

## SUPPORTING INFORMATION FOR

### Chiral Pyridoxal-Catalyzed Biomimetic Mannich Reaction:

#### Mechanism and Origin of Stereoselectivity

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## Part 1: Computational details

All the calculations were performed with the Gaussian09<sup>1</sup> program by using density functional theory, which has been identified to be a powerful and widely used method for exploring the reaction mechanisms. The solvent effect was considered using the implicit IEF-PCM model. All structures of the stationary points were completely optimized by the B3LYP-D3 functional at the 6-31G(d, p) basis set in the mixed solvent of H<sub>2</sub>O and CHCl<sub>3</sub> with a ratio of 1:1 using a dielectric constant value of 41.5. Frequency calculations were carried out at the same level to confirm the characteristics of all of the optimized structures as minima (no imaginary frequency) or transition states (only one imaginary frequency) and provided the thermal relative Gibbs free energy correction. All the energies discussed in the main text are the relative Gibbs free energies (GFE), which were obtained by the addition of the thermal Gibbs free energy corrections (GFEC) at the B3LYP-D3/6-31G(d, p)/IEF-PCM<sub>solvent</sub> level and the single-point energies (SPE) at a higher computational level of B3LYP-D3/6-311++G(2df, 2pd)/IEF-PCM<sub>solvent</sub>. Atom-in-molecule (AIM) quantitative analysis were plotted by using Multiwfn and VMD, and the computed 3D-structures were rendered using the CYLview software.

We have denoted the computational levels B3LYP-D3/6-31G(d, p)/IEF-PCM<sub>solvent</sub>, M06-2X/6-31G(d, p)/IEF-PCM<sub>solvent</sub>,  $\omega$ B97X-D/6-31G(d, p)/IEF-PCM<sub>solvent</sub>, B3LYP-D3/6-31G(d, p)/IEF-PCM<sub>solvent</sub>//B3LYP-D3/6-311++G(2df, 2pd)/IEF-PCM<sub>solvent</sub>, B3LYP-D3/6-31G(d, p)/IEF-PCM<sub>solvent</sub>//6-311+G(d, p) as L1-5 levels, respectively. To check whether the selected method is reliable, different DFT methods including M06-2X and  $\omega$ B97X-D have been performed additionally for the key transition states involved in the stereoselectivity-determining step, and the computed results were summarized as Table S1. There are small differences between the energies calculated by different methods. Thus, the selected DFT method is appropriate for the system studied in this work.

**Table S1.** The relative GFE (kcal/mol) of transition states **TS5RR/SS** calculated at L1, L2, and L3 levels.

	L1	L2	L3
<b>TS5RR</b>	0.0	0.0	0.0
<b>TS5SS</b>	2.1	3.8	2.9

To test the accuracy of the selected basis set, we also performed the single-point energy calculations using the other two different basis sets including 6-311++G(2df, 2pd) and 6-311+G(d, p)

for the key transition states **TS5RR/RS/SR/SS**. As summarized in Table S2, the relative GFEs of **TS5RR/RS/SR/SS** calculated by L5 level are close to those calculated by the selected L4 level. Thus, the calculated results should be reliable and the selected basis set is suitable for the systems studied in this work.

**Table S2.** The relative GFE (kcal/mol) of transition states **TS5RR/RS/SR/SS** calculated at L4 and L5 level.

	L4	L5
<b>TS5RR</b>	0	0
<b>TS5SS</b>	2.1	2.2
<b>TS5SR</b>	4.2	4.8
<b>TS5RS</b>	8.3	8.9

In addition, the extent of enantioselectivity, in terms of enantiomeric excess (ee %), was also calculated by using the Boltzmann distribution of diastereomeric transition states with the following equation:

$$\frac{[RR]}{[SS]} = \frac{\exp\left(\frac{-\Delta G_{[RR]}^\ddagger}{RT}\right)}{\exp\left(\frac{-\Delta G_{[SS]}^\ddagger}{RT}\right)} = \exp\left(\frac{\Delta\Delta G_{[SS]}^\ddagger - [RR]}{RT}\right)$$

