---|---|
| 3015.2786 | 3016.2440 | 3022.1431 |
| 3022.8136 | 3022.8418 | 3025.1883 |
| 3027.1195 | 3027.2222 | 3032.7425 |
| 3033.0452 | 3033.9381 | 3034.7343 |
| 3034.8623 | 3035.7468 | 3045.2904 |
| 3046.7993 | 3047.7400 | 3056.4503 |
| 3059.0207 | 3060.3142 | 3065.6278 |
| 3066.5272 | 3068.3209 | 3077.0080 |
| 3079.3503 | 3080.4203 | 3099.7393 |
| 3100.1898 | 3101.2539 | 3103.9458 |
| 3104.5525 | 3104.7209 | 3106.8650 |
| 3132.0823 | 3133.0631 | 3138.8983 |
| 3140.1646 | 3166.8972 | 3172.4082 |

**Pre-TS7**

Zero-point correction= 0.400990

Thermal correction to Energy= 0.428406

Thermal correction to Enthalpy= 0.429351

Thermal correction to Gibbs Free Energy= 0.338951

Sum of electronic and zero-point Energies= -1133.191238

Sum of electronic and thermal Energies= -1133.163821

Sum of electronic and thermal Enthalpies= -1133.162877

Sum of electronic and thermal Free Energies= -1133.253276

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.936484 | 0.226340 | -1.424077 |
| B | -0.045306 | 1.105869 | -0.871240 |
| O | -0.368422 | 1.662448 | 0.339026 |
| C | 1.349517 | 1.550283 | -1.424275 |
| C | 2.215873 | 0.826298 | -2.151837 |

| | | | |
|---|---|---|---|
| H | 1.720946 | 2.501614 | -1.033115 |
| H | 1.924722 | -0.155754 | -2.527284 |
| C | 3.654870 | 1.184640 | -2.396485 |
| C | 4.586034 | 0.290764 | -1.550542 |
| H | 3.830286 | 2.237906 | -2.144120 |
| H | 3.907040 | 1.055243 | -3.458702 |
| C | 6.074543 | 0.594890 | -1.746495 |
| H | 4.322919 | 0.411377 | -0.492257 |
| H | 4.395275 | -0.763808 | -1.797111 |
| H | 6.335719 | 0.478028 | -2.808020 |
| H | 6.264797 | 1.648503 | -1.497373 |
| C | 6.981944 | -0.301179 | -0.895382 |
| C | 8.475037 | 0.005249 | -1.061130 |
| H | 6.797892 | -1.354098 | -1.154409 |
| H | 6.704439 | -0.196171 | 0.163543 |
| C | 9.369433 | -0.900967 | -0.210365 |
| H | 8.749513 | -0.097055 | -2.120272 |
| H | 8.659488 | 1.055908 | -0.797695 |
| H | 10.430397 | -0.662818 | -0.346597 |
| H | 9.138322 | -0.794778 | 0.856504 |
| H | 9.228273 | -1.956063 | -0.474734 |
| C | 1.632821 | -1.378187 | 0.623892 |
| H | 2.041385 | -1.498898 | -0.368270 |
| C | 2.357239 | -0.626356 | 1.675892 |
| N | 0.404514 | -1.734118 | 0.833580 |
| N | -0.668094 | -2.073825 | 1.016570 |
| F | 2.397801 | 0.714439 | 1.465875 |
| F | 3.650701 | -1.025330 | 1.740265 |
| F | 1.794563 | -0.809778 | 2.894356 |
| C | -1.542356 | 1.308907 | 1.080371 |

| | | | |
|---|---|---|---|
| C | -1.181828 | 1.221662 | 2.554859 |
| H | -1.953482 | 0.360012 | 0.722183 |
| H | -2.301935 | 2.084948 | 0.915865 |
| H | -2.072063 | 0.991300 | 3.150465 |
| H | -0.437421 | 0.439038 | 2.728966 |
| H | -0.765396 | 2.171077 | 2.907539 |
| C | -0.847151 | -0.377368 | -2.714338 |
| C | -0.456128 | -1.842780 | -2.594912 |
| H | -0.144374 | 0.170343 | -3.351627 |
| H | -1.840508 | -0.293220 | -3.171112 |
| H | -0.460664 | -2.318048 | -3.581833 |
| H | 0.545944 | -1.951722 | -2.167145 |
| H | -1.163173 | -2.374737 | -1.950292 |

Vibrational frequencies

| | | |
|---|---|---|
| 13.2725 | 14.6647 | 34.5362 |
| 40.7086 | 46.3336 | 55.3551 |
| 59.2742 | 65.7640 | 69.6795 |
| 81.8543 | 95.4226 | 101.2700 |
| 107.6742 | 109.8200 | 115.5233 |
| 125.0439 | 135.8820 | 147.6950 |
| 154.6994 | 163.5627 | 181.5657 |
| 187.0780 | 245.9173 | 256.9882 |
| 264.5861 | 290.9678 | 300.4213 |
| 321.4802 | 340.0341 | 364.0199 |
| 367.5979 | 378.1636 | 421.9995 |
| 440.2415 | 457.6600 | 465.6622 |
| 488.4424 | 492.1453 | 538.1659 |
| 549.9433 | 591.4832 | 609.2804 |
| 646.1235 | 696.4232 | 744.2894 |

| | | |
|---|---|---|
| 746.5678 | 763.0715 | 811.5733 |
| 827.6285 | 830.1534 | 833.5120 |
| 869.4431 | 899.6198 | 905.5752 |
| 906.6366 | 945.3029 | 992.9500 |
| 1013.0869 | 1025.2014 | 1035.3111 |
| 1048.9611 | 1059.4814 | 1065.1148 |
| 1073.1939 | 1090.4071 | 1116.0196 |
| 1125.2511 | 1132.0173 | 1134.8170 |
| 1142.8241 | 1150.7676 | 1184.8561 |
| 1188.0503 | 1204.4810 | 1218.1015 |
| 1249.3847 | 1250.2285 | 1259.4021 |
| 1279.7249 | 1307.1001 | 1308.2547 |
| 1315.1337 | 1325.3208 | 1335.0542 |
| 1340.8854 | 1350.2360 | 1356.9834 |
| 1357.8972 | 1370.9671 | 1399.6639 |
| 1407.3644 | 1417.6475 | 1418.0757 |
| 1421.5620 | 1435.5107 | 1449.1338 |
| 1451.9394 | 1481.7828 | 1482.6589 |
| 1488.0212 | 1489.7754 | 1494.0978 |
| 1498.0043 | 1499.6885 | 1503.4132 |
| 1507.8320 | 1513.8475 | 1514.5018 |
| 1531.3726 | 1538.7878 | 1708.4017 |
| 2229.3780 | 3008.4677 | 3012.4809 |
| 3017.1237 | 3019.4545 | 3021.5820 |
| 3031.0919 | 3031.7919 | 3033.2642 |
| 3045.5009 | 3047.6129 | 3050.0461 |
| 3050.3936 | 3061.0392 | 3066.4957 |
| 3083.7272 | 3088.4355 | 3095.8825 |
| 3098.2891 | 3103.0822 | 3106.7529 |
| 3121.8361 | 3124.4114 | 3129.9936 |

3137.6291 3141.6678 3278.4600

**TS7**

Zero-point correction= 0.399187

Thermal correction to Energy= 0.425393

Thermal correction to Enthalpy= 0.426338

Thermal correction to Gibbs Free Energy= 0.341040

Sum of electronic and zero-point Energies= -1133.148845

Sum of electronic and thermal Energies= -1133.122639

Sum of electronic and thermal Enthalpies= -1133.121694

Sum of electronic and thermal Free Energies= -1133.206992

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.249011 | -0.739852 | -1.024752 |
| B | 0.372197 | 0.230611 | -0.161972 |
| O | -0.435874 | 1.306551 | 0.335675 |
| C | 1.811988 | 0.823326 | -0.672171 |
| C | 2.637956 | 0.182691 | -1.516947 |
| H | 2.099119 | 1.805018 | -0.291855 |
| H | 2.373678 | -0.829138 | -1.833228 |
| C | 3.943945 | 0.712343 | -2.035075 |
| C | 5.134874 | -0.005983 | -1.364210 |
| H | 4.016359 | 1.790555 | -1.846797 |
| H | 4.007758 | 0.564169 | -3.122096 |
| C | 6.495863 | 0.480731 | -1.873493 |
| H | 5.068174 | 0.146177 | -0.278471 |
| H | 5.045910 | -1.088363 | -1.531640 |
| H | 6.553319 | 0.326205 | -2.960394 |
| H | 6.576227 | 1.565181 | -1.712652 |
| C | 7.676958 | -0.222886 | -1.195065 |

| | | | |
|---|---|---|---|
| C | 9.044510 | 0.259916 | -1.693079 |
| H | 7.595692 | -1.307613 | -1.356654 |
| H | 7.613901 | -0.070757 | -0.107831 |
| C | 10.214756 | -0.448571 | -1.005070 |
| H | 9.108845 | 0.105861 | -2.779127 |
| H | 9.125440 | 1.343799 | -1.532022 |
| H | 11.180039 | -0.086367 | -1.376486 |
| H | 10.193279 | -0.285208 | 0.079307 |
| H | 10.177805 | -1.531314 | -1.176431 |
| C | 1.147940 | -0.686254 | 0.995836 |
| H | 1.837008 | -1.437310 | 0.609306 |
| C | 1.703975 | -0.093753 | 2.285678 |
| N | -0.045464 | -1.770629 | 1.585325 |
| N | -0.997850 | -2.234160 | 1.233383 |
| F | 2.715681 | 0.752451 | 2.019391 |
| F | 2.185731 | -1.058268 | 3.102799 |
| F | 0.770085 | 0.580441 | 2.980807 |
| C | -1.822434 | 1.126730 | 0.583167 |
| C | -2.146998 | 1.201450 | 2.072958 |
| H | -2.175706 | 0.171003 | 0.172939 |
| H | -2.368476 | 1.923312 | 0.055825 |
| H | -3.232372 | 1.170850 | 2.225982 |
| H | -1.699615 | 0.368682 | 2.622642 |
| H | -1.764632 | 2.133542 | 2.502068 |
| C | -0.771421 | -0.297888 | -2.266538 |
| C | -1.491848 | -1.455809 | -2.937913 |
| H | 0.046602 | 0.068084 | -2.908075 |
| H | -1.463317 | 0.546059 | -2.123806 |
| H | -1.898447 | -1.151462 | -3.908571 |
| H | -0.804530 | -2.293988 | -3.097218 |

| | | | |
|---|---|---|---|
| H | -2.318154 | -1.808140 | -2.310745 |

Vibrational frequencies

| | | |
|---|---|---|
| -464.9296 | 12.7636 | 27.8994 |
| 38.1749 | 61.5555 | 62.3349 |
| 72.9484 | 82.6780 | 86.7982 |
| 92.2888 | 102.0667 | 114.3053 |
| 119.1694 | 132.2571 | 140.0782 |
| 146.8513 | 150.7335 | 163.4644 |
| 172.8857 | 196.2059 | 207.9750 |
| 244.9585 | 246.2582 | 263.6519 |
| 273.2208 | 278.0075 | 286.9213 |
| 293.5297 | 296.7384 | 319.8392 |
| 343.5977 | 362.7519 | 368.5403 |
| 391.3224 | 437.7291 | 459.8815 |
| 469.6984 | 499.5029 | 508.3036 |
| 577.6429 | 600.9190 | 655.7213 |
| 689.6784 | 722.3742 | 746.0161 |
| 749.0279 | 764.9953 | 817.2153 |
| 832.2315 | 834.8896 | 848.7177 |
| 873.0713 | 900.9257 | 908.6320 |
| 910.1774 | 938.4540 | 990.5561 |
| 1011.0322 | 1019.4113 | 1026.9556 |
| 1038.1907 | 1052.6795 | 1056.2700 |
| 1064.3623 | 1075.2645 | 1100.9529 |
| 1107.7290 | 1124.0805 | 1132.7831 |
| 1137.7231 | 1139.9969 | 1156.6723 |
| 1175.9466 | 1190.5589 | 1196.0825 |
| 1212.3255 | 1217.8031 | 1246.5297 |
| 1256.0547 | 1271.5025 | 1290.3636 |

| | | |
|---|---|---|
| 1306.6086 | 1310.7997 | 1314.3597 |
| 1324.7222 | 1329.4729 | 1335.5059 |
| 1339.8254 | 1344.5044 | 1363.6060 |
| 1396.6312 | 1404.5779 | 1409.7275 |
| 1418.2385 | 1424.4228 | 1433.3731 |
| 1437.2237 | 1480.8475 | 1481.8041 |
| 1483.9441 | 1487.3862 | 1493.1019 |
| 1497.6906 | 1498.1332 | 1498.8064 |
| 1501.5864 | 1507.3822 | 1513.1196 |
| 1526.9242 | 1536.1876 | 1654.8294 |
| 2292.2637 | 2984.7576 | 2999.8207 |
| 3010.8662 | 3015.1375 | 3017.8662 |
| 3020.3727 | 3022.4937 | 3026.4127 |
| 3032.4899 | 3035.1527 | 3041.7327 |
| 3044.4829 | 3046.1638 | 3046.7594 |
| 3059.1672 | 3068.5754 | 3081.7554 |
| 3099.6638 | 3104.5166 | 3113.6320 |
| 3115.6241 | 3118.3690 | 3126.2684 |
| 3133.6176 | 3136.4257 | 3182.9109 |

**M7**

Zero-point correction= 0.247845

Thermal correction to Energy= 0.261583

Thermal correction to Enthalpy= 0.262528

Thermal correction to Gibbs Free Energy= 0.205992

Sum of electronic and zero-point Energies= -490.303610

Sum of electronic and thermal Energies= -490.289871

Sum of electronic and thermal Enthalpies= -490.288927

Sum of electronic and thermal Free Energies= -490.345463

Cartesian coordinates

| | | | |
|---|---|---|---|
| B | 7.392595 | 7.973693 | 0.361105 |
| O | 6.740946 | 9.099428 | 0.798420 |
| C | 8.887530 | 7.757303 | 0.749650 |
| C | 9.591710 | 8.629508 | 1.490486 |
| H | 9.404008 | 6.855481 | 0.407941 |
| H | 9.091654 | 9.533831 | 1.844416 |
| C | 11.022939 | 8.479980 | 1.917613 |
| C | 11.176916 | 8.434147 | 3.450813 |
| H | 11.602590 | 9.335064 | 1.537951 |
| H | 11.458131 | 7.575886 | 1.473023 |
| C | 12.637706 | 8.328888 | 3.903258 |
| H | 10.722483 | 9.334439 | 3.887196 |
| H | 10.607397 | 7.580648 | 3.842553 |
| H | 13.090401 | 7.429572 | 3.461602 |
| H | 13.203340 | 9.183357 | 3.504673 |
| C | 12.797025 | 8.281233 | 5.427286 |
| C | 14.256351 | 8.172051 | 5.885621 |
| H | 12.227982 | 7.428996 | 5.826172 |
| H | 12.345871 | 9.181945 | 5.868212 |
| C | 14.404345 | 8.133093 | 7.409290 |
| H | 14.705139 | 7.268528 | 5.450029 |
| H | 14.826502 | 9.020882 | 5.483255 |
| H | 15.455000 | 8.052055 | 7.710282 |
| H | 13.996080 | 9.040817 | 7.870135 |
| H | 13.868564 | 7.277001 | 7.837078 |
| O | 6.682453 | 7.081087 | -0.408161 |
| H | 5.822584 | 9.118919 | 0.492371 |
| H | 7.214625 | 6.320317 | -0.677264 |

Vibrational frequencies

| | | |
|---|---|---|
| 31.9937 | 45.4418 | 58.0278 |
| 79.6004 | 117.4937 | 124.2399 |
| 138.7783 | 160.9555 | 180.9344 |
| 240.3249 | 264.1289 | 279.0565 |
| 376.0078 | 402.7827 | 454.3838 |
| 482.8004 | 488.8178 | 546.9924 |
| 554.5807 | 634.2107 | 745.3613 |
| 757.7524 | 795.3838 | 837.9344 |
| 843.7398 | 907.9162 | 912.2746 |
| 991.4111 | 1012.6694 | 1021.0543 |
| 1030.6273 | 1042.7159 | 1046.6948 |
| 1056.9766 | 1065.3203 | 1073.5865 |
| 1135.6713 | 1143.6085 | 1218.0254 |
| 1247.5127 | 1263.0522 | 1289.8851 |
| 1311.3051 | 1323.7312 | 1336.9612 |
| 1341.9698 | 1347.4395 | 1365.2479 |
| 1384.2824 | 1402.3555 | 1411.1013 |
| 1418.8447 | 1419.5705 | 1477.2201 |
| 1482.6129 | 1487.3705 | 1496.2628 |
| 1497.2542 | 1507.1611 | 1513.7233 |
| 1705.3888 | 3008.7159 | 3010.7260 |
| 3013.3573 | 3021.3797 | 3024.3373 |
| 3031.7671 | 3033.6878 | 3045.0253 |
| 3056.2830 | 3064.6888 | 3076.1931 |
| 3099.3048 | 3102.1865 | 3105.9794 |
| 3133.5731 | 3805.6723 | 3828.0904 |

**R1′**

Zero-point correction= 0.304472

Thermal correction to Energy= 0.321085

Thermal correction to Enthalpy= 0.322030

Thermal correction to Gibbs Free Energy= 0.257732

Sum of electronic and zero-point Energies= -568.874651

Sum of electronic and thermal Energies= -568.858038

Sum of electronic and thermal Enthalpies= -568.857093

Sum of electronic and thermal Free Energies= -568.921391

Cartesian coordinates

| | | | |
|---|---|---|---|
| B | 7.416845 | 8.005814 | 0.330100 |
| O | 6.800704 | 9.160632 | 0.730083 |
| C | 8.909390 | 7.776793 | 0.728307 |
| C | 9.621938 | 8.649326 | 1.460480 |
| H | 9.414799 | 6.862339 | 0.403060 |
| H | 9.130763 | 9.564655 | 1.798063 |
| C | 11.048318 | 8.486154 | 1.898841 |
| C | 11.190847 | 8.447141 | 3.433335 |
| H | 11.640716 | 9.332135 | 1.518472 |
| H | 11.476530 | 7.574422 | 1.463091 |
| C | 12.647312 | 8.331521 | 3.897281 |
| H | 10.740993 | 9.353540 | 3.861775 |
| H | 10.610871 | 7.600675 | 3.825084 |
| H | 13.096373 | 7.427727 | 3.461071 |
| H | 13.222604 | 9.180630 | 3.501081 |
| C | 12.794910 | 8.285871 | 5.422507 |
| C | 14.250105 | 8.168146 | 5.891999 |
| H | 12.217447 | 7.438037 | 5.818657 |
| H | 12.346250 | 9.190254 | 5.858441 |
| C | 14.386322 | 8.129029 | 7.416729 |
| H | 14.696731 | 7.261667 | 5.460329 |

| | | | |
|---|---|---|---|
| H | 14.828451 | 9.013239 | 5.493480 |
| H | 15.434128 | 8.041572 | 7.725701 |
| H | 13.980174 | 9.039425 | 7.874137 |
| H | 13.842016 | 7.276409 | 7.840650 |
| C | 5.423814 | 9.420258 | 0.428118 |
| C | 4.504413 | 8.779012 | 1.457831 |
| H | 5.181427 | 9.061435 | -0.578956 |
| H | 5.306511 | 10.509596 | 0.435273 |
| H | 3.460605 | 9.041976 | 1.252533 |
| H | 4.596942 | 7.688710 | 1.429883 |
| H | 4.756356 | 9.123384 | 2.466331 |
| O | 6.698239 | 7.094502 | -0.409719 |
| H | 7.229471 | 6.325703 | -0.655816 |

Vibrational frequencies

| | | |
|---|---|---|
| 21.1484 | 31.9567 | 46.2729 |
| 61.0634 | 70.6142 | 84.6188 |
| 113.5772 | 126.8518 | 149.8587 |
| 157.1544 | 168.4512 | 222.2287 |
| 243.5272 | 264.3756 | 279.8102 |
| 300.9347 | 359.6408 | 404.0410 |
| 424.5390 | 459.6363 | 501.3969 |
| 522.9532 | 609.8068 | 632.1406 |
| 745.0779 | 753.8807 | 769.2485 |
| 808.3259 | 828.2167 | 841.2757 |
| 903.8202 | 908.3285 | 927.4608 |
| 990.1424 | 1009.1377 | 1014.1604 |
| 1030.1832 | 1041.7666 | 1056.4968 |
| 1065.1380 | 1073.4700 | 1082.9956 |
| 1125.1416 | 1136.1810 | 1144.3950 |

| | | |
|---|---|---|
| 1195.6144 | 1217.4949 | 1244.6006 |
| 1257.4736 | 1283.4205 | 1310.4212 |
| 1319.5137 | 1322.2742 | 1336.3498 |
| 1341.2453 | 1346.5603 | 1356.8491 |
| 1365.5234 | 1377.1785 | 1402.8334 |
| 1412.4884 | 1419.1504 | 1420.2643 |
| 1449.7364 | 1477.5504 | 1482.7237 |
| 1484.1003 | 1487.5713 | 1496.4233 |
| 1496.4816 | 1497.4860 | 1507.3408 |
| 1513.8323 | 1526.6156 | 1704.7407 |
| 3008.4114 | 3010.7156 | 3013.3595 |
| 3021.3060 | 3024.0927 | 3031.7970 |
| 3033.6360 | 3044.8243 | 3044.9439 |
| 3047.9930 | 3056.0027 | 3064.5352 |
| 3075.8484 | 3089.1971 | 3099.4096 |
| 3101.6988 | 3102.1848 | 3119.7586 |
| 3129.3591 | 3133.2732 | 3830.2791 |

**Cat+R1′**

Zero-point correction= 0.569044

Thermal correction to Energy= 0.606950

Thermal correction to Enthalpy= 0.607894

Thermal correction to Gibbs Free Energy= 0.494522

Sum of electronic and zero-point Energies= -1511.291340

Sum of electronic and thermal Energies= -1511.253433

Sum of electronic and thermal Enthalpies= -1511.252489

Sum of electronic and thermal Free Energies= -1511.365861

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | 0.761682 | -1.215415 | -0.517689 |
| B | 0.478960 | 2.302288 | -1.176725 |

| | | | |
|---|---|---|---|
| C | 0.541267 | -1.184523 | 0.817705 |
| O | -1.364952 | 1.946971 | 1.174201 |
| C | -0.643517 | -0.704969 | 1.374292 |
| C | 1.557788 | -1.704303 | 1.670187 |
| C | -2.103729 | 1.087134 | 0.428769 |
| C | -1.753007 | -0.261325 | 0.476121 |
| C | 1.421410 | -1.702402 | 3.034810 |
| C | -0.811930 | -0.695139 | 2.796582 |
| C | 0.241999 | -1.186735 | 3.633751 |
| C | -3.205741 | 1.503695 | -0.373555 |
| C | -2.472170 | -1.211312 | -0.315545 |
| C | -3.899944 | 0.608257 | -1.149339 |
| C | -3.542220 | -0.763078 | -1.156924 |
| H | 2.210375 | -2.088834 | 3.671459 |
| H | -4.730727 | 0.938268 | -1.763808 |
| C | -4.234811 | -1.695142 | -1.978046 |
| C | -3.889230 | -3.026886 | -1.972380 |
| C | -2.842417 | -3.478830 | -1.130459 |
| C | -2.155618 | -2.599774 | -0.322306 |
| H | -5.041658 | -1.332791 | -2.609696 |
| H | -4.418126 | -3.733842 | -2.604792 |
| H | -2.579971 | -4.532910 | -1.121242 |
| H | -1.363317 | -2.963939 | 0.320975 |
| C | 0.086077 | -1.172643 | 5.046814 |
| C | -1.071855 | -0.700203 | 5.622251 |
| C | -2.125053 | -0.231482 | 4.799098 |
| C | -2.000452 | -0.229489 | 3.426715 |
| H | 0.900103 | -1.545851 | 5.663075 |
| H | -1.183842 | -0.691632 | 6.702535 |
| H | -3.041809 | 0.130994 | 5.255831 |

| | | | |
|---|---|---|---|
| H | -2.820101 | 0.126934 | 2.813140 |
| I | -3.830126 | 3.563961 | -0.377216 |
| I | 3.346857 | -2.498720 | 0.793785 |
| H | -1.557495 | 2.867233 | 0.928314 |
| O | -0.272420 | 3.426587 | -1.398799 |
| C | 1.603700 | 2.379303 | -0.111010 |
| C | 2.539531 | 1.436256 | 0.084388 |
| H | 1.623286 | 3.260024 | 0.535423 |
| H | 2.537579 | 0.551929 | -0.553042 |
| C | 3.605698 | 1.449111 | 1.139105 |
| C | 5.019532 | 1.242999 | 0.567533 |
| H | 3.395924 | 0.627952 | 1.840920 |
| H | 3.561270 | 2.380785 | 1.717026 |
| C | 6.087087 | 1.105024 | 1.657914 |
| H | 5.022271 | 0.341107 | -0.059141 |
| H | 5.270126 | 2.083180 | -0.094195 |
| H | 6.073604 | 1.999085 | 2.297781 |
| H | 5.825507 | 0.258648 | 2.309003 |
| C | 7.500790 | 0.899630 | 1.102095 |
| C | 8.568611 | 0.751176 | 2.192605 |
| H | 7.763161 | 1.746988 | 0.452182 |
| H | 7.512113 | 0.007290 | 0.459462 |
| C | 9.979114 | 0.555166 | 1.629592 |
| H | 8.551574 | 1.640778 | 2.837485 |
| H | 8.309875 | -0.099326 | 2.838436 |
| H | 10.723185 | 0.466469 | 2.429366 |
| H | 10.038879 | -0.353016 | 1.017531 |
| H | 10.272645 | 1.400243 | 0.995021 |
| C | -0.598992 | -0.403585 | -3.515736 |
| C | -0.644863 | 1.013117 | -2.974503 |

| | | | |
|---|---|---|---|
| H | -1.266229 | -0.492422 | -4.378870 |
| H | 0.416260 | -0.662810 | -3.831722 |
| H | -0.924008 | -1.123023 | -2.759032 |
| H | -0.339322 | 1.732871 | -3.743762 |
| H | -1.660246 | 1.263147 | -2.647612 |
| O | 0.263329 | 1.112585 | -1.855391 |
| H | 0.409509 | -0.405963 | -0.950803 |
| H | -0.998172 | 3.319380 | -2.029026 |

Vibrational frequencies

| | | |
|---|---|---|
| 11.8212 | 18.2942 | 21.7742 |
| 23.9478 | 39.1179 | 45.5377 |
| 50.7876 | 53.9604 | 59.6824 |
| 67.9460 | 77.1507 | 78.6234 |
| 86.1495 | 90.5324 | 99.4376 |
| 102.8213 | 111.2592 | 123.6235 |
| 136.7244 | 139.1666 | 149.4128 |
| 153.1171 | 154.5379 | 160.0985 |
| 162.3966 | 175.0670 | 179.8287 |
| 198.2219 | 200.3014 | 215.1464 |
| 227.5313 | 236.1871 | 256.7245 |
| 256.9361 | 282.6650 | 286.3211 |
| 289.7922 | 297.5650 | 326.3281 |
| 345.0185 | 349.9957 | 357.1236 |
| 379.1142 | 381.5585 | 387.5790 |
| 431.2350 | 441.2274 | 444.6543 |
| 454.5355 | 455.6272 | 460.7878 |
| 503.5345 | 531.7548 | 538.7479 |
| 546.5101 | 554.8239 | 556.3924 |
| 567.5076 | 580.3497 | 596.7464 |

| | | |
|---|---|---|
| 614.3761 | 636.0352 | 639.8282 |
| 640.9739 | 667.9772 | 697.6597 |
| 716.7932 | 725.0340 | 737.8465 |
| 741.0587 | 751.8272 | 761.6817 |
| 766.4921 | 768.1357 | 778.4387 |
| 786.5092 | 790.5528 | 809.3902 |
| 820.9429 | 840.4020 | 844.5137 |
| 875.0968 | 876.2219 | 881.2248 |
| 903.0751 | 906.1978 | 907.4315 |
| 908.9872 | 938.4069 | 941.2880 |
| 969.3953 | 971.9922 | 991.7972 |
| 996.2044 | 999.2413 | 1001.8428 |
| 1010.0710 | 1013.2301 | 1017.8996 |
| 1036.9124 | 1048.4940 | 1058.5598 |
| 1060.9347 | 1061.8705 | 1073.3809 |
| 1080.3166 | 1087.0314 | 1100.5538 |
| 1133.9639 | 1138.0484 | 1144.0809 |
| 1163.7407 | 1179.4649 | 1182.4041 |
| 1186.2967 | 1187.6978 | 1218.1488 |
| 1238.0572 | 1240.8388 | 1243.5902 |
| 1244.7531 | 1258.5518 | 1261.8404 |
| 1280.7404 | 1284.0678 | 1299.6700 |
| 1310.2451 | 1311.5333 | 1320.4627 |
| 1329.5753 | 1333.7771 | 1338.2997 |
| 1341.1678 | 1345.9397 | 1355.6702 |
| 1364.7434 | 1370.3459 | 1374.7699 |
| 1387.0893 | 1405.0914 | 1406.2982 |
| 1411.1210 | 1413.4130 | 1417.7840 |
| 1420.9004 | 1422.8527 | 1428.5901 |
| 1448.8032 | 1457.9750 | 1472.8242 |

| | | |
|---|---|---|
| 1474.6652 | 1481.6999 | 1485.5424 |
| 1486.6480 | 1488.6640 | 1493.3121 |
| 1495.0238 | 1496.5143 | 1503.5327 |
| 1505.5442 | 1512.3895 | 1527.9813 |
| 1542.0331 | 1549.3944 | 1602.5117 |
| 1614.6168 | 1623.5511 | 1626.0737 |
| 1667.0563 | 1669.0460 | 1712.8355 |
| 3008.4511 | 3011.3195 | 3012.4233 |
| 3020.7089 | 3026.7927 | 3031.6187 |
| 3032.8156 | 3040.6265 | 3044.6846 |
| 3056.8761 | 3057.0618 | 3064.1774 |
| 3077.4514 | 3090.3250 | 3098.5024 |
| 3103.1752 | 3115.6525 | 3133.1031 |
| 3142.0293 | 3158.7449 | 3182.9102 |
| 3184.8453 | 3191.0329 | 3195.1136 |
| 3206.6608 | 3209.6048 | 3209.9314 |
| 3213.5067 | 3221.5050 | 3227.2103 |
| 3473.6079 | 3724.5060 | 3815.0392 |

**TS1′**

Zero-point correction= 0.646283

Thermal correction to Energy= 0.688140

Thermal correction to Enthalpy= 0.689084

Thermal correction to Gibbs Free Energy= 0.564564

Sum of electronic and zero-point Energies= -1666.257963

Sum of electronic and thermal Energies= -1666.216107

Sum of electronic and thermal Enthalpies= -1666.215163

Sum of electronic and thermal Free Energies= -1666.339683

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.154932 | -0.900493 | -0.560899 |
| B | 0.803274 | 0.354283 | -0.925750 |
| C | -0.333940 | -1.371894 | 0.710700 |
| O | -1.320637 | 1.913836 | 1.343020 |
| C | -1.407138 | -0.921482 | 1.465707 |
| C | 0.547437 | -2.355764 | 1.248013 |
| C | -2.416426 | 1.282538 | 0.841971 |
| C | -2.485524 | -0.103343 | 0.831600 |
| C | 0.427723 | -2.778646 | 2.548850 |
| C | -1.551668 | -1.344996 | 2.825170 |
| C | -0.601096 | -2.261412 | 3.378909 |
| C | -3.500371 | 2.034599 | 0.300163 |
| C | -3.613777 | -0.771845 | 0.257496 |
| C | -4.604642 | 1.425313 | -0.242089 |
| C | -4.684046 | 0.008173 | -0.288973 |
| H | 1.102574 | -3.525420 | 2.953401 |
| H | -5.419533 | 2.011711 | -0.653640 |
| C | -5.802687 | -0.648536 | -0.871407 |
| C | -5.864701 | -2.023303 | -0.920170 |
| C | -4.808761 | -2.798473 | -0.380433 |
| C | -3.714048 | -2.190669 | 0.196173 |
| H | -6.606983 | -0.042975 | -1.280959 |
| H | -6.721542 | -2.516219 | -1.370176 |
| H | -4.863706 | -3.882737 | -0.420308 |
| H | -2.913934 | -2.795328 | 0.609077 |
| C | -0.731327 | -2.672451 | 4.733548 |
| C | -1.762755 | -2.200053 | 5.513828 |
| C | -2.708846 | -1.298016 | 4.967350 |
| C | -2.609116 | -0.882934 | 3.657051 |
| H | -0.001554 | -3.368193 | 5.139161 |

| | | | |
|---|---|---|---|
| H | -1.854540 | -2.517087 | 6.548613 |
| H | -3.519528 | -0.929447 | 5.589428 |
| H | -3.334592 | -0.187245 | 3.249662 |
| I | -3.369029 | 4.176219 | 0.308071 |
| I | 1.981909 | -3.331658 | -0.013701 |
| H | -0.656205 | 1.890564 | 0.597413 |
| O | -0.003591 | 1.562941 | -0.897320 |
| C | 1.984897 | 0.492545 | 0.130041 |
| C | 3.255551 | 0.131105 | -0.083343 |
| H | 1.749198 | 0.934668 | 1.103935 |
| H | 3.512212 | -0.317551 | -1.046003 |
| C | 4.400253 | 0.267186 | 0.882446 |
| C | 5.518115 | 1.189145 | 0.360509 |
| H | 4.831755 | -0.727934 | 1.072818 |
| H | 4.033867 | 0.641439 | 1.847345 |
| C | 6.724654 | 1.268059 | 1.302744 |
| H | 5.848591 | 0.834637 | -0.626339 |
| H | 5.105776 | 2.195100 | 0.202465 |
| H | 6.389902 | 1.606203 | 2.293935 |
| H | 7.135977 | 0.258615 | 1.447737 |
| C | 7.832669 | 2.199600 | 0.797679 |
| C | 9.046920 | 2.268533 | 1.732020 |
| H | 7.423071 | 3.210979 | 0.661772 |
| H | 8.160899 | 1.867724 | -0.198169 |
| C | 10.145616 | 3.203899 | 1.219012 |
| H | 8.719019 | 2.599040 | 2.727415 |
| H | 9.457993 | 1.258261 | 1.865482 |
| H | 11.000580 | 3.235573 | 1.903810 |
| H | 10.516042 | 2.879278 | 0.239043 |
| H | 9.771666 | 4.228875 | 1.106856 |

| | | | |
|---|---|---|---|
| C | 2.305398 | 0.287956 | -4.390213 |
| C | 1.771310 | 0.956510 | -3.135327 |
| H | 2.768647 | 1.027252 | -5.052077 |
| H | 3.054823 | -0.467981 | -4.133803 |
| H | 1.496964 | -0.204321 | -4.943839 |
| H | 2.580580 | 1.453946 | -2.586866 |
| H | 1.029060 | 1.725725 | -3.389855 |
| O | 1.179531 | -0.042407 | -2.299309 |
| H | 0.069521 | -1.003869 | -2.930723 |
| C | -1.369367 | -3.918003 | -2.358500 |
| C | -0.436492 | -3.002358 | -3.120790 |
| H | -1.198541 | -4.952203 | -2.672867 |
| H | -1.184362 | -3.856107 | -1.281304 |
| H | -2.414699 | -3.661187 | -2.552540 |
| H | 0.612519 | -3.213796 | -2.895985 |
| H | -0.595145 | -3.062042 | -4.200086 |
| O | -0.725206 | -1.616281 | -2.739548 |
| H | -0.620076 | -1.437871 | -1.616867 |
| H | -0.736791 | 1.505707 | -1.527094 |

Vibrational frequencies

| | | |
|---|---|---|
| -372.1423 | 8.3817 | 9.9463 |
| 15.1096 | 21.0027 | 26.3134 |
| 33.6005 | 44.9811 | 49.2226 |
| 52.0810 | 53.8269 | 58.7215 |
| 60.8857 | 68.2214 | 73.4830 |
| 84.4599 | 87.5523 | 87.9087 |
| 96.7736 | 102.1824 | 115.1724 |
| 127.8130 | 131.2874 | 137.6142 |
| 141.4997 | 151.3059 | 160.2893 |

| | | |
|---|---|---|
| 163.3572 | 166.2479 | 171.0325 |
| 184.1770 | 188.2833 | 212.7810 |
| 223.4418 | 231.0809 | 236.4145 |
| 249.6501 | 259.3594 | 261.5019 |
| 280.9288 | 284.5022 | 288.5526 |
| 311.4649 | 322.3471 | 330.9663 |
| 346.9430 | 356.7378 | 364.5905 |
| 378.9670 | 385.3637 | 399.9844 |
| 439.2804 | 447.2090 | 455.4959 |
| 457.5224 | 472.3219 | 473.0517 |
| 501.9896 | 511.8396 | 520.6179 |
| 532.7212 | 545.9910 | 560.6523 |
| 564.7213 | 566.5869 | 575.0176 |
| 582.3326 | 597.9797 | 631.1569 |
| 632.4697 | 652.4238 | 699.8324 |
| 715.4399 | 719.1459 | 733.9551 |
| 745.0854 | 745.7515 | 755.3520 |
| 759.0407 | 766.2547 | 770.4548 |
| 777.7164 | 780.5354 | 792.4053 |
| 800.9110 | 809.5739 | 826.9858 |
| 827.5111 | 829.4124 | 843.1703 |
| 872.6310 | 879.5685 | 882.5238 |
| 898.8704 | 904.2876 | 904.5295 |
| 908.7165 | 910.8631 | 929.2191 |
| 948.8551 | 961.1030 | 968.5794 |
| 974.9623 | 982.7998 | 996.6903 |
| 1000.2566 | 1002.4214 | 1005.8770 |
| 1007.4593 | 1021.6052 | 1033.9616 |
| 1036.7145 | 1044.1910 | 1051.4844 |
| 1055.3463 | 1058.5300 | 1062.2596 |

| | | |
|---|---|---|
| 1066.8400 | 1073.8764 | 1096.6352 |
| 1108.3575 | 1122.5952 | 1133.2377 |
| 1136.3243 | 1146.6407 | 1164.9296 |
| 1173.0037 | 1183.3213 | 1186.6908 |
| 1188.1009 | 1188.8842 | 1195.2064 |
| 1220.6542 | 1239.4716 | 1245.1590 |
| 1250.7360 | 1270.7105 | 1272.0431 |
| 1279.2614 | 1282.4370 | 1290.2092 |
| 1302.8182 | 1305.0156 | 1311.6694 |
| 1314.1862 | 1330.7932 | 1333.3591 |
| 1334.4003 | 1339.6344 | 1340.7572 |
| 1341.8697 | 1346.4370 | 1363.7104 |
| 1369.3598 | 1395.2870 | 1400.3073 |
| 1404.0286 | 1405.5198 | 1409.6914 |
| 1414.1649 | 1417.0923 | 1420.7231 |
| 1422.1869 | 1433.3031 | 1435.4934 |
| 1452.8081 | 1461.8696 | 1475.9674 |
| 1478.5777 | 1481.9513 | 1483.3404 |
| 1485.3132 | 1487.8502 | 1488.7944 |
| 1491.8044 | 1494.0901 | 1497.1914 |
| 1497.6323 | 1503.2769 | 1507.4258 |
| 1514.0444 | 1528.8284 | 1536.2228 |
| 1539.2340 | 1545.0110 | 1605.7288 |
| 1612.8923 | 1621.5625 | 1623.8228 |
| 1666.3701 | 1668.4697 | 1725.1755 |
| 1903.4459 | 2894.5723 | 2998.2704 |
| 3008.7993 | 3010.7289 | 3018.2251 |
| 3021.2165 | 3021.9117 | 3030.9219 |
| 3032.1006 | 3040.7285 | 3041.6211 |
| 3050.7042 | 3055.3664 | 3061.2402 |

| | | |
|---|---|---|
| 3066.5773 | 3070.5361 | 3082.6232 |
| 3085.7704 | 3098.4814 | 3101.6007 |
| 3112.4061 | 3120.3042 | 3124.5753 |
| 3125.2434 | 3137.8497 | 3148.1240 |
| 3184.4048 | 3185.5705 | 3191.1916 |
| 3193.0800 | 3194.3986 | 3207.6802 |
| 3207.7935 | 3209.7716 | 3211.4334 |
| 3219.1806 | 3219.4138 | 3792.6870 |