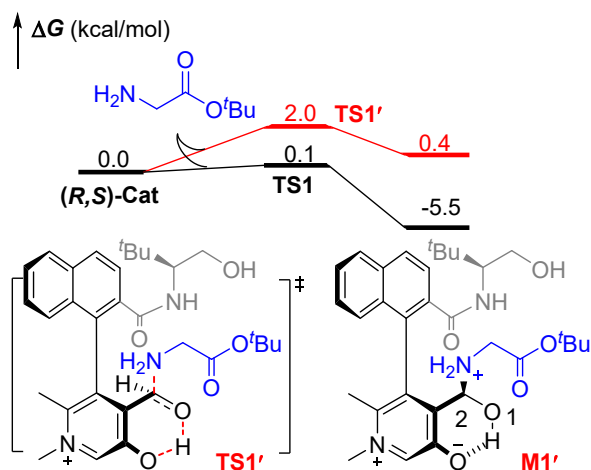
$$ee = \frac{[RR] - [SS]}{[RR] + [SS]} \times 100\% = \frac{\frac{[RR]}{[SS]} - 1}{\frac{[RR]}{[SS]} + 1} \times 100\%$$

Where  $\Delta G^\ddagger$  is the GFE barrier of the competing diastereomeric transition state and  $\Delta\Delta G^\ddagger$  is the GFE barrier difference between the two diastereomeric transition states.

## Part 2: Additional computational results

### 2.1 Other unfavorable pathway for the formation of **M1'**

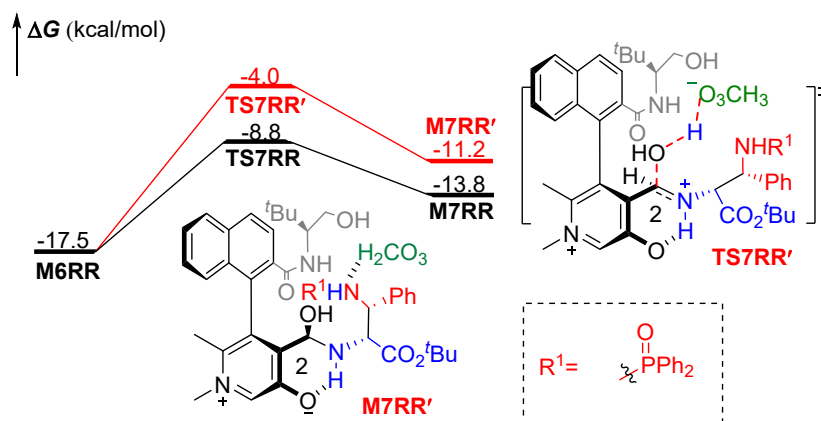
Other possible pathways of nucleophilic addition were considered and discussed as follows. Both the attack modes on *Re*- and *Si*-faces of C2=O1 of (**R,S**)-**Cat** were investigated. As shown in Fig. S1, the reactant **R1** and catalyst (**R,S**)-**Cat** were transformed to quaternary ammonium salt **M1'** via transition state **TS1'** ( $\Delta G^\ddagger = 2.0$  kcal/mol). The energy barrier of the nucleophilic addition pathway is higher than that of the pathway via **TS1** ( $\Delta G^\ddagger = 0.1$  kcal/mol), so the pathway cannot be safely excluded.