**M1′**

Zero-point correction= 0.651561

Thermal correction to Energy= 0.694035

Thermal correction to Enthalpy= 0.694980

Thermal correction to Gibbs Free Energy= 0.568880

Sum of electronic and zero-point Energies= -1666.265300

Sum of electronic and thermal Energies= -1666.222826

Sum of electronic and thermal Enthalpies= -1666.221882

Sum of electronic and thermal Free Energies= -1666.347981

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.141338 | -0.943853 | -0.436416 |
| B | 0.742513 | 0.235374 | -0.700355 |
| C | -0.330262 | -1.413556 | 0.823742 |
| O | -1.251988 | 1.857464 | 1.449515 |
| C | -1.415039 | -0.974413 | 1.574320 |
| C | 0.529706 | -2.415167 | 1.366376 |
| C | -2.355702 | 1.252816 | 0.920544 |
| C | -2.465659 | -0.129407 | 0.929221 |
| C | 0.380866 | -2.865935 | 2.654850 |
| C | -1.594901 | -1.427211 | 2.918626 |
| C | -0.663281 | -2.362235 | 3.473954 |

| | | | |
|---|---|---|---|
| C | -3.391081 | 2.032034 | 0.325489 |
| C | -3.596904 | -0.769134 | 0.327521 |
| C | -4.494291 | 1.449835 | -0.247929 |
| C | -4.619953 | 0.035417 | -0.270987 |
| H | 1.043515 | -3.624910 | 3.057123 |
| H | -5.272371 | 2.054719 | -0.701822 |
| C | -5.736429 | -0.595317 | -0.885580 |
| C | -5.838195 | -1.968164 | -0.919134 |
| C | -4.826361 | -2.767658 | -0.332574 |
| C | -3.735980 | -2.185249 | 0.277397 |
| H | -6.505523 | 0.028471 | -1.333579 |
| H | -6.692452 | -2.441381 | -1.394529 |
| H | -4.911830 | -3.850139 | -0.363713 |
| H | -2.968650 | -2.806734 | 0.725954 |
| C | -0.828324 | -2.803485 | 4.815297 |
| C | -1.875204 | -2.343120 | 5.582236 |
| C | -2.802642 | -1.422472 | 5.034239 |
| C | -2.668876 | -0.977470 | 3.736816 |
| H | -0.112513 | -3.513323 | 5.221661 |
| H | -1.993517 | -2.683597 | 6.606849 |
| H | -3.625974 | -1.063293 | 5.645248 |
| H | -3.380493 | -0.267667 | 3.328793 |
| I | -3.185025 | 4.167846 | 0.296916 |
| I | 1.988756 | -3.369027 | 0.113086 |
| H | -0.608135 | 1.899900 | 0.698002 |
| O | -0.017673 | 1.451491 | -0.892999 |
| C | 1.935059 | 0.499137 | 0.315911 |
| C | 3.216147 | 0.150116 | 0.147754 |
| H | 1.681741 | 1.036008 | 1.235666 |
| H | 3.495293 | -0.392887 | -0.757892 |

| | | | |
|---|---|---|---|
| C | 4.354566 | 0.427478 | 1.090353 |
| C | 5.489494 | 1.223908 | 0.420764 |
| H | 4.766765 | -0.528853 | 1.448564 |
| H | 3.990464 | 0.965788 | 1.974910 |
| C | 6.694728 | 1.459009 | 1.337980 |
| H | 5.818796 | 0.688199 | -0.481016 |
| H | 5.094536 | 2.189686 | 0.076309 |
| H | 6.369339 | 2.006450 | 2.233977 |
| H | 7.074444 | 0.489952 | 1.692848 |
| C | 7.831211 | 2.229197 | 0.655415 |
| C | 9.044709 | 2.465498 | 1.562588 |
| H | 7.451457 | 3.197827 | 0.299309 |
| H | 8.152613 | 1.679931 | -0.241444 |
| C | 10.175352 | 3.225178 | 0.862695 |
| H | 8.726609 | 3.021236 | 2.455316 |
| H | 9.420678 | 1.497765 | 1.922771 |
| H | 11.028544 | 3.384719 | 1.531619 |
| H | 10.537707 | 2.674617 | -0.013942 |
| H | 9.835589 | 4.208926 | 0.516632 |
| C | 2.583633 | 0.137895 | -4.161462 |
| C | 1.865504 | 0.808535 | -3.009109 |
| H | 3.008593 | 0.902543 | -4.819541 |
| H | 3.395135 | -0.499333 | -3.797779 |
| H | 1.895081 | -0.474463 | -4.753873 |
| H | 2.541644 | 1.399657 | -2.390730 |
| H | 1.047161 | 1.451273 | -3.344956 |
| O | 1.321872 | -0.217183 | -2.122703 |
| H | 0.613667 | -0.767053 | -2.606546 |
| C | -1.655675 | -3.798054 | -3.018582 |
| C | -0.446864 | -2.933105 | -3.331306 |

| | | | |
|---|---|---|---|
| H | -1.466604 | -4.834926 | -3.316193 |
| H | -1.871361 | -3.787721 | -1.943689 |
| H | -2.541544 | -3.436173 | -3.550085 |
| H | 0.439068 | -3.291712 | -2.791960 |
| H | -0.220394 | -2.938330 | -4.401415 |
| O | -0.694507 | -1.548653 | -2.992219 |
| H | -0.961374 | -1.523695 | -2.050539 |
| H | -0.836528 | 1.276372 | -1.380394 |

Vibrational frequencies

| | | |
|---|---|---|
| 8.0179 | 12.6710 | 14.8689 |
| 21.6114 | 28.3784 | 30.8475 |
| 35.7459 | 40.7918 | 48.0370 |
| 52.3034 | 59.9572 | 61.3269 |
| 65.9308 | 69.1331 | 81.9633 |
| 83.1890 | 88.1953 | 96.7706 |
| 109.0860 | 111.6672 | 120.5446 |
| 127.7930 | 134.3880 | 137.8881 |
| 141.9833 | 152.0908 | 161.1807 |
| 163.8197 | 166.2317 | 175.6131 |
| 185.7197 | 203.2496 | 213.8945 |
| 218.7401 | 223.3888 | 237.4957 |
| 249.4186 | 270.7802 | 271.4637 |
| 282.0696 | 284.8386 | 289.9468 |
| 303.9582 | 316.3984 | 349.0160 |
| 350.3893 | 357.2827 | 368.2332 |
| 376.4305 | 386.2756 | 435.1416 |
| 444.0692 | 446.0886 | 456.7807 |
| 460.1224 | 467.4774 | 479.2673 |
| 489.1255 | 529.1942 | 536.2748 |

| | | |
|---|---|---|
| 545.9321 | 550.8473 | 564.0796 |
| 565.6368 | 573.8658 | 583.7617 |
| 596.4600 | 620.4209 | 630.8257 |
| 636.3633 | 654.7618 | 680.4995 |
| 696.3081 | 702.6030 | 718.0606 |
| 731.7486 | 741.8136 | 746.6775 |
| 750.2534 | 758.0616 | 768.3404 |
| 769.0656 | 789.1593 | 796.1201 |
| 800.9468 | 824.1791 | 828.5305 |
| 829.4775 | 833.1412 | 843.5998 |
| 875.7447 | 876.4226 | 882.4502 |
| 893.6224 | 900.8872 | 903.5720 |
| 905.8152 | 907.0969 | 909.4049 |
| 947.4454 | 960.4298 | 970.9729 |
| 972.0869 | 990.9363 | 998.8872 |
| 1002.3137 | 1002.4672 | 1014.6932 |
| 1019.2556 | 1024.9574 | 1035.0941 |
| 1042.2468 | 1048.2927 | 1053.3492 |
| 1057.9505 | 1058.1414 | 1059.9293 |
| 1063.6479 | 1071.7603 | 1076.5109 |
| 1107.8533 | 1116.3087 | 1131.1619 |
| 1137.6765 | 1145.1158 | 1159.2483 |
| 1164.2256 | 1175.4956 | 1185.5896 |
| 1187.0935 | 1187.8091 | 1218.4504 |
| 1226.2269 | 1238.8802 | 1244.9375 |
| 1250.0850 | 1266.6071 | 1273.8910 |
| 1279.5036 | 1284.0683 | 1299.3677 |
| 1305.1644 | 1306.1778 | 1314.6644 |
| 1320.1910 | 1332.5053 | 1335.8688 |
| 1340.8827 | 1343.5769 | 1353.5461 |

| | | |
|---|---|---|
| 1361.8041 | 1369.9867 | 1381.9052 |
| 1394.3919 | 1399.1253 | 1400.6372 |
| 1401.2760 | 1406.7421 | 1410.6580 |
| 1418.6240 | 1420.9958 | 1424.2493 |
| 1430.5788 | 1431.6913 | 1445.4827 |
| 1451.8701 | 1456.5072 | 1476.7885 |
| 1478.4720 | 1483.3731 | 1483.5427 |
| 1487.8252 | 1489.2340 | 1491.0985 |
| 1493.3370 | 1495.1859 | 1497.4015 |
| 1499.6492 | 1507.8339 | 1514.7696 |
| 1520.7897 | 1524.3300 | 1536.2340 |
| 1543.0682 | 1592.5951 | 1604.6320 |
| 1611.2762 | 1621.7319 | 1622.3178 |
| 1666.2529 | 1667.9478 | 1727.4565 |
| 2814.3545 | 3000.1128 | 3009.4052 |
| 3011.6658 | 3017.4044 | 3021.8707 |
| 3032.4299 | 3033.3338 | 3042.1852 |
| 3044.4393 | 3049.8230 | 3051.4877 |
| 3053.2049 | 3062.9941 | 3071.6065 |
| 3093.0577 | 3095.1256 | 3099.4761 |
| 3104.6822 | 3104.8891 | 3122.5258 |
| 3123.9965 | 3124.9341 | 3130.7313 |
| 3135.8454 | 3165.3736 | 3184.1818 |
| 3184.5627 | 3192.7068 | 3193.7385 |
| 3205.9680 | 3207.5902 | 3209.4433 |
| 3209.7741 | 3216.2411 | 3219.6446 |
| 3360.6403 | 3597.1032 | 3785.4755 |

**TS2′**

Zero-point correction= 0.648010

Thermal correction to Energy= 0.689735

Thermal correction to Enthalpy= 0.690679

Thermal correction to Gibbs Free Energy= 0.568613

Sum of electronic and zero-point Energies= -1666.260814

Sum of electronic and thermal Energies= -1666.219089

Sum of electronic and thermal Enthalpies= -1666.218145

Sum of electronic and thermal Free Energies= -1666.340211

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.905132 | -0.548313 | -1.504076 |
| B | -0.643883 | -1.418713 | -0.379998 |
| C | -2.069109 | 0.154612 | -1.393111 |
| O | -0.146725 | -0.216546 | 0.940400 |
| C | -2.097000 | 1.279875 | -0.585447 |
| C | -3.244452 | -0.295844 | -2.051529 |
| C | 0.055741 | 1.099036 | 0.735829 |
| C | -0.816486 | 1.849642 | -0.071708 |
| C | -4.452286 | 0.318775 | -1.839583 |
| C | -3.362858 | 1.887159 | -0.277619 |
| C | -4.547381 | 1.394222 | -0.916457 |
| C | 1.142343 | 1.798136 | 1.364754 |
| C | -0.486004 | 3.201251 | -0.435925 |
| C | 1.415338 | 3.116870 | 1.101560 |
| C | 0.640163 | 3.843448 | 0.166664 |
| H | -5.350933 | -0.028391 | -2.338312 |
| H | 2.240892 | 3.618430 | 1.595231 |
| C | 0.971001 | 5.182188 | -0.177370 |
| C | 0.229329 | 5.870836 | -1.109780 |
| C | -0.868987 | 5.233403 | -1.736957 |
| C | -1.219407 | 3.941303 | -1.409795 |

| | | | |
|---|---|---|---|
| H | 1.828238 | 5.645188 | 0.304641 |
| H | 0.488845 | 6.891621 | -1.374740 |
| H | -1.439706 | 5.767711 | -2.491429 |
| H | -2.055912 | 3.473387 | -1.914568 |
| C | -5.808989 | 1.968389 | -0.600286 |
| C | -5.909890 | 2.978738 | 0.329470 |
| C | -4.744885 | 3.457223 | 0.977196 |
| C | -3.506230 | 2.930950 | 0.679234 |
| H | -6.694761 | 1.579295 | -1.095385 |
| H | -6.878943 | 3.404178 | 0.573481 |
| H | -4.829211 | 4.243834 | 1.721692 |
| H | -2.626334 | 3.302421 | 1.191525 |
| I | 2.397349 | 0.865515 | 2.845300 |
| I | -3.122393 | -1.978132 | -3.372789 |
| H | 0.615405 | -1.079070 | 1.604677 |
| O | 0.510237 | -2.220089 | -0.590598 |
| C | -1.858143 | -2.172102 | 0.305966 |
| C | -2.636389 | -1.719803 | 1.298204 |
| H | -2.130950 | -3.131080 | -0.145909 |
| H | -2.387272 | -0.760392 | 1.752481 |
| C | -3.905720 | -2.350254 | 1.800238 |
| C | -5.121667 | -1.479849 | 1.423309 |
| H | -3.872193 | -2.455765 | 2.894855 |
| H | -4.027592 | -3.357592 | 1.381469 |
| C | -6.457196 | -2.003899 | 1.958210 |
| H | -4.959664 | -0.457668 | 1.791795 |
| H | -5.167786 | -1.400183 | 0.330048 |
| H | -6.616888 | -3.032288 | 1.603643 |
| H | -6.415396 | -2.060737 | 3.055542 |
| C | -7.644943 | -1.129929 | 1.537364 |

| | | | |
|---|---|---|---|
| C | -8.993486 | -1.621004 | 2.075960 |
| H | -7.688373 | -1.084882 | 0.439352 |
| H | -7.473265 | -0.097635 | 1.874968 |
| C | -10.166247 | -0.736067 | 1.644462 |
| H | -9.166101 | -2.651434 | 1.735578 |
| H | -8.950462 | -1.664224 | 3.173173 |
| H | -11.119073 | -1.107907 | 2.037913 |
| H | -10.037790 | 0.292865 | 2.001862 |
| H | -10.250615 | -0.697332 | 0.551623 |
| C | 1.419923 | -4.102636 | 3.053392 |
| C | 0.554369 | -2.880245 | 2.837990 |
| H | 0.980974 | -4.724458 | 3.840180 |
| H | 1.482802 | -4.704321 | 2.140526 |
| H | 2.431259 | -3.816898 | 3.357368 |
| H | -0.461921 | -3.134571 | 2.526287 |
| H | 0.507662 | -2.248903 | 3.727914 |
| O | 1.160311 | -2.038580 | 1.804421 |
| H | 1.050338 | -2.415024 | 0.860707 |
| C | 2.800251 | 1.626355 | -1.982336 |
| C | 2.720985 | 0.190521 | -1.491409 |
| H | 3.506842 | 2.200152 | -1.373700 |
| H | 3.130146 | 1.659737 | -3.025809 |
| H | 1.822499 | 2.114165 | -1.909801 |
| H | 3.694906 | -0.303555 | -1.567137 |
| H | 2.415952 | 0.158745 | -0.437196 |
| O | 1.824722 | -0.604034 | -2.292283 |
| H | 0.960444 | -0.154411 | -2.318217 |
| H | 1.122523 | -1.794301 | -1.240097 |