**Fig. S1** The relative GFE profiles for the formation of intermediates **M1/M1'** via transition states **TS1/TS1'**.

## 2.2 Other unfavorable pathway for the formation of **M7RR'**

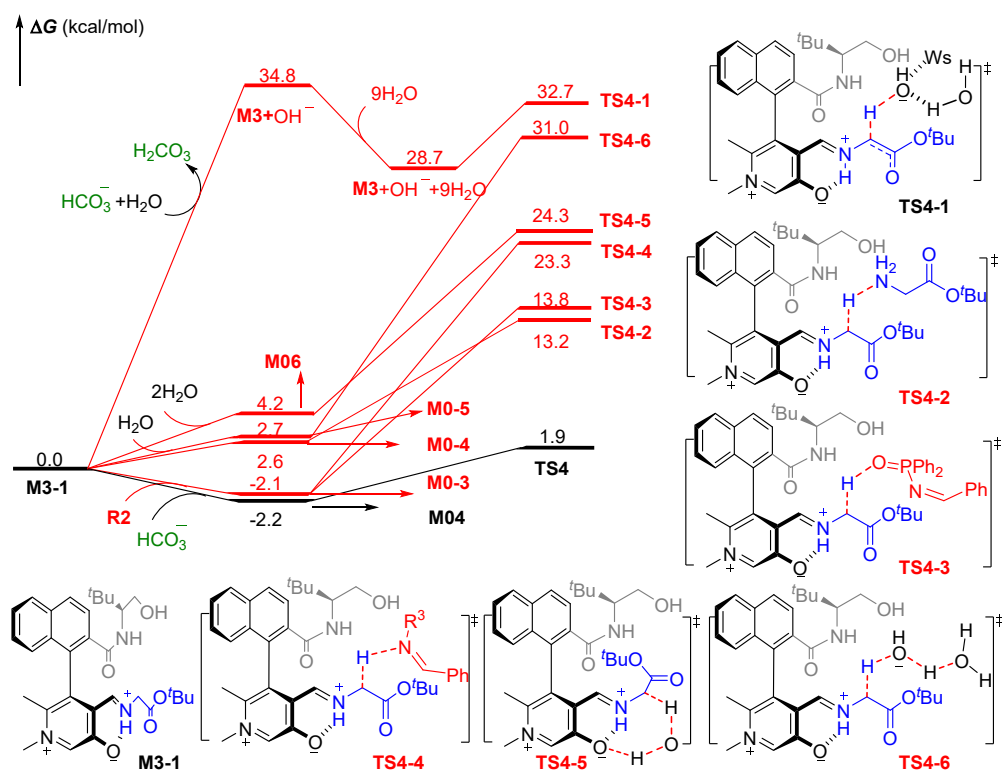
Next, we considered and discussed other possible pathway of hydrolysis. Both the attack modes on *Re*- and *Si*-faces of  $C2=N$  of **(R,S)-Cat** were investigated. As shown in Fig. S2, after we obtained the intermediate **M6RR**, the pathway of the  $HCO_3^-$  assisted dehydration to form secondary amine intermediate **M7RR'** via transition state **TS7RR'** ( $\Delta G^\ddagger = 13.5$  kcal/mol). The energy barrier of the pathway is higher than that of the pathway via **TS7RR** ( $\Delta G^\ddagger = 8.7$  kcal/mol), so the pathway cannot be safely excluded.



**Fig. S2** The relative GFE profiles for hydrolysis from intermediate **M6RR** to intermediates **M7RR/M7RR'** via transition states **TS7RR/TS7RR'**.

### Part 3: Other unfavorable deprotonation pathways of M4

As shown in Fig. S3, the  $\alpha$ -C-H of intermediate **M3-1** was deprotonated by  $\text{HCO}_3^-$  via transition state **TS4** ( $\Delta G^\ddagger = 5.3$  kcal/mol). The  $\alpha$ -C-H of intermediate **M3-1** was deprotonated by glycine **R1** via transition state **TS4-2** ( $\Delta G^\ddagger = 10.5$  kcal/mol). The  $\alpha$ -C-H of intermediate **M3-1** was deprotonated by the oxygen of phenyl N-diphenylphosphinimine **R2** via transition state **TS4-3** ( $\Delta G^\ddagger = 15.9$  kcal/mol). The  $\alpha$ -C-H of intermediate **M3-1** was deprotonated the nitrogen of phenyl N-diphenylphosphinimine **R2** via transition state **TS4-4** ( $\Delta G^\ddagger = 25.4$  kcal/mol). The  $\alpha$ -C-H of intermediate **M3-1** was deprotonated by oxygen negative with the assistance of  $\text{H}_2\text{O}$  via transition state **TS4-5** ( $\Delta G^\ddagger = 19.2$  kcal/mol). The  $\alpha$ -C-H of intermediate **M3-1** was deprotonated by hydroxide anion with the assistance of  $\text{H}_2\text{O}$  via transition state **TS4-6** ( $\Delta G^\ddagger = 33.7$  kcal/mol).