Vibrational frequencies

| | | |
|---|---|---|
| -358.7172 | 11.6155 | 14.5116 |
| 24.9211 | 31.9308 | 33.1202 |
| 40.8868 | 41.8732 | 48.7252 |
| 54.9253 | 60.1041 | 62.9066 |
| 72.3969 | 76.8812 | 81.4412 |
| 87.2309 | 93.5845 | 97.6971 |
| 99.6432 | 102.2616 | 107.5099 |
| 116.8257 | 121.0460 | 136.6592 |
| 144.2659 | 150.7951 | 153.8035 |
| 160.5428 | 166.6449 | 168.1884 |
| 176.8433 | 189.6860 | 198.6336 |
| 204.9878 | 218.0708 | 242.7302 |
| 252.6639 | 261.6185 | 266.7180 |
| 282.3215 | 286.1626 | 289.1444 |
| 292.7170 | 299.9781 | 319.5073 |
| 339.7916 | 355.5371 | 373.0103 |
| 390.1123 | 406.3254 | 415.0532 |
| 432.3723 | 442.2149 | 450.4902 |
| 456.8873 | 462.8496 | 479.0133 |
| 491.2130 | 509.9591 | 522.5621 |
| 530.9336 | 558.1894 | 560.8237 |
| 562.8391 | 569.5155 | 580.0710 |
| 596.6423 | 619.9690 | 634.9860 |
| 639.9585 | 658.6136 | 664.2315 |
| 698.1336 | 717.3768 | 742.1310 |
| 749.8178 | 753.9015 | 757.7903 |
| 760.9379 | 766.3269 | 767.9180 |
| 783.6334 | 801.1793 | 801.9977 |
| 824.8564 | 825.9953 | 831.6767 |
| 833.2643 | 834.6770 | 870.4791 |

| | | |
|---|---|---|
| 873.8764 | 881.9397 | 884.5862 |
| 891.9787 | 896.6597 | 903.1949 |
| 904.6120 | 906.4622 | 911.2944 |
| 952.4193 | 968.9437 | 970.1885 |
| 979.1296 | 988.8561 | 998.0344 |
| 999.8847 | 1015.9216 | 1019.8570 |
| 1026.5309 | 1031.6075 | 1048.6928 |
| 1053.4984 | 1057.9955 | 1061.3578 |
| 1064.7686 | 1066.7995 | 1073.5436 |
| 1076.1134 | 1087.2323 | 1099.1123 |
| 1104.5472 | 1125.3327 | 1132.3364 |
| 1138.0493 | 1152.7384 | 1165.5055 |
| 1168.4953 | 1178.4775 | 1185.5396 |
| 1192.4927 | 1192.6959 | 1220.5037 |
| 1238.5596 | 1246.3067 | 1252.0825 |
| 1268.9340 | 1274.0014 | 1284.6590 |
| 1286.4132 | 1293.8055 | 1296.4152 |
| 1305.6219 | 1312.5331 | 1316.5979 |
| 1327.3859 | 1337.6155 | 1342.0046 |
| 1343.9985 | 1349.9396 | 1355.6930 |
| 1366.6013 | 1370.9819 | 1383.1634 |
| 1390.6380 | 1403.4704 | 1405.3687 |
| 1405.6811 | 1409.4392 | 1411.1151 |
| 1418.4472 | 1419.3261 | 1420.5822 |
| 1425.7205 | 1434.9614 | 1441.0077 |
| 1452.8345 | 1460.7626 | 1467.2158 |
| 1478.7613 | 1482.0555 | 1483.8261 |
| 1484.4770 | 1485.4140 | 1487.7831 |
| 1493.6085 | 1494.2324 | 1496.6050 |
| 1497.3754 | 1506.6863 | 1511.5063 |

| | | |
|---|---|---|
| 1514.2486 | 1530.0401 | 1532.4999 |
| 1540.5946 | 1547.6055 | 1592.0577 |
| 1611.3567 | 1620.8662 | 1626.0580 |
| 1666.9679 | 1667.1755 | 1721.8808 |
| 1820.9188 | 2853.0858 | 3007.1846 |
| 3010.3859 | 3012.4023 | 3021.5074 |
| 3030.3656 | 3031.7853 | 3034.3599 |
| 3046.1930 | 3047.0189 | 3047.9776 |
| 3053.9317 | 3056.8106 | 3064.0847 |
| 3080.9605 | 3093.7525 | 3095.7631 |
| 3097.8050 | 3098.7521 | 3103.7095 |
| 3125.1349 | 3125.5756 | 3129.3888 |
| 3136.1377 | 3147.8836 | 3156.9092 |
| 3183.9397 | 3184.7719 | 3192.0578 |
| 3194.3246 | 3207.1742 | 3207.3997 |
| 3209.2041 | 3211.0295 | 3224.2611 |
| 3229.0765 | 3368.1851 | 3686.0997 |

**M2′**

Zero-point correction= 0.651918

Thermal correction to Energy= 0.693932

Thermal correction to Enthalpy= 0.694876

Thermal correction to Gibbs Free Energy= 0.572343

Sum of electronic and zero-point Energies= -1666.280493

Sum of electronic and thermal Energies= -1666.238479

Sum of electronic and thermal Enthalpies= -1666.237535

Sum of electronic and thermal Free Energies= -1666.360068

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -1.064226 | -0.413254 | -0.820384 |
| B | -0.705981 | -0.894777 | 0.552037 |

| | | | |
|---|---|---|---|
| C | -2.152328 | 0.396162 | -0.848386 |
| O | -0.417076 | 0.225288 | 1.466824 |
| C | -2.053736 | 1.687377 | -0.340305 |
| C | -3.385032 | -0.074302 | -1.377222 |
| C | 0.006556 | 1.426428 | 1.037700 |
| C | -0.713371 | 2.172846 | 0.097318 |
| C | -4.516442 | 0.701405 | -1.336280 |
| C | -3.237157 | 2.491174 | -0.218068 |
| C | -4.477341 | 1.985543 | -0.730767 |
| C | 1.189983 | 1.991813 | 1.600406 |
| C | -0.146143 | 3.375141 | -0.442731 |
| C | 1.700092 | 3.191432 | 1.171953 |
| C | 1.070845 | 3.891353 | 0.109904 |
| H | -5.456167 | 0.337140 | -1.737758 |
| H | 2.601073 | 3.603176 | 1.614136 |
| C | 1.642290 | 5.079429 | -0.423365 |
| C | 1.052795 | 5.729199 | -1.484176 |
| C | -0.135300 | 5.209210 | -2.053798 |
| C | -0.720458 | 4.069416 | -1.546684 |
| H | 2.562374 | 5.455887 | 0.016323 |
| H | 1.499397 | 6.631123 | -1.892426 |
| H | -0.587434 | 5.710859 | -2.904743 |
| H | -1.622963 | 3.681963 | -2.004479 |
| C | -5.658304 | 2.769708 | -0.616932 |
| C | -5.630748 | 3.999504 | 0.000740 |
| C | -4.414728 | 4.490961 | 0.534912 |
| C | -3.251395 | 3.759726 | 0.428357 |
| H | -6.586558 | 2.370973 | -1.017807 |
| H | -6.538779 | 4.588756 | 0.089777 |
| H | -4.400145 | 5.452631 | 1.040046 |

| | | | |
|---|---|---|---|
| H | -2.333494 | 4.148269 | 0.853008 |
| I | 2.200922 | 0.956924 | 3.187555 |
| I | -3.471495 | -2.027518 | -2.251624 |
| H | 1.748224 | -1.819325 | 2.951993 |
| O | 0.591329 | -1.674495 | 0.239427 |
| C | -1.795846 | -1.864956 | 1.178682 |
| C | -2.744838 | -1.468227 | 2.037904 |
| H | -1.881842 | -2.875898 | 0.770951 |
| H | -2.697948 | -0.449950 | 2.430269 |
| C | -3.965800 | -2.255419 | 2.428251 |
| C | -5.229076 | -1.670542 | 1.763283 |
| H | -4.102755 | -2.245144 | 3.519581 |
| H | -3.849589 | -3.304872 | 2.127206 |
| C | -6.512862 | -2.432327 | 2.106003 |
| H | -5.336406 | -0.616233 | 2.054928 |
| H | -5.082327 | -1.670581 | 0.675640 |
| H | -6.396607 | -3.486646 | 1.815896 |
| H | -6.663362 | -2.429137 | 3.195228 |
| C | -7.754284 | -1.852504 | 1.417824 |
| C | -9.044957 | -2.616324 | 1.736864 |
| H | -7.595414 | -1.849000 | 0.329510 |
| H | -7.873789 | -0.799247 | 1.710899 |
| C | -10.275722 | -2.030961 | 1.038642 |
| H | -8.923151 | -3.668752 | 1.445018 |
| H | -9.205200 | -2.617434 | 2.823989 |
| H | -11.183288 | -2.595901 | 1.279712 |
| H | -10.442545 | -0.989376 | 1.339063 |
| H | -10.155211 | -2.044136 | -0.051425 |
| C | 0.608320 | -4.715392 | 2.018236 |
| C | 0.741826 | -3.536233 | 2.960355 |

| | | | |
|---|---|---|---|
| H | -0.087979 | -5.448332 | 2.437874 |
| H | 0.222095 | -4.394007 | 1.045920 |
| H | 1.576394 | -5.202596 | 1.864307 |
| H | -0.228240 | -3.051339 | 3.119925 |
| H | 1.143989 | -3.848870 | 3.931122 |
| O | 1.663532 | -2.587086 | 2.361013 |
| H | 1.087885 | -2.015615 | 1.061806 |
| C | 2.018712 | 1.696099 | -2.955951 |
| C | 2.306890 | 0.795626 | -1.766438 |
| H | 2.662213 | 2.581840 | -2.926242 |
| H | 2.193739 | 1.166513 | -3.897962 |
| H | 0.979404 | 2.041784 | -2.936610 |
| H | 3.343178 | 0.444638 | -1.781301 |
| H | 2.147612 | 1.334840 | -0.826888 |
| O | 1.493090 | -0.395403 | -1.799368 |
| H | 0.552165 | -0.128449 | -1.830062 |
| H | 1.168678 | -1.220487 | -0.453538 |

Vibrational frequencies

| | | |
|---|---|---|
| 10.6301 | 19.5184 | 24.9947 |
| 29.2978 | 31.7919 | 42.4948 |
| 45.2011 | 48.3941 | 50.4784 |
| 54.4448 | 61.6769 | 68.4043 |
| 78.5989 | 87.2306 | 88.1440 |
| 88.7325 | 93.5661 | 98.6963 |
| 100.3098 | 106.8229 | 108.7151 |
| 134.4466 | 137.3279 | 139.6279 |
| 154.8783 | 156.8747 | 158.8522 |
| 163.2557 | 171.4623 | 179.5876 |
| 185.2867 | 197.6459 | 206.5114 |

| | | |
|---|---|---|
| 219.4981 | 221.6908 | 256.4459 |
| 269.5640 | 276.0239 | 279.9887 |
| 283.2395 | 285.6068 | 293.2019 |
| 304.6394 | 329.4597 | 343.1671 |
| 345.4697 | 366.3536 | 380.6846 |
| 402.5018 | 416.9218 | 421.6247 |
| 428.2754 | 450.3734 | 457.3102 |
| 459.3576 | 470.6251 | 477.1887 |
| 496.4398 | 509.3013 | 519.9988 |
| 522.0348 | 542.6251 | 563.1121 |
| 566.7067 | 570.3116 | 583.3743 |
| 589.7664 | 611.6839 | 637.1671 |
| 656.5344 | 673.0063 | 682.3250 |
| 714.9768 | 733.2781 | 747.0117 |
| 750.3398 | 751.9562 | 761.4571 |
| 765.3249 | 769.1563 | 782.0373 |
| 790.5794 | 808.0622 | 822.1039 |
| 823.6106 | 825.5138 | 829.0527 |
| 841.7564 | 857.9712 | 871.4367 |
| 878.8493 | 882.5129 | 888.0132 |
| 895.0050 | 903.1269 | 907.0585 |
| 907.8669 | 908.8503 | 911.2163 |
| 923.8947 | 956.1010 | 967.1354 |
| 973.9224 | 981.4967 | 995.0674 |
| 998.3498 | 1002.2117 | 1013.0670 |
| 1018.0631 | 1026.7516 | 1032.2315 |
| 1037.8562 | 1053.9760 | 1057.1475 |
| 1060.6636 | 1065.1585 | 1067.1753 |
| 1069.7149 | 1073.9175 | 1081.7753 |
| 1100.7378 | 1110.8768 | 1135.4424 |

| | | |
|---|---|---|
| 1136.9066 | 1145.8135 | 1154.4225 |
| 1165.3744 | 1185.1832 | 1190.9958 |
| 1191.9347 | 1194.4857 | 1220.6585 |
| 1241.6236 | 1242.9020 | 1250.8943 |
| 1258.0902 | 1272.2238 | 1276.3654 |
| 1285.4217 | 1290.1664 | 1292.8587 |
| 1302.4085 | 1307.6698 | 1311.9563 |
| 1316.2765 | 1320.6492 | 1334.2311 |
| 1336.9750 | 1341.4649 | 1347.6053 |
| 1349.2361 | 1367.5596 | 1368.6921 |
| 1391.0493 | 1396.0262 | 1402.7365 |
| 1403.9955 | 1406.3368 | 1411.7514 |
| 1414.0315 | 1419.1431 | 1419.4923 |
| 1423.9168 | 1439.5386 | 1454.3874 |
| 1457.0499 | 1461.7815 | 1478.7095 |
| 1482.3141 | 1484.0452 | 1484.2020 |
| 1485.3499 | 1487.5101 | 1489.7159 |
| 1491.5699 | 1497.1097 | 1499.3809 |
| 1501.4817 | 1508.4349 | 1515.2420 |
| 1528.2122 | 1529.8074 | 1538.1200 |
| 1541.6778 | 1590.3225 | 1606.5838 |
| 1620.1165 | 1621.3215 | 1666.7983 |
| 1667.6228 | 1679.2656 | 1714.6633 |
| 2789.4982 | 2985.4657 | 3009.5091 |
| 3011.0500 | 3012.7752 | 3021.4546 |
| 3025.6958 | 3032.2307 | 3033.6746 |
| 3045.6393 | 3046.3755 | 3048.9362 |
| 3053.1318 | 3056.1829 | 3063.8205 |
| 3077.2879 | 3078.6960 | 3093.9431 |
| 3099.5972 | 3103.9537 | 3104.6058 |

| | | |
|---|---|---|
| 3111.5708 | 3122.1204 | 3126.7874 |
| 3132.0070 | 3132.7207 | 3134.3631 |
| 3182.4219 | 3184.7055 | 3192.8400 |
| 3193.8405 | 3207.6963 | 3208.4458 |
| 3210.4464 | 3211.9774 | 3225.8008 |
| 3225.8373 | 3607.8668 | 3723.9334 |

**TS3S-L2**

Zero-point correction= 0.497575

Thermal correction to Energy= 0.534923

Thermal correction to Enthalpy= 0.535867

Thermal correction to Gibbs Free Energy= 0.422296

Sum of electronic and zero-point Energies= -2337.138214

Sum of electronic and thermal Energies= -2337.100866

Sum of electronic and thermal Enthalpies= -2337.099922

Sum of electronic and thermal Free Energies= -2337.213492

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.094615 | -0.856305 | -0.781379 |
| B | 0.427632 | 0.049854 | 0.246870 |
| C | -1.306517 | -1.421092 | -0.623672 |
| O | -0.604100 | 0.898950 | 0.831716 |
| C | -2.466201 | -0.638846 | -0.583625 |
| C | -1.404466 | -2.841706 | -0.505129 |
| C | -1.426558 | 1.545710 | -0.021118 |
| C | -2.340198 | 0.832267 | -0.804055 |
| C | -2.614455 | -3.464739 | -0.308823 |
| C | -3.728409 | -1.261261 | -0.284180 |
| C | -3.799239 | -2.691550 | -0.171440 |
| C | -1.372226 | 2.969871 | -0.110549 |

| | | | |
|---|---|---|---|
| C | -3.108799 | 1.525047 | -1.802934 |
| C | -2.164136 | 3.659206 | -0.999624 |
| C | -3.028169 | 2.956355 | -1.882768 |
| H | -2.677745 | -4.551586 | -0.225468 |
| H | -2.122621 | 4.748760 | -1.056270 |
| C | -3.802142 | 3.653426 | -2.854554 |
| C | -4.608302 | 2.969797 | -3.739833 |
| C | -4.661343 | 1.553858 | -3.692284 |
| C | -3.933857 | 0.852510 | -2.751910 |
| H | -3.735423 | 4.744327 | -2.889777 |
| H | -5.194868 | 3.513009 | -4.485173 |
| H | -5.280337 | 1.010978 | -4.411465 |
| H | -3.979810 | -0.236530 | -2.741059 |
| C | -5.048586 | -3.318046 | 0.103751 |
| C | -6.189292 | -2.567762 | 0.294167 |
| C | -6.118292 | -1.153512 | 0.226332 |
| C | -4.924758 | -0.519447 | -0.054382 |
| H | -5.081162 | -4.408889 | 0.172511 |
| H | -7.142569 | -3.057160 | 0.509557 |
| H | -7.017533 | -0.557746 | 0.404039 |
| H | -4.892780 | 0.569248 | -0.090519 |
| C | 1.778969 | 0.772194 | -0.262813 |
| C | 2.599281 | 0.230512 | -1.186549 |
| H | 2.052838 | 1.728279 | 0.199677 |
| H | 2.344306 | -0.757209 | -1.594660 |
| C | 3.867212 | 0.836657 | -1.702969 |
| C | 5.098044 | 0.009370 | -1.282084 |
| H | 3.972916 | 1.874035 | -1.342968 |
| H | 3.831777 | 0.874605 | -2.807554 |
| C | 6.414051 | 0.552511 | -1.842053 |

| | | | |
|---|---|---|---|
| H | 5.144921 | -0.020868 | -0.178820 |
| H | 4.962007 | -1.036776 | -1.611967 |
| H | 6.352863 | 0.585334 | -2.945614 |
| H | 6.546432 | 1.600197 | -1.514334 |
| C | 7.636807 | -0.268753 | -1.426090 |
| C | 8.957755 | 0.259840 | -1.991886 |
| H | 7.497929 | -1.318108 | -1.747676 |
| H | 7.698553 | -0.297646 | -0.321989 |
| C | 10.170620 | -0.571705 | -1.575392 |
| H | 8.892480 | 0.291062 | -3.095111 |
| H | 9.098569 | 1.307262 | -1.667594 |
| H | 11.105941 | -0.167000 | -1.996356 |
| H | 10.282621 | -0.594465 | -0.477671 |
| H | 10.076627 | -1.616654 | -1.918286 |
| C | 1.221128 | -0.767343 | 1.420437 |
| H | 1.742373 | -1.665997 | 1.070741 |
| C | 2.023001 | -0.095564 | 2.543395 |
| N | -0.067248 | -1.564925 | 2.354210 |
| N | -1.159707 | -1.662527 | 2.494135 |
| I | -0.056712 | 4.042383 | 1.177336 |
| I | 0.382820 | -4.001122 | -0.595876 |
| F | 3.284192 | 0.112461 | 2.137850 |
| F | 2.080603 | -0.870442 | 3.639393 |
| F | 1.506630 | 1.081094 | 2.908075 |

Vibrational frequencies

| | | |
|---|---|---|
| -460.0886 | 8.4156 | 13.8536 |
| 20.7227 | 30.7460 | 36.3136 |
| 39.6552 | 46.9573 | 49.9104 |
| 54.7578 | 58.2840 | 67.0849 |

| | | |
|---|---|---|
| 76.3777 | 84.9206 | 92.1492 |
| 95.3956 | 100.4164 | 101.1138 |
| 112.7470 | 124.2266 | 136.8265 |
| 143.7898 | 148.2609 | 160.0845 |
| 167.3295 | 168.6502 | 193.1080 |
| 198.5013 | 215.8867 | 224.0704 |
| 244.4600 | 262.8076 | 269.0193 |
| 271.6231 | 278.8107 | 285.2021 |
| 294.0249 | 300.4281 | 319.5890 |
| 337.2959 | 343.7720 | 361.7591 |
| 367.7209 | 402.3710 | 411.9801 |
| 423.4624 | 446.7602 | 455.5570 |
| 458.1450 | 465.3595 | 474.0233 |
| 504.6858 | 520.0482 | 526.0007 |
| 531.5842 | 568.9773 | 571.7186 |
| 574.6211 | 579.5643 | 588.2411 |
| 596.1396 | 602.5230 | 632.0425 |
| 643.6394 | 662.6689 | 673.8848 |
| 681.1455 | 722.2422 | 744.8679 |
| 753.6193 | 760.9935 | 763.6108 |
| 767.5024 | 772.4579 | 777.6481 |
| 789.2028 | 803.3277 | 808.3785 |
| 829.9524 | 830.7333 | 837.4260 |
| 871.3594 | 881.3898 | 887.3648 |
| 890.3214 | 903.4357 | 906.8762 |
| 912.4881 | 927.0479 | 927.5539 |
| 951.5494 | 978.4526 | 993.1253 |
| 995.8403 | 997.8136 | 1000.0639 |
| 1018.2180 | 1021.1048 | 1026.1949 |
| 1031.2111 | 1031.7688 | 1038.0400 |

| | | |
|---|---|---|
| 1047.4372 | 1057.5288 | 1065.0014 |
| 1067.0144 | 1074.0389 | 1079.0753 |
| 1105.5955 | 1122.4949 | 1128.8849 |
| 1138.5153 | 1142.1960 | 1154.0315 |
| 1168.7164 | 1174.2224 | 1178.8822 |
| 1183.4783 | 1202.0483 | 1229.9202 |
| 1234.1151 | 1236.3503 | 1246.6661 |
| 1263.8934 | 1266.4287 | 1275.4540 |
| 1280.5551 | 1282.5950 | 1291.5997 |
| 1294.6338 | 1304.2268 | 1310.1195 |
| 1320.8265 | 1322.8895 | 1329.4647 |
| 1342.6880 | 1352.7002 | 1368.5719 |
| 1385.4741 | 1394.8647 | 1398.3147 |
| 1406.0654 | 1409.1423 | 1411.5809 |
| 1419.8775 | 1442.9533 | 1445.9135 |
| 1449.6437 | 1450.8155 | 1452.6354 |
| 1455.8953 | 1461.4866 | 1469.6188 |
| 1470.4759 | 1475.7209 | 1476.0734 |
| 1533.0310 | 1536.8354 | 1593.9927 |
| 1607.0186 | 1621.1203 | 1622.5734 |
| 1653.0424 | 1668.2470 | 1669.2612 |
| 2389.7605 | 3002.5271 | 3007.3025 |
| 3011.9171 | 3012.2540 | 3016.4133 |
| 3017.8037 | 3032.3033 | 3044.3022 |
| 3055.7046 | 3064.5354 | 3078.7565 |
| 3092.8652 | 3098.4093 | 3127.5003 |
| 3144.2829 | 3174.2567 | 3175.2259 |
| 3183.0199 | 3185.2360 | 3187.1840 |
| 3196.5004 | 3196.7237 | 3197.8123 |
| 3198.9738 | 3217.6390 | 3221.0789 |

**TS3R-L2**

Zero-point correction= 0.497628

Thermal correction to Energy= 0.534887

Thermal correction to Enthalpy= 0.535831

Thermal correction to Gibbs Free Energy= 0.423716

Sum of electronic and zero-point Energies= -2337.133860

Sum of electronic and thermal Energies= -2337.096600

Sum of electronic and thermal Enthalpies= -2337.095656

Sum of electronic and thermal Free Energies= -2337.207772

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.184201 | -1.259867 | -0.134866 |
| B | 0.274473 | -0.138011 | 0.685635 |
| C | -1.467817 | -1.665500 | -0.140673 |
| O | -0.803127 | 0.779869 | 1.066123 |
| C | -2.517762 | -0.790993 | -0.452428 |
| C | -1.764830 | -3.037050 | 0.145101 |
| C | -1.419717 | 1.375967 | 0.021653 |
| C | -2.210045 | 0.615887 | -0.841872 |
| C | -3.057959 | -3.505339 | 0.169342 |
| C | -3.880499 | -1.238158 | -0.327956 |
| C | -4.146654 | -2.617857 | -0.038599 |
| C | -1.256396 | 2.775209 | -0.205195 |
| C | -2.706584 | 1.208809 | -2.053208 |
| C | -1.802281 | 3.383834 | -1.312325 |
| C | -2.506840 | 2.612979 | -2.277759 |
| H | -3.266019 | -4.555785 | 0.381664 |
| H | -1.681684 | 4.456416 | -1.477555 |
| C | -3.010540 | 3.213611 | -3.467353 |
| C | -3.665141 | 2.459152 | -4.417973 |

| | | | |
|---|---|---|---|
| C | -3.834245 | 1.065752 | -4.217062 |
| C | -3.370424 | 0.458536 | -3.067550 |
| H | -2.857646 | 4.286114 | -3.616062 |
| H | -4.043972 | 2.928104 | -5.329703 |
| H | -4.332909 | 0.465260 | -4.982474 |
| H | -3.502451 | -0.615690 | -2.935372 |
| C | -5.492079 | -3.075224 | 0.062447 |
| C | -6.548254 | -2.201304 | -0.083552 |
| C | -6.292963 | -0.827957 | -0.325172 |
| C | -4.999562 | -0.360515 | -0.444691 |
| H | -5.669058 | -4.133817 | 0.271694 |
| H | -7.577689 | -2.558812 | 0.000820 |
| H | -7.128996 | -0.128896 | -0.412086 |
| H | -4.830413 | 0.701927 | -0.617388 |
| C | 1.597899 | 0.588304 | 0.089450 |
| C | 2.393544 | 0.004641 | -0.829435 |
| H | 1.840611 | 1.595779 | 0.447598 |
| H | 2.161736 | -1.022868 | -1.138607 |
| C | 3.612861 | 0.604994 | -1.455460 |
| C | 4.875810 | -0.200361 | -1.089342 |
| H | 3.730353 | 1.656524 | -1.143337 |
| H | 3.501370 | 0.600258 | -2.555722 |
| C | 6.152385 | 0.347484 | -1.730135 |
| H | 4.984915 | -0.213657 | 0.009529 |
| H | 4.732945 | -1.253551 | -1.392429 |
| H | 6.029052 | 0.367811 | -2.828801 |
| H | 6.294224 | 1.399704 | -1.421132 |
| C | 7.403208 | -0.460108 | -1.374773 |
| C | 8.689060 | 0.079868 | -2.006780 |
| H | 7.258730 | -1.511597 | -1.686614 |

| | | | |
|---|---|---|---|
| H | 7.520686 | -0.485723 | -0.275129 |
| C | 9.927402 | -0.744582 | -1.656157 |
| H | 8.566639 | 0.113895 | -3.105000 |
| H | 8.839367 | 1.127273 | -1.686552 |
| H | 10.837239 | -0.332351 | -2.123176 |
| H | 10.095413 | -0.769935 | -0.565587 |
| H | 9.822911 | -1.789174 | -1.996981 |
| C | 1.041684 | -0.547346 | 2.055074 |
| H | 1.173198 | 0.298951 | 2.742522 |
| C | 2.262466 | -1.468226 | 2.178617 |
| N | -0.232342 | -1.371161 | 3.022379 |
| N | -1.318041 | -1.556208 | 3.111522 |
| I | -0.181439 | 3.937702 | 1.220826 |
| I | -0.177524 | -4.390966 | 0.565045 |
| F | 2.422451 | -2.298406 | 1.148222 |
| F | 2.208198 | -2.209963 | 3.295631 |
| F | 3.368141 | -0.705150 | 2.257646 |

Vibrational frequencies

| | | |
|---|---|---|
| -458.8694 | 12.9317 | 18.4457 |
| 24.2241 | 31.7536 | 34.5505 |
| 39.2307 | 51.3818 | 54.0632 |
| 62.2004 | 69.9523 | 79.2078 |
| 82.3938 | 86.2548 | 91.8901 |
| 98.1906 | 102.0986 | 104.6110 |
| 107.7601 | 115.1020 | 141.5270 |
| 149.4710 | 158.0838 | 160.4953 |
| 167.4200 | 181.5099 | 191.6230 |
| 198.6188 | 215.0681 | 218.5217 |
| 228.7363 | 252.5575 | 268.7064 |

| | | |
|---|---|---|
| 272.2441 | 274.9757 | 285.3526 |
| 290.5162 | 294.3591 | 315.2056 |
| 338.9489 | 343.3418 | 354.7114 |
| 369.1005 | 393.5660 | 417.8488 |
| 432.1399 | 446.9008 | 456.4807 |
| 461.4557 | 465.4981 | 477.4038 |
| 504.9043 | 521.7733 | 525.7676 |
| 531.5901 | 567.2372 | 571.6439 |
| 574.3852 | 580.0967 | 588.8515 |
| 594.6344 | 600.7464 | 634.5040 |
| 646.2075 | 659.0014 | 672.6702 |
| 674.5237 | 726.0746 | 743.5904 |
| 751.7831 | 753.2940 | 760.2530 |
| 764.4328 | 772.5363 | 775.0848 |
| 784.4968 | 800.7501 | 807.7001 |
| 829.2577 | 831.2344 | 833.2290 |
| 864.5977 | 881.9125 | 886.6720 |
| 889.5399 | 898.6905 | 909.0584 |
| 911.2808 | 926.9543 | 927.4948 |
| 951.7603 | 978.0387 | 992.1301 |
| 995.9830 | 997.6897 | 998.3492 |
| 1017.0425 | 1019.7502 | 1026.6560 |
| 1029.3521 | 1033.6964 | 1036.0961 |
| 1055.0561 | 1058.4688 | 1062.6954 |
| 1069.0876 | 1073.7931 | 1080.1063 |
| 1106.1920 | 1113.6005 | 1129.1580 |
| 1133.7122 | 1141.1970 | 1153.2736 |
| 1166.9891 | 1173.4351 | 1175.6711 |
| 1182.6026 | 1201.8401 | 1228.5932 |
| 1233.2120 | 1235.6313 | 1248.0186 |

| | | |
|---|---|---|
| 1262.9726 | 1271.7613 | 1276.7855 |
| 1279.7968 | 1280.7077 | 1295.2440 |
| 1297.2009 | 1307.3441 | 1313.3428 |
| 1325.9216 | 1328.2037 | 1337.5488 |
| 1341.8769 | 1355.0001 | 1366.7296 |
| 1389.4642 | 1393.6449 | 1401.3556 |
| 1406.4486 | 1409.3855 | 1412.4221 |
| 1420.2991 | 1443.6788 | 1445.7642 |
| 1448.1253 | 1451.2402 | 1451.7585 |
| 1456.9619 | 1462.3963 | 1468.7331 |
| 1471.1120 | 1476.2957 | 1476.5099 |
| 1531.6848 | 1536.4990 | 1594.8825 |
| 1608.2917 | 1620.1214 | 1622.2984 |
| 1650.3847 | 1667.4591 | 1668.8810 |
| 2400.5281 | 3003.9463 | 3008.2183 |
| 3011.9656 | 3012.9593 | 3017.3360 |
| 3022.0296 | 3032.8881 | 3045.8586 |
| 3057.8169 | 3066.0848 | 3080.4169 |
| 3093.9391 | 3099.0551 | 3141.3193 |
| 3149.3493 | 3159.9444 | 3174.1698 |
| 3174.2551 | 3182.6967 | 3183.6261 |
| 3195.8097 | 3196.2682 | 3197.0622 |
| 3198.8091 | 3214.2345 | 3220.2064 |

**TS3S-L3**

Zero-point correction= 0.503158

Thermal correction to Energy= 0.540452

Thermal correction to Enthalpy= 0.541396

Thermal correction to Gibbs Free Energy= 0.428966

Sum of electronic and zero-point Energies= -1764.737648

Sum of electronic and thermal Energies= -1764.700354

Sum of electronic and thermal Enthalpies= -1764.699410

Sum of electronic and thermal Free Energies= -1764.811840

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.071435 | -0.759516 | -0.870507 |
| B | 0.431952 | 0.130692 | 0.177107 |
| C | -1.265060 | -1.356354 | -0.677929 |
| O | -0.606055 | 0.951213 | 0.792903 |
| C | -2.433853 | -0.610523 | -0.610248 |
| C | -1.324518 | -2.773783 | -0.557377 |
| C | -1.443170 | 1.583119 | -0.058369 |
| C | -2.348931 | 0.860911 | -0.822002 |
| C | -2.505753 | -3.424118 | -0.336793 |
| C | -3.671577 | -1.262213 | -0.295370 |
| C | -3.704037 | -2.681044 | -0.180480 |
| C | -1.417309 | 3.002511 | -0.146337 |
| C | -3.153130 | 1.537383 | -1.795847 |
| C | -2.232193 | 3.674641 | -1.013560 |
| C | -3.100309 | 2.956876 | -1.875763 |
| H | -2.540006 | -4.505662 | -0.250013 |
| H | -2.212662 | 4.758476 | -1.069195 |
| C | -3.905489 | 3.642597 | -2.824146 |
| C | -4.718231 | 2.949526 | -3.683137 |
| C | -4.747531 | 1.535000 | -3.633426 |
| C | -3.988939 | 0.848115 | -2.718599 |
| H | -3.854324 | 4.727527 | -2.857264 |
| H | -5.327851 | 3.478191 | -4.408878 |
| H | -5.371734 | 0.986607 | -4.332120 |
| H | -4.012389 | -0.236009 | -2.705407 |
| C | -4.927148 | -3.340916 | 0.114934 |

| | | | |
|---|---|---|---|
| C | -6.076636 | -2.623633 | 0.320015 |
| C | -6.043205 | -1.210181 | 0.247697 |
| C | -4.878478 | -0.548222 | -0.050607 |
| H | -4.925855 | -4.425284 | 0.184714 |
| H | -7.007624 | -3.132169 | 0.549110 |
| H | -6.948994 | -0.643050 | 0.438802 |
| H | -4.870693 | 0.535222 | -0.086576 |
| C | 1.788132 | 0.855382 | -0.305950 |
| C | 2.615119 | 0.299611 | -1.205553 |
| H | 2.077102 | 1.802450 | 0.155009 |
| H | 2.345699 | -0.670498 | -1.631881 |
| C | 3.912120 | 0.880588 | -1.678453 |
| C | 5.099628 | -0.003064 | -1.268906 |
| H | 4.041239 | 1.889917 | -1.271094 |
| H | 3.900299 | 0.964943 | -2.773450 |
| C | 6.433692 | 0.525769 | -1.789816 |
| H | 5.128050 | -0.074985 | -0.173760 |
| H | 4.938116 | -1.021756 | -1.645877 |
| H | 6.385712 | 0.606899 | -2.884355 |
| H | 6.593960 | 1.544140 | -1.410635 |
| C | 7.619994 | -0.353176 | -1.400265 |
| C | 8.953711 | 0.169905 | -1.930254 |
| H | 7.456135 | -1.372271 | -1.777209 |
| H | 7.671106 | -0.433630 | -0.305587 |
| C | 10.129410 | -0.725778 | -1.552000 |
| H | 8.895454 | 0.261349 | -3.022415 |
| H | 9.122135 | 1.183151 | -1.543958 |
| H | 11.075279 | -0.332384 | -1.935575 |
| H | 10.220714 | -0.813727 | -0.464214 |
| H | 9.999167 | -1.735029 | -1.956677 |

| | | | |
|---|---|---|---|
| C | 1.225483 | -0.692317 | 1.338983 |
| H | 1.775263 | -1.577764 | 1.012411 |
| C | 1.949732 | 0.000100 | 2.495047 |
| N | -0.058289 | -1.518854 | 2.271162 |
| N | -1.119356 | -1.738380 | 2.458676 |
| I | -0.116092 | 4.091445 | 1.122562 |
| I | 0.480584 | -3.880314 | -0.681818 |
| F | 3.190386 | 0.322226 | 2.123114 |
| F | 2.046294 | -0.803303 | 3.562642 |
| F | 1.325918 | 1.111110 | 2.880650 |

Vibrational frequencies

| | | |
|---|---|---|
| -463.6534 | 9.9055 | 19.6997 |
| 30.2418 | 37.1119 | 38.5387 |
| 39.4982 | 50.4027 | 54.1345 |
| 56.6046 | 60.6078 | 64.7922 |
| 71.0287 | 87.2206 | 93.2202 |
| 99.4413 | 101.3124 | 101.6180 |
| 112.6778 | 121.5554 | 134.3873 |
| 139.0416 | 146.6899 | 160.2345 |
| 162.2939 | 168.6928 | 192.9193 |
| 199.0479 | 215.9680 | 224.4956 |
| 238.3268 | 253.3390 | 265.2339 |
| 271.6790 | 278.7660 | 285.7855 |
| 294.4826 | 301.4028 | 317.5755 |
| 335.4424 | 343.1956 | 364.5815 |
| 367.0472 | 404.3645 | 410.8466 |
| 420.2892 | 443.8287 | 449.5825 |
| 457.2038 | 463.6224 | 470.4035 |
| 500.0939 | 518.9404 | 523.6086 |

| | | |
|---|---|---|
| 534.9628 | 563.2915 | 569.0081 |
| 571.1985 | 581.5225 | 588.1832 |
| 598.6199 | 602.4004 | 629.4303 |
| 641.4137 | 662.1122 | 676.5645 |
| 687.8054 | 725.4295 | 725.7848 |
| 739.9004 | 744.5840 | 762.8886 |
| 765.8126 | 775.6991 | 778.9540 |
| 782.0124 | 789.2253 | 797.9059 |
| 820.0085 | 832.6913 | 836.7069 |
| 883.6238 | 887.8294 | 889.5050 |
| 893.6016 | 900.9188 | 915.9396 |
| 922.5263 | 922.9986 | 934.6719 |
| 949.7012 | 986.4951 | 993.6618 |
| 996.7154 | 998.4432 | 1020.1653 |
| 1025.6794 | 1026.3260 | 1036.7201 |
| 1040.7150 | 1046.8582 | 1054.8853 |
| 1062.3114 | 1068.5998 | 1077.8073 |
| 1083.4783 | 1088.5450 | 1094.2892 |
| 1120.2276 | 1143.8413 | 1151.8993 |
| 1164.7659 | 1171.4036 | 1173.3776 |
| 1176.5753 | 1178.5837 | 1197.3401 |
| 1212.7135 | 1229.5556 | 1231.2849 |
| 1237.8156 | 1254.0936 | 1261.2744 |
| 1275.6906 | 1284.6496 | 1289.6250 |
| 1292.3136 | 1298.4075 | 1308.3054 |
| 1318.9199 | 1322.5798 | 1329.2253 |
| 1331.2257 | 1333.9443 | 1350.2889 |
| 1357.3124 | 1361.7418 | 1388.8544 |
| 1399.1960 | 1418.7619 | 1418.8888 |
| 1423.7040 | 1425.5216 | 1427.1264 |

| | | |
|---|---|---|
| 1445.3943 | 1471.1318 | 1473.0981 |
| 1476.2930 | 1478.4398 | 1482.3140 |
| 1493.2863 | 1496.8400 | 1499.9843 |
| 1504.1380 | 1507.5080 | 1510.0588 |
| 1556.3885 | 1563.7455 | 1642.2491 |
| 1652.5348 | 1665.2774 | 1668.1342 |
| 1697.7997 | 1711.0134 | 1712.1655 |
| 2506.0139 | 3042.1990 | 3046.7411 |
| 3050.6231 | 3056.6930 | 3058.3793 |
| 3067.6019 | 3075.3339 | 3086.6022 |
| 3099.3410 | 3106.6968 | 3117.5812 |
| 3140.8293 | 3145.6055 | 3151.8448 |
| 3153.5423 | 3202.8509 | 3203.5040 |
| 3211.2597 | 3214.7865 | 3222.4298 |
| 3222.7546 | 3225.7857 | 3226.3244 |
| 3226.6079 | 3232.5600 | 3237.1721 |

**TS3R-L3**

Zero-point correction= 0.503257

Thermal correction to Energy= 0.540367

Thermal correction to Enthalpy= 0.541311

Thermal correction to Gibbs Free Energy= 0.430187

Sum of electronic and zero-point Energies= -1764.732534

Sum of electronic and thermal Energies= -1764.695424

Sum of electronic and thermal Enthalpies= -1764.694480

Sum of electronic and thermal Free Energies= -1764.805604

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.157799 | -1.246304 | -0.130592 |
| B | 0.276717 | -0.112491 | 0.684213 |
| C | -1.444862 | -1.648941 | -0.115786 |

| | | | |
|---|---|---|---|
| O | -0.811482 | 0.779361 | 1.084027 |
| C | -2.488400 | -0.791333 | -0.444818 |
| C | -1.738152 | -3.008953 | 0.202132 |
| C | -1.412504 | 1.370659 | 0.026149 |
| C | -2.187530 | 0.613035 | -0.835552 |
| C | -3.019960 | -3.481427 | 0.225843 |
| C | -3.846204 | -1.242703 | -0.331910 |
| C | -4.106533 | -2.605327 | -0.018473 |
| C | -1.247685 | 2.763700 | -0.202031 |
| C | -2.681917 | 1.201425 | -2.043877 |
| C | -1.779929 | 3.366027 | -1.307991 |
| C | -2.479439 | 2.591872 | -2.270837 |
| H | -3.224641 | -4.521490 | 0.460070 |
| H | -1.658234 | 4.431744 | -1.476230 |
| C | -2.975387 | 3.190748 | -3.460173 |
| C | -3.626986 | 2.438467 | -4.402821 |
| C | -3.802215 | 1.048762 | -4.196255 |
| C | -3.345631 | 0.446626 | -3.050630 |
| H | -2.817079 | 4.255510 | -3.608590 |
| H | -4.000224 | 2.899777 | -5.311554 |
| H | -4.298531 | 0.452943 | -4.956008 |
| H | -3.476884 | -0.621093 | -2.911088 |
| C | -5.445414 | -3.070916 | 0.077483 |
| C | -6.498332 | -2.211901 | -0.099593 |
| C | -6.248070 | -0.844861 | -0.368242 |
| C | -4.963956 | -0.373093 | -0.481959 |
| H | -5.613434 | -4.119692 | 0.306675 |
| H | -7.519604 | -2.570345 | -0.020241 |
| H | -7.081786 | -0.158324 | -0.478330 |
| H | -4.796599 | 0.680819 | -0.671434 |

| | | | |
|---|---|---|---|
| C | 1.594317 | 0.623978 | 0.086738 |
| C | 2.352526 | 0.052934 | -0.862371 |
| H | 1.873428 | 1.612736 | 0.454635 |
| H | 2.087371 | -0.948289 | -1.208358 |
| C | 3.581899 | 0.646660 | -1.476106 |
| C | 4.819851 | -0.186266 | -1.106432 |
| H | 3.712086 | 1.681379 | -1.138854 |
| H | 3.482165 | 0.662956 | -2.569345 |
| C | 6.104711 | 0.354604 | -1.728621 |
| H | 4.916852 | -0.211160 | -0.013691 |
| H | 4.663656 | -1.224698 | -1.427877 |
| H | 5.993826 | 0.383364 | -2.821139 |
| H | 6.256060 | 1.393454 | -1.404857 |
| C | 7.335566 | -0.473842 | -1.366199 |
| C | 8.626872 | 0.065700 | -1.977987 |
| H | 7.184842 | -1.511332 | -1.695459 |
| H | 7.440722 | -0.509949 | -0.273019 |
| C | 9.844539 | -0.781041 | -1.620056 |
| H | 8.517166 | 0.111619 | -3.069005 |
| H | 8.783174 | 1.097774 | -1.639057 |
| H | 10.760332 | -0.377473 | -2.061814 |
| H | 9.987419 | -0.822023 | -0.534988 |
| H | 9.726177 | -1.809292 | -1.977935 |
| C | 1.069092 | -0.513015 | 2.026359 |
| H | 1.219012 | 0.306959 | 2.734035 |
| C | 2.272127 | -1.457519 | 2.086925 |
| N | -0.192315 | -1.370738 | 3.012567 |
| N | -1.259027 | -1.605498 | 3.143167 |
| I | -0.203788 | 3.915365 | 1.238790 |
| I | -0.154728 | -4.337339 | 0.663884 |

| | | | |
|---|---|---|---|
| F | 2.423236 | -2.202803 | 0.997450 |
| F | 2.199305 | -2.281694 | 3.138295 |
| F | 3.381092 | -0.719286 | 2.227265 |

Vibrational frequencies

| | | |
|---|---|---|
| -471.5150 | 12.7702 | 18.1165 |
| 28.3471 | 33.3271 | 38.3815 |
| 47.0656 | 52.2006 | 60.4339 |
| 68.4605 | 71.0654 | 76.4974 |
| 88.3490 | 92.6296 | 97.6958 |
| 102.4663 | 104.7854 | 106.9535 |
| 110.5424 | 123.7898 | 143.3642 |
| 145.7536 | 157.5837 | 159.9688 |
| 166.8595 | 176.3708 | 192.2441 |
| 199.2805 | 218.2997 | 221.6987 |
| 231.5340 | 249.4906 | 257.0051 |
| 274.8804 | 281.0477 | 284.7655 |
| 290.0260 | 295.1932 | 314.2558 |
| 336.9097 | 340.7295 | 353.7920 |
| 368.3243 | 394.9736 | 415.5909 |
| 432.5942 | 442.6323 | 451.7609 |
| 457.7617 | 463.0221 | 473.7930 |
| 499.7173 | 521.9742 | 522.2417 |
| 530.7778 | 561.5951 | 568.7452 |
| 570.1923 | 583.2056 | 588.8074 |
| 594.5660 | 602.9859 | 630.5635 |
| 648.2704 | 658.0166 | 675.8194 |
| 680.0685 | 728.1500 | 729.0749 |
| 740.9293 | 746.7785 | 753.9818 |
| 758.8071 | 774.1575 | 777.5047 |

| | | |
|---|---|---|
| 782.9324 | 788.3053 | 800.2981 |
| 820.7272 | 829.5046 | 836.3569 |
| 881.1359 | 886.3308 | 887.6625 |
| 891.3710 | 901.8584 | 914.6785 |
| 921.9970 | 926.0678 | 930.3775 |
| 949.6809 | 990.2936 | 995.1579 |
| 997.0776 | 998.5767 | 1022.2075 |
| 1023.5703 | 1025.7888 | 1035.8222 |
| 1039.0315 | 1048.6524 | 1054.0021 |
| 1065.0709 | 1068.8608 | 1073.5394 |
| 1084.8086 | 1094.5862 | 1103.5454 |
| 1122.6423 | 1138.5754 | 1148.5689 |
| 1162.0007 | 1167.0880 | 1171.6152 |
| 1172.1480 | 1180.7837 | 1192.5221 |
| 1213.7585 | 1228.2049 | 1230.5079 |
| 1237.3789 | 1255.7724 | 1257.7851 |
| 1273.4779 | 1285.8275 | 1288.3085 |
| 1289.6050 | 1299.9372 | 1306.9192 |
| 1318.5585 | 1329.5673 | 1332.9553 |
| 1335.9482 | 1340.0214 | 1353.9186 |
| 1356.8542 | 1361.4705 | 1387.3828 |
| 1399.4661 | 1418.3920 | 1421.4405 |
| 1423.2201 | 1425.9071 | 1427.2190 |
| 1443.4644 | 1471.6735 | 1472.0048 |
| 1476.1763 | 1477.3813 | 1482.3994 |
| 1493.8738 | 1494.2623 | 1499.2280 |
| 1504.4100 | 1506.2840 | 1509.8449 |
| 1554.7840 | 1562.8280 | 1642.4761 |
| 1652.6773 | 1665.7639 | 1667.3323 |
| 1690.8519 | 1708.4780 | 1710.8476 |

| | | |
|---|---|---|
| 2496.6912 | 3041.7593 | 3047.0585 |
| 3054.0562 | 3056.1917 | 3060.0612 |
| 3060.5990 | 3075.2610 | 3088.3582 |
| 3100.5484 | 3106.2637 | 3118.5353 |
| 3136.0416 | 3143.4532 | 3157.5267 |
| 3164.4409 | 3194.1547 | 3204.5539 |
| 3205.5256 | 3211.0428 | 3213.7615 |
| 3220.6022 | 3225.4997 | 3227.2189 |
| 3233.9693 | 3234.8996 | 3241.4343 |

**TS3S-L4**

Zero-point correction= 0.501841

Thermal correction to Energy= 0.539034

Thermal correction to Enthalpy= 0.539978

Thermal correction to Gibbs Free Energy= 0.427455

Sum of electronic and zero-point Energies= -2336.026962

Sum of electronic and thermal Energies= -2335.989769

Sum of electronic and thermal Enthalpies= -2335.988825

Sum of electronic and thermal Free Energies= -2336.101348

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.082314 | -0.806758 | -0.812082 |
| B | 0.420154 | 0.079915 | 0.238226 |
| C | -1.281400 | -1.386867 | -0.643865 |
| O | -0.617325 | 0.916254 | 0.828084 |
| C | -2.443868 | -0.624745 | -0.595239 |
| C | -1.362400 | -2.807059 | -0.520772 |
| C | -1.429928 | 1.558029 | -0.031071 |
| C | -2.335410 | 0.845939 | -0.809206 |
| C | -2.559629 | -3.439797 | -0.315826 |
| C | -3.696330 | -1.258607 | -0.295781 |

| | | | |
|---|---|---|---|
| C | -3.751454 | -2.678914 | -0.179541 |
| C | -1.378201 | 2.980408 | -0.126355 |
| C | -3.113315 | 1.530572 | -1.801066 |
| C | -2.170723 | 3.660595 | -1.013264 |
| C | -3.037724 | 2.951190 | -1.886794 |
| H | -2.610340 | -4.526255 | -0.226405 |
| H | -2.133504 | 4.749509 | -1.073989 |
| C | -3.819658 | 3.643236 | -2.853130 |
| C | -4.630360 | 2.955682 | -3.722410 |
| C | -4.681030 | 1.540628 | -3.666248 |
| C | -3.945132 | 0.847501 | -2.734271 |
| H | -3.753386 | 4.732684 | -2.891774 |
| H | -5.223728 | 3.492504 | -4.464208 |
| H | -5.304896 | 0.993597 | -4.375226 |
| H | -3.985050 | -0.241805 | -2.715502 |
| C | -4.991108 | -3.319447 | 0.098801 |
| C | -6.134398 | -2.582626 | 0.285145 |
| C | -6.078420 | -1.168579 | 0.211480 |
| C | -4.896885 | -0.524718 | -0.070645 |
| H | -5.008711 | -4.409069 | 0.170409 |
| H | -7.081250 | -3.079910 | 0.501549 |
| H | -6.982652 | -0.583538 | 0.388473 |
| H | -4.872410 | 0.564176 | -0.109631 |
| C | 1.788396 | 0.803178 | -0.236532 |
| C | 2.606400 | 0.256694 | -1.154162 |
| H | 2.074514 | 1.756478 | 0.227173 |
| H | 2.333861 | -0.720443 | -1.577747 |
| C | 3.884197 | 0.852797 | -1.655077 |
| C | 5.097202 | -0.001260 | -1.264156 |
| H | 4.002760 | 1.874891 | -1.262319 |

| | | | |
|---|---|---|---|
| H | 3.844405 | 0.923008 | -2.755654 |
| C | 6.409397 | 0.539316 | -1.822136 |
| H | 5.154687 | -0.056968 | -0.163806 |
| H | 4.944537 | -1.034504 | -1.620673 |
| H | 6.340985 | 0.589378 | -2.922836 |
| H | 6.552829 | 1.577517 | -1.475433 |
| C | 7.622239 | -0.297957 | -1.428689 |
| C | 8.935631 | 0.230412 | -1.998352 |
| H | 7.472038 | -1.338589 | -1.766790 |
| H | 7.693759 | -0.341288 | -0.327508 |
| C | 10.139075 | -0.617557 | -1.605485 |
| H | 8.858127 | 0.277867 | -3.097782 |
| H | 9.085888 | 1.268475 | -1.656731 |
| H | 11.073043 | -0.215876 | -2.025136 |
| H | 10.254241 | -0.657007 | -0.511193 |
| H | 10.028786 | -1.652337 | -1.965403 |
| C | 1.215467 | -0.734017 | 1.387681 |
| H | 1.745679 | -1.635928 | 1.055428 |
| C | 1.970560 | -0.051866 | 2.533501 |
| N | -0.094534 | -1.583266 | 2.342482 |
| N | -1.152002 | -1.798136 | 2.529095 |
| I | -0.088319 | 4.042592 | 1.152043 |
| I | 0.416263 | -3.930278 | -0.611314 |
| F | 3.241739 | 0.128263 | 2.185766 |
| F | 1.963683 | -0.798760 | 3.637329 |
| F | 1.455975 | 1.129133 | 2.842445 |

Vibrational frequencies

| | | |
|---|---|---|
| -482.1209 | 8.1677 | 17.5541 |
| 23.7201 | 36.8970 | 37.5652 |

| | | |
|---|---|---|
| 46.3807 | 50.3568 | 53.2037 |
| 54.8025 | 64.2933 | 67.5424 |
| 69.8453 | 87.3314 | 93.0629 |
| 95.1077 | 99.7782 | 102.4858 |
| 122.7887 | 129.1185 | 137.0490 |
| 141.2895 | 147.1146 | 161.9844 |
| 165.8437 | 168.2928 | 195.3998 |
| 199.1758 | 217.2639 | 226.4092 |
| 239.2399 | 261.0698 | 267.7914 |
| 272.5496 | 278.8756 | 284.3130 |
| 295.6527 | 302.2321 | 318.4023 |
| 334.9716 | 343.3710 | 359.3950 |
| 368.5157 | 405.3043 | 411.8532 |
| 422.6598 | 444.9900 | 445.8283 |
| 461.4246 | 466.1136 | 469.9973 |
| 498.8146 | 522.4848 | 529.1095 |
| 542.5236 | 569.8430 | 573.5678 |
| 575.0076 | 584.2979 | 591.9444 |
| 602.0903 | 606.8945 | 628.0128 |
| 643.0675 | 665.7316 | 677.7864 |
| 694.6672 | 725.8031 | 732.1646 |
| 737.0869 | 753.7628 | 768.7676 |
| 774.7272 | 780.2625 | 780.8898 |
| 782.3127 | 803.4509 | 810.4842 |
| 824.5995 | 839.8567 | 843.5422 |
| 882.7385 | 889.5906 | 895.3576 |
| 898.3906 | 900.4853 | 910.4638 |
| 934.3569 | 935.5915 | 938.6044 |
| 951.4971 | 978.3574 | 997.1062 |
| 1010.8437 | 1013.1065 | 1025.4675 |

| | | |
|---|---|---|
| 1031.1723 | 1038.2571 | 1039.8865 |
| 1042.5295 | 1047.6959 | 1053.0092 |
| 1056.2814 | 1062.9996 | 1072.5285 |
| 1078.1523 | 1082.7748 | 1092.6042 |
| 1115.9297 | 1136.5697 | 1139.3976 |
| 1144.1990 | 1150.0984 | 1154.0187 |
| 1163.2778 | 1166.1308 | 1182.9038 |
| 1197.1263 | 1215.8556 | 1218.7479 |
| 1224.1344 | 1233.2319 | 1256.2058 |
| 1265.1449 | 1265.5466 | 1275.7949 |
| 1282.9820 | 1289.3266 | 1297.9990 |
| 1300.2821 | 1305.0287 | 1309.4411 |
| 1311.7850 | 1323.1989 | 1344.8930 |
| 1348.0084 | 1353.8595 | 1381.9522 |
| 1387.6128 | 1397.1013 | 1414.6747 |
| 1415.0190 | 1427.0564 | 1429.1585 |
| 1434.2718 | 1439.4680 | 1442.9172 |
| 1444.8149 | 1456.6379 | 1457.5535 |
| 1466.4711 | 1470.7635 | 1473.4861 |
| 1479.4066 | 1494.3211 | 1507.7103 |
| 1554.2774 | 1564.3624 | 1646.5516 |
| 1656.1256 | 1667.0855 | 1670.2087 |
| 1692.3285 | 1712.9973 | 1714.5691 |
| 2539.9105 | 3031.8922 | 3037.3378 |
| 3043.2257 | 3045.4163 | 3048.0538 |
| 3049.0906 | 3070.0126 | 3082.2650 |
| 3093.9918 | 3099.8485 | 3113.9657 |
| 3132.9735 | 3137.2008 | 3142.4166 |
| 3147.3854 | 3202.1821 | 3203.1624 |
| 3210.4240 | 3211.5119 | 3218.4559 |

| | | |
|---|---|---|
| 3219.2225 | 3220.9587 | 3222.8046 |
| 3224.3540 | 3232.6937 | 3234.3234 |

**TS3R-L4**

Zero-point correction= 0.501844

Thermal correction to Energy= 0.538934

Thermal correction to Enthalpy= 0.539878

Thermal correction to Gibbs Free Energy= 0.428577

Sum of electronic and zero-point Energies= -2336.022778

Sum of electronic and thermal Energies= -2335.985688

Sum of electronic and thermal Enthalpies= -2335.984744

Sum of electronic and thermal Free Energies= -2336.096045

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.180121 | -1.280995 | -0.090155 |
| B | 0.267279 | -0.159224 | 0.731363 |
| C | -1.465486 | -1.669696 | -0.090584 |
| O | -0.809171 | 0.757730 | 1.099259 |
| C | -2.495878 | -0.799563 | -0.438085 |
| C | -1.781329 | -3.025511 | 0.239983 |
| C | -1.391654 | 1.350595 | 0.038722 |
| C | -2.169379 | 0.599666 | -0.831279 |
| C | -3.072897 | -3.480739 | 0.250094 |
| C | -3.862505 | -1.231907 | -0.337026 |
| C | -4.145986 | -2.591465 | -0.018700 |
| C | -1.203581 | 2.744013 | -0.195381 |
| C | -2.641711 | 1.189978 | -2.049732 |
| C | -1.717041 | 3.348220 | -1.313188 |
| C | -2.418564 | 2.578845 | -2.281024 |
| H | -3.295092 | -4.521148 | 0.493949 |
| H | -1.577910 | 4.417057 | -1.485424 |

| | | | |
|---|---|---|---|
| C | -2.896976 | 3.178631 | -3.479547 |
| C | -3.551642 | 2.428996 | -4.425699 |
| C | -3.746705 | 1.041273 | -4.214499 |
| C | -3.306783 | 0.438179 | -3.060071 |
| H | -2.723738 | 4.246036 | -3.632600 |
| H | -3.913697 | 2.894115 | -5.344017 |
| H | -4.247479 | 0.444425 | -4.978796 |
| H | -3.456044 | -0.632407 | -2.915974 |
| C | -5.494948 | -3.036966 | 0.060862 |
| C | -6.534582 | -2.162108 | -0.135960 |
| C | -6.261175 | -0.798699 | -0.407651 |
| C | -4.966506 | -0.346058 | -0.506198 |
| H | -5.683107 | -4.087272 | 0.293776 |
| H | -7.567379 | -2.507807 | -0.069089 |
| H | -7.086763 | -0.096078 | -0.533613 |
| H | -4.781128 | 0.709939 | -0.700417 |
| C | 1.605279 | 0.565955 | 0.149799 |
| C | 2.359044 | 0.000006 | -0.809109 |
| H | 1.880389 | 1.562105 | 0.518652 |
| H | 2.094613 | -1.009827 | -1.150342 |
| C | 3.569727 | 0.608452 | -1.443045 |
| C | 4.831171 | -0.196461 | -1.102321 |
| H | 3.687126 | 1.652207 | -1.111694 |
| H | 3.443072 | 0.619318 | -2.538935 |
| C | 6.091298 | 0.365309 | -1.751820 |
| H | 4.956248 | -0.216825 | -0.006664 |
| H | 4.688775 | -1.244963 | -1.416054 |
| H | 5.958498 | 0.384181 | -2.847552 |
| H | 6.224320 | 1.415979 | -1.439796 |
| C | 7.348336 | -0.427442 | -1.407531 |

| | | | |
|---|---|---|---|
| C | 8.615597 | 0.133278 | -2.046295 |
| H | 7.215073 | -1.477317 | -1.723281 |
| H | 7.473958 | -0.451894 | -0.310626 |
| C | 9.862339 | -0.672373 | -1.701980 |
| H | 8.484400 | 0.164083 | -3.141136 |
| H | 8.749782 | 1.179813 | -1.724262 |
| H | 10.762550 | -0.247498 | -2.169696 |
| H | 10.029645 | -0.695274 | -0.613901 |
| H | 9.767329 | -1.714469 | -2.044838 |
| C | 1.047290 | -0.564471 | 2.070641 |
| H | 1.206452 | 0.261880 | 2.776790 |
| C | 2.228714 | -1.538401 | 2.150998 |
| N | -0.254681 | -1.390150 | 3.080323 |
| N | -1.320383 | -1.598317 | 3.223875 |
| I | -0.166376 | 3.881358 | 1.239987 |
| I | -0.226395 | -4.347111 | 0.751096 |
| F | 2.379426 | -2.282142 | 1.067434 |
| F | 2.118853 | -2.357818 | 3.194264 |
| F | 3.349085 | -0.832715 | 2.312229 |

Vibrational frequencies

| | | |
|---|---|---|
| -494.4373 | 11.5931 | 17.3853 |
| 29.3742 | 33.1193 | 36.8877 |
| 42.7617 | 52.0736 | 58.3616 |
| 67.6446 | 73.0877 | 79.4636 |
| 87.6157 | 91.8896 | 97.7215 |
| 101.6294 | 103.9129 | 106.9233 |
| 108.9804 | 124.8228 | 146.3567 |
| 147.1631 | 157.5242 | 159.9083 |
| 166.7380 | 178.6232 | 191.4768 |

| | | |
|---|---|---|
| 197.7962 | 218.4074 | 221.7720 |
| 231.7354 | 250.6408 | 265.5320 |
| 271.5962 | 274.3590 | 283.0605 |
| 288.3661 | 296.6739 | 314.1367 |
| 337.4732 | 341.3159 | 349.7446 |
| 370.3732 | 394.9180 | 415.7403 |
| 432.2926 | 441.6678 | 451.0431 |
| 459.5512 | 465.3770 | 473.3005 |
| 499.9034 | 524.8045 | 526.9538 |
| 537.9951 | 567.0953 | 572.7197 |
| 573.6341 | 585.2649 | 591.8058 |
| 598.6672 | 604.8636 | 629.9301 |
| 651.9153 | 661.3790 | 677.0909 |
| 686.9786 | 729.0670 | 734.9413 |
| 740.0623 | 754.0303 | 760.1919 |
| 768.0435 | 779.3482 | 780.4383 |
| 782.6320 | 804.8245 | 808.1201 |
| 819.5033 | 838.9187 | 840.1883 |
| 880.8135 | 886.9241 | 894.0215 |
| 896.8038 | 899.7119 | 908.9469 |
| 921.2761 | 935.7030 | 939.2282 |
| 951.4282 | 982.1131 | 998.2764 |
| 1012.7100 | 1013.9701 | 1020.2371 |
| 1030.7706 | 1037.7044 | 1041.8864 |
| 1043.5806 | 1047.0353 | 1049.3084 |
| 1058.7049 | 1061.5653 | 1069.4762 |
| 1084.8734 | 1093.4097 | 1104.2014 |
| 1119.4717 | 1130.6323 | 1136.1222 |
| 1142.5184 | 1144.4732 | 1147.0316 |
| 1157.0232 | 1176.1425 | 1178.8475 |

| | | |
|---|---|---|
| 1199.4710 | 1213.6990 | 1220.3106 |
| 1221.8015 | 1238.0803 | 1249.5179 |
| 1261.1324 | 1267.6396 | 1276.7045 |
| 1280.0773 | 1288.4579 | 1298.6143 |
| 1302.5774 | 1310.3494 | 1311.6580 |
| 1318.6640 | 1328.3429 | 1344.5690 |
| 1350.7528 | 1355.8190 | 1382.4809 |
| 1386.2247 | 1398.6430 | 1413.7942 |
| 1417.1683 | 1426.6791 | 1427.8227 |
| 1437.1971 | 1439.9561 | 1440.2195 |
| 1445.9134 | 1457.1542 | 1458.1571 |
| 1467.9254 | 1471.5195 | 1472.0193 |
| 1477.6844 | 1491.7518 | 1506.3020 |
| 1552.3696 | 1562.8240 | 1647.3091 |
| 1656.1506 | 1666.8401 | 1668.7696 |
| 1690.1042 | 1709.9134 | 1712.3238 |
| 2535.9268 | 3032.1607 | 3036.8589 |
| 3044.6642 | 3045.0986 | 3046.6453 |
| 3051.0488 | 3069.9278 | 3082.7858 |
| 3094.4546 | 3099.7586 | 3114.1225 |
| 3132.6587 | 3138.6224 | 3154.2361 |
| 3158.9085 | 3196.9425 | 3202.7013 |
| 3204.0606 | 3211.1120 | 3211.5370 |
| 3214.5465 | 3220.4616 | 3220.9972 |
| 3223.8260 | 3228.0785 | 3240.2677 |

**TS3S-L5**

Zero-point correction= 0.504551

Thermal correction to Energy= 0.541599

Thermal correction to Enthalpy= 0.542543

Thermal correction to Gibbs Free Energy= 0.430615

Sum of electronic and zero-point Energies= -1764.990294

Sum of electronic and thermal Energies= -1764.953247

Sum of electronic and thermal Enthalpies= -1764.952302

Sum of electronic and thermal Free Energies= -1765.064230

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.076068 | -0.845955 | -0.728361 |
| B | 0.412186 | 0.073410 | 0.304424 |
| C | -1.286645 | -1.410218 | -0.583311 |
| O | -0.632753 | 0.913196 | 0.882318 |
| C | -2.437677 | -0.635587 | -0.562989 |
| C | -1.389129 | -2.824754 | -0.467063 |
| C | -1.429816 | 1.549374 | 0.001105 |
| C | -2.312333 | 0.830816 | -0.791288 |
| C | -2.593403 | -3.443049 | -0.286763 |
| C | -3.700702 | -1.252384 | -0.284885 |
| C | -3.775488 | -2.668865 | -0.169374 |
| C | -1.384034 | 2.966579 | -0.101852 |
| C | -3.053780 | 1.503659 | -1.815824 |
| C | -2.144746 | 3.638167 | -1.016607 |
| C | -2.974826 | 2.920556 | -1.914572 |
| H | -2.660779 | -4.522674 | -0.202418 |
| H | -2.107496 | 4.720317 | -1.085893 |
| C | -3.715945 | 3.601796 | -2.917317 |
| C | -4.489414 | 2.906429 | -3.809435 |
| C | -4.544122 | 1.494559 | -3.738673 |
| C | -3.848580 | 0.812697 | -2.772701 |
| H | -3.647060 | 4.685021 | -2.967903 |
| H | -5.049222 | 3.431992 | -4.576697 |
| H | -5.138736 | 0.943591 | -4.460928 |

| | | | |
|---|---|---|---|
| H | -3.893480 | -0.269941 | -2.742929 |
| C | -5.025543 | -3.293570 | 0.086589 |
| C | -6.161176 | -2.545048 | 0.251329 |
| C | -6.086737 | -1.134113 | 0.178140 |
| C | -4.895282 | -0.505841 | -0.081020 |
| H | -5.059371 | -4.377163 | 0.159726 |
| H | -7.112983 | -3.027804 | 0.449089 |
| H | -6.983112 | -0.542263 | 0.336482 |
| H | -4.858443 | 0.576606 | -0.118670 |
| C | 1.761618 | 0.795847 | -0.195932 |
| C | 2.582627 | 0.260371 | -1.111043 |
| H | 2.037293 | 1.750448 | 0.254802 |
| H | 2.328131 | -0.712126 | -1.537284 |
| C | 3.854050 | 0.873113 | -1.613197 |
| C | 5.073587 | 0.001717 | -1.275616 |
| H | 3.982703 | 1.874844 | -1.186334 |
| H | 3.794993 | 0.988201 | -2.704218 |
| C | 6.381904 | 0.575739 | -1.818197 |
| H | 5.141683 | -0.110520 | -0.185764 |
| H | 4.920129 | -1.006107 | -1.684284 |
| H | 6.296239 | 0.702264 | -2.906136 |
| H | 6.536438 | 1.580601 | -1.401929 |
| C | 7.598119 | -0.295253 | -1.503875 |
| C | 8.908469 | 0.277700 | -2.045724 |
| H | 7.442815 | -1.299095 | -1.923362 |
| H | 7.682817 | -0.426172 | -0.416132 |
| C | 10.115668 | -0.607714 | -1.745149 |
| H | 8.818445 | 0.419825 | -3.130589 |
| H | 9.069807 | 1.275266 | -1.616826 |
| H | 11.039269 | -0.172454 | -2.140398 |

| | | | |
|---|---|---|---|
| H | 10.246749 | -0.745575 | -0.665955 |
| H | 9.996980 | -1.600577 | -2.193970 |
| C | 1.186067 | -0.736401 | 1.494988 |
| H | 1.725494 | -1.626173 | 1.164203 |
| C | 1.927074 | -0.064566 | 2.656402 |
| N | -0.100110 | -1.552758 | 2.411888 |
| N | -1.159394 | -1.782679 | 2.609896 |
| I | -0.137298 | 4.065091 | 1.221696 |
| I | 0.389805 | -3.988261 | -0.545721 |
| F | 3.160458 | 0.271071 | 2.269295 |
| F | 2.046149 | -0.900259 | 3.700465 |
| F | 1.306643 | 1.032740 | 3.088162 |

Vibrational frequencies

| | | |
|---|---|---|
| -472.9258 | 10.5457 | 20.0742 |
| 25.4825 | 33.9777 | 35.9228 |
| 38.8909 | 42.9072 | 52.3582 |
| 61.1045 | 61.7087 | 67.2305 |
| 86.9151 | 93.0432 | 93.4986 |
| 98.9903 | 101.3379 | 105.5625 |
| 121.2103 | 130.1389 | 137.7515 |
| 145.7062 | 152.6900 | 161.3593 |
| 169.8639 | 171.6812 | 191.3342 |
| 202.3312 | 214.5114 | 224.3839 |
| 241.2936 | 264.4308 | 270.0156 |
| 278.6918 | 283.8300 | 288.2930 |
| 295.4483 | 299.2654 | 319.8509 |
| 339.5019 | 345.0308 | 365.2188 |
| 368.6483 | 402.9292 | 414.2920 |
| 421.4518 | 445.4446 | 454.5955 |

| | | |
|---|---|---|
| 459.5551 | 465.7252 | 475.6529 |
| 506.0373 | 521.1651 | 526.7389 |
| 531.2069 | 566.5165 | 573.1144 |
| 574.3698 | 580.1764 | 591.5711 |
| 600.8332 | 605.2065 | 634.2519 |
| 646.0075 | 665.8188 | 678.9837 |
| 683.9973 | 730.4292 | 742.0680 |
| 745.5475 | 757.6773 | 765.7177 |
| 770.3573 | 775.5876 | 779.8142 |
| 789.5007 | 799.8355 | 802.3144 |
| 830.2779 | 838.7546 | 841.0853 |
| 883.2143 | 887.0697 | 888.4882 |
| 891.8686 | 914.9635 | 919.5055 |
| 920.5141 | 924.9963 | 937.9015 |
| 958.9854 | 990.6117 | 992.6967 |
| 995.9799 | 1005.0596 | 1018.6136 |
| 1021.0185 | 1024.6635 | 1033.3060 |
| 1044.1537 | 1050.5327 | 1053.2758 |
| 1066.3594 | 1073.8176 | 1080.4247 |
| 1082.4057 | 1091.2762 | 1093.2976 |
| 1122.2386 | 1148.2727 | 1151.0743 |
| 1158.6517 | 1175.4569 | 1181.5950 |
| 1183.9803 | 1192.1413 | 1206.7984 |
| 1224.6153 | 1227.5698 | 1236.7789 |
| 1238.8189 | 1251.1360 | 1272.7649 |
| 1288.0922 | 1296.8567 | 1297.4189 |
| 1301.4578 | 1305.7243 | 1315.5791 |
| 1318.3525 | 1325.3370 | 1331.5902 |
| 1337.5789 | 1345.7070 | 1350.1126 |
| 1363.7754 | 1379.9916 | 1388.3373 |

| | | |
|---|---|---|
| 1415.2941 | 1420.3844 | 1430.5126 |
| 1431.7504 | 1434.7329 | 1436.6609 |
| 1449.8500 | 1477.0335 | 1480.2014 |
| 1482.7647 | 1489.1501 | 1494.2991 |
| 1501.3423 | 1503.7821 | 1507.1281 |
| 1509.9469 | 1512.5685 | 1519.2089 |
| 1561.5616 | 1568.0265 | 1639.4554 |
| 1648.8238 | 1661.7882 | 1663.0818 |
| 1703.9489 | 1708.7187 | 1710.5610 |
| 2465.3642 | 3035.2441 | 3039.2862 |
| 3044.5280 | 3046.5715 | 3049.3747 |
| 3052.5267 | 3066.9614 | 3079.3703 |
| 3090.9901 | 3097.5848 | 3109.3617 |
| 3128.5836 | 3137.5432 | 3164.9834 |
| 3174.2129 | 3190.6750 | 3213.2164 |
| 3216.1021 | 3227.8305 | 3230.1635 |
| 3235.3040 | 3239.0122 | 3240.3967 |
| 3242.0401 | 3260.7031 | 3262.3588 |

**TS3R-L5**

Zero-point correction= 0.504580

Thermal correction to Energy= 0.541708

Thermal correction to Enthalpy= 0.542652

Thermal correction to Gibbs Free Energy= 0.430957

Sum of electronic and zero-point Energies= -1764.985323

Sum of electronic and thermal Energies= -1764.948195

Sum of electronic and thermal Enthalpies= -1764.947251

Sum of electronic and thermal Free Energies= -1765.058947

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.171719 | -1.273579 | -0.124163 |

| | | | |
|---|---|---|---|
| B | 0.268353 | -0.143117 | 0.693626 |
| C | -1.456706 | -1.667082 | -0.132904 |
| O | -0.809098 | 0.775235 | 1.074553 |
| C | -2.491535 | -0.793380 | -0.443594 |
| C | -1.764647 | -3.032319 | 0.139789 |
| C | -1.401881 | 1.365232 | 0.016710 |
| C | -2.179780 | 0.606734 | -0.839837 |
| C | -3.051843 | -3.489118 | 0.165026 |
| C | -3.852819 | -1.227392 | -0.320857 |
| C | -4.129533 | -2.591755 | -0.034260 |
| C | -1.232967 | 2.755417 | -0.222224 |
| C | -2.666375 | 1.185093 | -2.055297 |
| C | -1.760003 | 3.350471 | -1.333890 |
| C | -2.458887 | 2.572537 | -2.292929 |
| H | -3.266441 | -4.533442 | 0.365754 |
| H | -1.633749 | 4.413611 | -1.510191 |
| C | -2.950446 | 3.163104 | -3.488156 |
| C | -3.601899 | 2.405779 | -4.426325 |
| C | -3.781579 | 1.019232 | -4.209589 |
| C | -3.329150 | 0.425428 | -3.058879 |
| H | -2.790100 | 4.225948 | -3.646645 |
| H | -3.972649 | 2.862211 | -5.338707 |
| H | -4.278948 | 0.418317 | -4.964862 |
| H | -3.467577 | -0.639760 | -2.912273 |
| C | -5.474583 | -3.037625 | 0.071100 |
| C | -6.515413 | -2.158035 | -0.071388 |
| C | -6.247568 | -0.790832 | -0.316039 |
| C | -4.958455 | -0.337950 | -0.438808 |
| H | -5.658298 | -4.088304 | 0.278134 |
| H | -7.541201 | -2.501934 | 0.017016 |

| | | | |
|---|---|---|---|
| H | -7.071344 | -0.088555 | -0.400602 |
| H | -4.777630 | 0.716097 | -0.613121 |
| C | 1.586449 | 0.581289 | 0.089648 |
| C | 2.358626 | 0.008934 | -0.845271 |
| H | 1.848167 | 1.578988 | 0.443240 |
| H | 2.113932 | -1.000085 | -1.179747 |
| C | 3.578055 | 0.617817 | -1.464133 |
| C | 4.830055 | -0.206303 | -1.121691 |
| H | 3.702699 | 1.650664 | -1.118247 |
| H | 3.462319 | 0.648711 | -2.555841 |
| C | 6.110424 | 0.371659 | -1.722799 |
| H | 4.928675 | -0.266878 | -0.030733 |
| H | 4.689875 | -1.235911 | -1.476772 |
| H | 5.996130 | 0.452308 | -2.812449 |
| H | 6.255495 | 1.395226 | -1.351006 |
| C | 7.349357 | -0.464780 | -1.402728 |
| C | 8.641300 | 0.117823 | -1.977025 |
| H | 7.208222 | -1.482994 | -1.791205 |
| H | 7.451042 | -0.563658 | -0.313019 |
| C | 9.866648 | -0.741569 | -1.674364 |
| H | 8.533584 | 0.234577 | -3.063289 |
| H | 8.792728 | 1.126975 | -1.572267 |
| H | 10.778461 | -0.299307 | -2.088740 |
| H | 10.012252 | -0.856227 | -0.594258 |
| H | 9.758919 | -1.744872 | -2.102207 |
| C | 1.030959 | -0.528514 | 2.063195 |
| H | 1.136821 | 0.312284 | 2.753315 |
| C | 2.255908 | -1.438884 | 2.203201 |
| N | -0.233717 | -1.394140 | 3.056464 |
| N | -1.284106 | -1.682941 | 3.221075 |

| | | | |
|---|---|---|---|
| I | -0.182582 | 3.927610 | 1.204505 |
| I | -0.191425 | -4.408436 | 0.509275 |
| F | 2.426613 | -2.278602 | 1.187561 |
| F | 2.197077 | -2.164896 | 3.328608 |
| F | 3.348378 | -0.663635 | 2.280047 |

Vibrational frequencies

| | | |
|---|---|---|
| -445.5331 | 13.0707 | 19.0458 |
| 28.4591 | 32.1938 | 34.9508 |
| 38.7478 | 51.0323 | 56.8785 |
| 66.1801 | 69.0270 | 76.2290 |
| 82.3507 | 91.1732 | 95.0901 |
| 98.8246 | 101.3110 | 105.4876 |
| 109.4158 | 119.0170 | 139.5379 |
| 141.6811 | 153.7918 | 160.2181 |
| 166.6306 | 171.8492 | 188.7560 |
| 198.4375 | 210.6737 | 219.5244 |
| 225.5485 | 249.8150 | 269.6068 |
| 276.3293 | 283.5759 | 286.7203 |
| 292.2216 | 295.6419 | 313.8800 |
| 340.7730 | 343.0978 | 354.8379 |
| 369.9315 | 398.1689 | 417.8939 |
| 429.0890 | 445.4614 | 454.4319 |
| 462.3739 | 467.7032 | 479.3434 |
| 505.5596 | 521.1833 | 529.2503 |
| 531.8805 | 566.1444 | 572.9531 |
| 574.9502 | 580.3601 | 591.1126 |
| 597.8447 | 607.5617 | 636.5952 |
| 648.7702 | 663.1738 | 677.4612 |
| 680.3484 | 731.9422 | 732.6008 |

| | | |
|---|---|---|
| 745.1507 | 750.3950 | 757.9240 |
| 762.4046 | 778.9990 | 782.0684 |
| 785.5472 | 796.0808 | 803.6574 |
| 825.2604 | 833.0704 | 838.5644 |
| 877.9670 | 891.4585 | 898.5432 |
| 900.2964 | 911.3604 | 918.7734 |
| 925.3720 | 935.8141 | 939.9255 |
| 959.4924 | 993.5890 | 1003.1248 |
| 1004.9037 | 1005.5499 | 1016.9740 |
| 1026.9349 | 1028.4780 | 1031.1651 |
| 1032.4270 | 1043.6147 | 1048.6536 |
| 1069.2686 | 1073.6920 | 1079.3026 |
| 1084.5380 | 1092.8893 | 1101.9568 |
| 1124.5297 | 1142.1913 | 1152.4744 |
| 1162.2834 | 1165.3080 | 1172.1011 |
| 1186.7338 | 1189.3424 | 1204.3393 |
| 1212.3727 | 1223.1361 | 1237.1767 |
| 1241.2406 | 1254.9595 | 1273.0773 |
| 1285.8534 | 1297.1568 | 1299.5188 |
| 1302.7894 | 1311.0805 | 1319.8651 |
| 1323.2626 | 1331.5247 | 1337.7357 |
| 1346.6025 | 1349.9650 | 1357.3531 |
| 1363.2839 | 1379.6468 | 1387.8498 |
| 1416.0061 | 1420.0345 | 1430.1884 |
| 1432.4466 | 1434.7051 | 1437.9605 |
| 1447.4362 | 1473.3583 | 1476.6513 |
| 1483.1514 | 1483.6310 | 1489.3080 |
| 1498.4716 | 1499.3130 | 1507.3030 |
| 1508.0030 | 1509.9776 | 1515.7889 |
| 1560.0972 | 1566.8492 | 1640.3984 |

| | | |
|---|---|---|
| 1650.1142 | 1662.0052 | 1663.0800 |
| 1698.7131 | 1709.1965 | 1710.9229 |
| 2473.7400 | 3037.3945 | 3042.3256 |
| 3047.2961 | 3053.3400 | 3054.1009 |
| 3058.1092 | 3069.8681 | 3083.3203 |
| 3095.1663 | 3103.1193 | 3118.5282 |
| 3129.7197 | 3139.6175 | 3180.2822 |
| 3187.4528 | 3190.9380 | 3216.2950 |
| 3217.1889 | 3226.4435 | 3229.0431 |
| 3235.7620 | 3238.7473 | 3241.4537 |
| 3242.1566 | 3253.9302 | 3258.7947 |

**TS3S-L6**

Zero-point correction= 0.502926

Thermal correction to Energy= 0.540093

Thermal correction to Enthalpy= 0.541037

Thermal correction to Gibbs Free Energy= 0.428390

Sum of electronic and zero-point Energies= -2336.487967

Sum of electronic and thermal Energies= -2336.450801

Sum of electronic and thermal Enthalpies= -2336.449856

Sum of electronic and thermal Free Energies= -2336.562503

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.085730 | -0.852870 | -0.715655 |
| B | 0.408482 | 0.059166 | 0.319243 |
| C | -1.293722 | -1.414377 | -0.582042 |
| O | -0.633639 | 0.911379 | 0.879019 |
| C | -2.444831 | -0.635197 | -0.560831 |
| C | -1.395935 | -2.834364 | -0.471787 |
| C | -1.427615 | 1.549099 | 0.003289 |
| C | -2.314653 | 0.831640 | -0.789890 |

| | | | |
|---|---|---|---|
| C | -2.608166 | -3.446336 | -0.291142 |
| C | -3.711070 | -1.249755 | -0.281938 |
| C | -3.790026 | -2.668560 | -0.168417 |
| C | -1.371505 | 2.971032 | -0.099835 |
| C | -3.052276 | 1.506601 | -1.818732 |
| C | -2.132673 | 3.641267 | -1.021583 |
| C | -2.966767 | 2.925307 | -1.920721 |
| H | -2.680796 | -4.532979 | -0.210977 |
| H | -2.091617 | 4.730075 | -1.094145 |
| C | -3.705616 | 3.606486 | -2.928419 |
| C | -4.482372 | 2.910520 | -3.821211 |
| C | -4.543117 | 1.497608 | -3.746817 |
| C | -3.849959 | 0.815530 | -2.775798 |
| H | -3.633141 | 4.695772 | -2.983097 |
| H | -5.042513 | 3.439969 | -4.595199 |
| H | -5.142582 | 0.942951 | -4.472393 |
| H | -3.900321 | -0.273470 | -2.742636 |
| C | -5.044765 | -3.288732 | 0.088171 |
| C | -6.179862 | -2.534999 | 0.254512 |
| C | -6.100811 | -1.122791 | 0.182327 |
| C | -4.904582 | -0.498436 | -0.077323 |
| H | -5.084084 | -4.378695 | 0.160307 |
| H | -7.138940 | -3.018175 | 0.453627 |
| H | -7.000235 | -0.523528 | 0.341785 |
| H | -4.863880 | 0.590617 | -0.115800 |
| C | 1.767071 | 0.782022 | -0.177746 |
| C | 2.594387 | 0.244880 | -1.090794 |
| H | 2.035265 | 1.747317 | 0.270994 |
| H | 2.344847 | -0.740937 | -1.507291 |
| C | 3.857461 | 0.861460 | -1.604332 |

| | | | |
|---|---|---|---|
| C | 5.086192 | 0.003874 | -1.277029 |
| H | 3.982455 | 1.873529 | -1.185569 |
| H | 3.783334 | 0.970407 | -2.701084 |
| C | 6.388255 | 0.580589 | -1.825090 |
| H | 5.163094 | -0.109456 | -0.181578 |
| H | 4.936636 | -1.012748 | -1.681971 |
| H | 6.297751 | 0.705042 | -2.918997 |
| H | 6.537882 | 1.595246 | -1.414729 |
| C | 7.611716 | -0.276678 | -1.512645 |
| C | 8.918410 | 0.296686 | -2.056653 |
| H | 7.460523 | -1.290262 | -1.926412 |
| H | 7.698691 | -0.405872 | -0.418601 |
| C | 10.131935 | -0.575528 | -1.757597 |
| H | 8.824980 | 0.437900 | -3.147732 |
| H | 9.075134 | 1.304090 | -1.632857 |
| H | 11.056682 | -0.133106 | -2.159357 |
| H | 10.271044 | -0.710297 | -0.672585 |
| H | 10.022056 | -1.577706 | -2.203410 |
| C | 1.186307 | -0.742171 | 1.496668 |
| H | 1.714436 | -1.646266 | 1.164051 |
| C | 1.928600 | -0.088368 | 2.669440 |
| N | -0.134881 | -1.595104 | 2.439184 |
| N | -1.186289 | -1.837709 | 2.639755 |
| I | -0.130575 | 4.051645 | 1.214037 |
| I | 0.364867 | -3.988329 | -0.564567 |
| F | 3.164607 | 0.233008 | 2.297861 |
| F | 2.029578 | -0.930527 | 3.700974 |
| F | 1.325591 | 1.009298 | 3.105663 |

Vibrational frequencies

| | | |
|---|---|---|
| -476.9394 | 10.9997 | 20.2441 |
| 21.6825 | 32.2711 | 35.0271 |
| 39.4165 | 40.5195 | 51.3996 |
| 58.2734 | 60.8725 | 63.2537 |
| 83.8589 | 86.5206 | 92.6771 |
| 98.1580 | 100.5383 | 105.6818 |
| 108.6728 | 128.1860 | 136.4971 |
| 138.3115 | 151.5649 | 162.3905 |
| 167.5880 | 172.7591 | 185.6052 |
| 195.2430 | 217.6162 | 226.5157 |
| 240.0862 | 258.9549 | 268.9485 |
| 274.3801 | 284.3341 | 286.7177 |
| 292.9896 | 295.8728 | 317.3183 |
| 338.5242 | 346.1352 | 352.0555 |
| 368.9149 | 403.3732 | 414.5845 |
| 421.2288 | 446.3181 | 452.8410 |
| 462.3165 | 464.1739 | 475.2890 |
| 506.5477 | 525.2107 | 531.0766 |
| 539.3839 | 572.6216 | 577.9981 |
| 581.1181 | 585.3987 | 595.9576 |
| 604.0108 | 606.6369 | 634.0571 |
| 647.9248 | 669.3688 | 680.0227 |
| 691.5579 | 736.7909 | 742.1810 |
| 754.5470 | 758.2691 | 772.3017 |
| 773.9171 | 777.6234 | 780.6666 |
| 789.4989 | 807.7177 | 815.8076 |
| 832.8355 | 844.6177 | 847.2864 |
| 886.9754 | 890.1853 | 891.7752 |
| 893.3324 | 908.4855 | 920.4482 |
| 932.4933 | 935.1719 | 938.8080 |

| | | |
|---|---|---|
| 960.5252 | 991.4270 | 1002.4774 |
| 1004.6886 | 1008.0730 | 1019.0538 |
| 1026.7564 | 1033.4224 | 1035.3301 |
| 1038.2465 | 1050.6636 | 1053.9457 |
| 1061.5596 | 1065.2346 | 1078.0339 |
| 1084.0104 | 1087.6591 | 1096.4486 |
| 1119.5687 | 1136.9335 | 1143.1097 |
| 1151.4961 | 1156.5509 | 1161.5487 |
| 1165.1601 | 1172.7605 | 1191.5528 |
| 1208.4580 | 1219.0664 | 1223.7478 |
| 1231.6921 | 1235.3743 | 1254.3947 |
| 1271.4223 | 1279.9387 | 1289.5590 |
| 1294.0543 | 1297.3657 | 1300.9978 |
| 1311.7877 | 1314.9532 | 1319.7682 |
| 1328.1792 | 1330.8685 | 1334.1505 |
| 1358.0403 | 1365.1412 | 1385.8988 |
| 1401.1475 | 1415.5929 | 1416.1689 |
| 1431.9101 | 1433.0768 | 1433.4254 |
| 1444.6093 | 1447.6650 | 1454.6300 |
| 1459.1492 | 1468.9127 | 1469.8063 |
| 1476.3887 | 1477.5075 | 1479.8647 |
| 1482.2690 | 1495.6247 | 1508.0468 |
| 1556.1488 | 1565.9114 | 1645.3860 |
| 1652.7848 | 1662.3806 | 1663.7543 |
| 1699.5512 | 1710.0985 | 1713.0081 |
| 2497.5733 | 3030.2932 | 3034.5936 |
| 3039.3991 | 3040.2265 | 3043.1272 |
| 3043.8092 | 3070.1766 | 3082.0760 |
| 3092.7496 | 3098.3362 | 3111.4998 |
| 3131.3345 | 3141.1448 | 3152.2634 |

| | | |
|---|---|---|
| 3165.1721 | 3189.4747 | 3204.5346 |
| 3206.8602 | 3217.2489 | 3218.9909 |
| 3219.9075 | 3223.4258 | 3228.7150 |
| 3230.0317 | 3245.1955 | 3246.6516 |

**TS3R-L6**

Zero-point correction= 0.503225

Thermal correction to Energy= 0.540333

Thermal correction to Enthalpy= 0.541277

Thermal correction to Gibbs Free Energy= 0.429321

Sum of electronic and zero-point Energies= -2336.483216

Sum of electronic and thermal Energies= -2336.446108

Sum of electronic and thermal Enthalpies= -2336.445164

Sum of electronic and thermal Free Energies= -2336.557120

Cartesian coordinates

| | | | |
|---|---|---|---|
| O | -0.183292 | -1.276721 | -0.109109 |
| B | 0.260412 | -0.160170 | 0.722249 |
| C | -1.463064 | -1.672299 | -0.128841 |
| O | -0.811685 | 0.772981 | 1.073315 |
| C | -2.495914 | -0.795159 | -0.447188 |
| C | -1.771923 | -3.040680 | 0.151308 |
| C | -1.396440 | 1.361437 | 0.015781 |
| C | -2.175184 | 0.603459 | -0.845250 |
| C | -3.066418 | -3.489629 | 0.173658 |
| C | -3.860868 | -1.224718 | -0.326698 |
| C | -4.143121 | -2.589310 | -0.034231 |
| C | -1.216117 | 2.755354 | -0.223120 |
| C | -2.651682 | 1.181931 | -2.067261 |
| C | -1.736661 | 3.346778 | -1.344946 |
| C | -2.435068 | 2.569802 | -2.308133 |

| | | | |
|---|---|---|---|
| H | -3.287705 | -4.538635 | 0.380552 |
| H | -1.605065 | 4.415801 | -1.524937 |
| C | -2.918810 | 3.158965 | -3.509925 |
| C | -3.571653 | 2.401115 | -4.450430 |
| C | -3.760159 | 1.014841 | -4.230056 |
| C | -3.314924 | 0.422091 | -3.073048 |
| H | -2.752098 | 4.226802 | -3.672725 |
| H | -3.937972 | 2.860058 | -5.371419 |
| H | -4.260538 | 0.409817 | -4.989747 |
| H | -3.461895 | -0.648438 | -2.923910 |
| C | -5.492881 | -3.028891 | 0.067976 |
| C | -6.531841 | -2.144427 | -0.082985 |
| C | -6.258066 | -0.777829 | -0.333036 |
| C | -4.964052 | -0.330682 | -0.452992 |
| H | -5.683918 | -4.083931 | 0.280194 |
| H | -7.565549 | -2.486654 | 0.003456 |
| H | -7.083546 | -0.068051 | -0.424784 |
| H | -4.777947 | 0.728477 | -0.632467 |
| C | 1.601940 | 0.558659 | 0.147455 |
| C | 2.374605 | -0.000917 | -0.798335 |
| H | 1.865491 | 1.556555 | 0.519971 |
| H | 2.123544 | -1.011461 | -1.146805 |
| C | 3.588539 | 0.615852 | -1.417736 |
| C | 4.848542 | -0.205909 | -1.115795 |
| H | 3.715674 | 1.649524 | -1.056462 |
| H | 3.451412 | 0.667763 | -2.512312 |
| C | 6.116723 | 0.379618 | -1.729621 |
| H | 4.971241 | -0.285407 | -0.022119 |
| H | 4.704251 | -1.237672 | -1.481880 |
| H | 5.985912 | 0.468988 | -2.822857 |

| | | | |
|---|---|---|---|
| H | 6.260641 | 1.408950 | -1.355154 |
| C | 7.366068 | -0.445619 | -1.433459 |
| C | 8.647300 | 0.142116 | -2.020572 |
| H | 7.224949 | -1.470384 | -1.822267 |
| H | 7.483074 | -0.550976 | -0.339654 |
| C | 9.883232 | -0.703511 | -1.737320 |
| H | 8.524269 | 0.263200 | -3.111104 |
| H | 8.796532 | 1.159101 | -1.617417 |
| H | 10.790927 | -0.249998 | -2.164753 |
| H | 10.047758 | -0.821026 | -0.653787 |
| H | 9.782110 | -1.713596 | -2.167034 |
| C | 1.005332 | -0.553858 | 2.092741 |
| H | 1.109029 | 0.292205 | 2.786638 |
| C | 2.214366 | -1.484677 | 2.258046 |
| N | -0.302166 | -1.403819 | 3.091525 |
| N | -1.350467 | -1.682840 | 3.258188 |
| I | -0.187256 | 3.917608 | 1.200401 |
| I | -0.212656 | -4.399828 | 0.535479 |
| F | 2.400343 | -2.311847 | 1.242287 |
| F | 2.112828 | -2.218322 | 3.366693 |
| F | 3.312425 | -0.733452 | 2.374282 |

Vibrational frequencies

| | | |
|---|---|---|
| -465.0360 | 12.3823 | 17.9573 |
| 26.4153 | 33.2606 | 35.5991 |
| 38.4492 | 51.6528 | 54.3904 |
| 64.0749 | 67.5286 | 70.9526 |
| 81.8054 | 88.8867 | 93.1327 |
| 96.6544 | 101.8690 | 104.8480 |
| 107.1401 | 121.6736 | 141.0684 |

| | | |
|---|---|---|
| 142.0158 | 153.9690 | 160.8977 |
| 165.3690 | 171.4090 | 188.0219 |
| 194.8014 | 210.2597 | 222.8744 |
| 230.8468 | 249.5365 | 270.9284 |
| 271.7792 | 285.1792 | 286.4871 |
| 289.8026 | 295.6045 | 313.2810 |
| 339.7055 | 342.6244 | 349.7756 |
| 372.3376 | 400.3966 | 419.6713 |
| 430.7042 | 446.1453 | 455.7404 |
| 464.3994 | 470.1654 | 480.2362 |
| 505.8317 | 528.5041 | 534.3142 |
| 537.2108 | 572.6046 | 578.0124 |
| 581.2955 | 586.8679 | 595.6593 |
| 601.2561 | 611.6014 | 637.5138 |
| 654.7659 | 665.6730 | 681.3230 |
| 685.6706 | 735.4443 | 740.6695 |
| 746.8507 | 758.7924 | 767.3418 |
| 773.7460 | 782.7392 | 784.2947 |
| 785.6689 | 807.4790 | 817.0788 |
| 827.3473 | 843.8934 | 848.2518 |
| 882.0119 | 890.4176 | 903.2588 |
| 905.6217 | 907.0990 | 918.1325 |
| 923.3804 | 945.9761 | 948.0087 |
| 961.2260 | 992.8196 | 1002.3450 |
| 1013.5059 | 1016.4721 | 1018.7582 |
| 1029.7498 | 1036.3915 | 1041.8036 |
| 1042.9820 | 1049.0846 | 1051.7701 |
| 1061.9548 | 1069.3868 | 1075.7647 |
| 1087.5778 | 1096.7279 | 1100.5609 |
| 1121.4996 | 1125.1073 | 1135.9725 |

| | | |
|---|---|---|
| 1147.8879 | 1156.6944 | 1160.3584 |
| 1168.9204 | 1171.2081 | 1190.0702 |
| 1205.6012 | 1208.3628 | 1227.4591 |
| 1232.0659 | 1237.9312 | 1254.2207 |
| 1271.8285 | 1282.0564 | 1286.9884 |
| 1295.4900 | 1298.0400 | 1305.2107 |
| 1314.3979 | 1316.9038 | 1321.9464 |
| 1329.8743 | 1336.2799 | 1336.9674 |
| 1357.0547 | 1364.9156 | 1385.5119 |
| 1400.7987 | 1416.0045 | 1416.9083 |
| 1431.4894 | 1433.7536 | 1434.5241 |
| 1441.6206 | 1442.6608 | 1451.2350 |
| 1455.9291 | 1465.3633 | 1470.8777 |
| 1474.1071 | 1475.8513 | 1480.1337 |
| 1480.9615 | 1494.2385 | 1508.2791 |
| 1554.4820 | 1564.9255 | 1645.9678 |
| 1653.8354 | 1662.3972 | 1663.9860 |
| 1697.1818 | 1710.5225 | 1713.1764 |
| 2501.5720 | 3031.5937 | 3036.4469 |
| 3040.1189 | 3044.2292 | 3046.1763 |
| 3050.1063 | 3071.8092 | 3084.6271 |
| 3094.9575 | 3101.7737 | 3116.9869 |
| 3132.3924 | 3142.9627 | 3168.3615 |
| 3175.3878 | 3183.6542 | 3207.4114 |
| 3208.1087 | 3216.7358 | 3218.7366 |
| 3221.4451 | 3223.5644 | 3229.7141 |
| 3230.6143 | 3241.3154 | 3246.1562 |