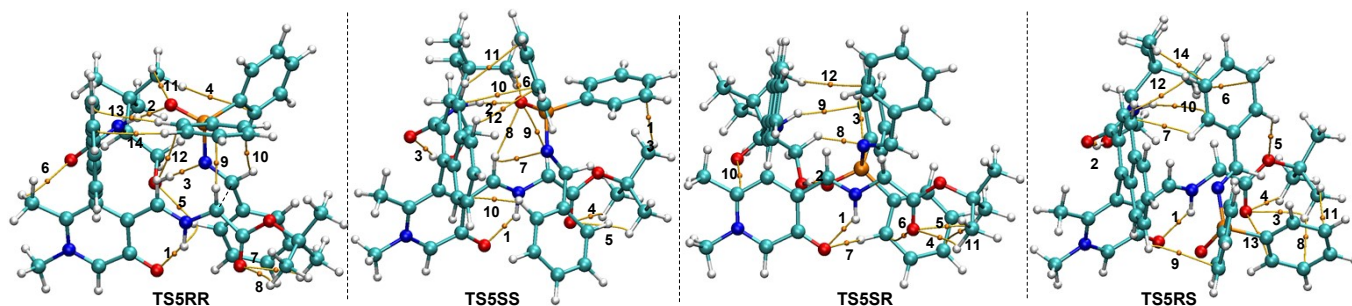


**Fig. S3** Relative Gibbs free energy profiles of transition states **TS4**/**TS4-1**/**TS4-2**/**TS4-3**/**TS4-4**/**TS4-5**/**TS4-6** and structures, the red and black path represent the deprotonation via different pathways, respectively. (Ws represents the other nine water molecules)

## Part 4: AIM analyses for transition states TS5RR, TS5SS, TS5SR and TS5RS

Herein, all the weak interactions with the values of Laplacian of electron densities were summarized in Table S3. Two N–H...O (1.67 Å, 1.73 Å), one O–H...N (1.86 Å), six C–H... $\pi$  (2.25 Å, 2.55 Å, 2.73 Å, 2.68 Å, 2.75 Å, 3.16 Å) and five C–H...O (2.26 Å, 2.58 Å, 2.44 Å, 2.47 Å, 2.68 Å) interactions can be found in **TS5RR**. Two N–H...O (1.75 Å, 1.80 Å), one O–H...O (1.93 Å), three C–H... $\pi$  (3.05 Å, 2.96 Å, 3.37 Å), one C–H...N (2.54 Å), one  $\pi$ - $\pi$  stacking and five C–H...O (2.44 Å, 2.45 Å, 2.30 Å, 2.45 Å, 2.49 Å) interactions exist in **TS5SS**. One O–H...O (1.72 Å), one N–H...O (1.80 Å), two C–H... $\pi$  (2.93 Å, 2.75 Å), three C–H...N (2.55 Å, 2.32 Å, 2.70 Å), three C–H...O (2.43 Å, 2.44 Å, 2.46 Å) and two LP... $\pi$  (3.34 Å, 2.86 Å) interactions exist in **TS5SR**, and one N–H...O (1.81 Å), one O–H...O (1.81 Å), three four C–H...O (2.44 Å, 2.45 Å, 2.63 Å, 2.90 Å), one LP... $\pi$  (3.48 Å), one N–H... $\pi$  (3.00 Å) and six C–H... $\pi$  (2.94 Å, 2.17 Å, 3.00 Å, 2.94 Å, 3.10 Å, 3.20 Å) interactions exist in **TS5RS**.

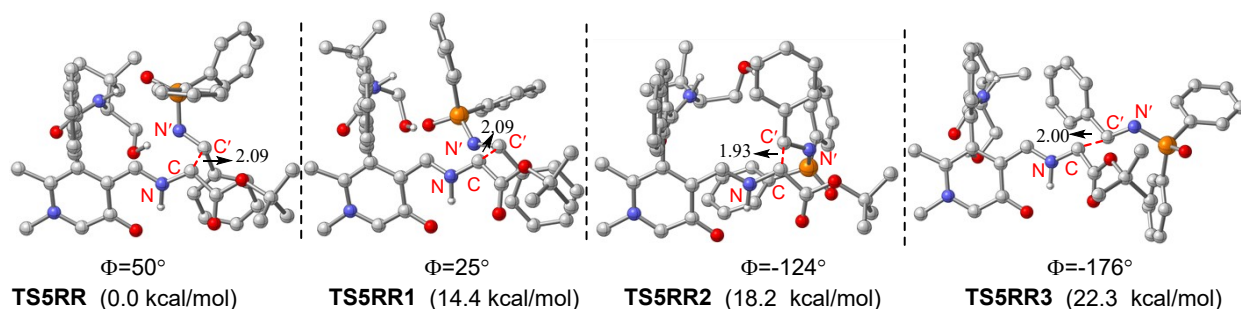
**Table S3.** AIM analyses of the transition states **TS5RR/SS/SR/RS** and the summary of Laplacian of electron density. Bond critical points (BCPs, orange color) along the bond paths (yellow color) ( $\nabla^2\rho$  in  $10^{-1}$  a.u.).



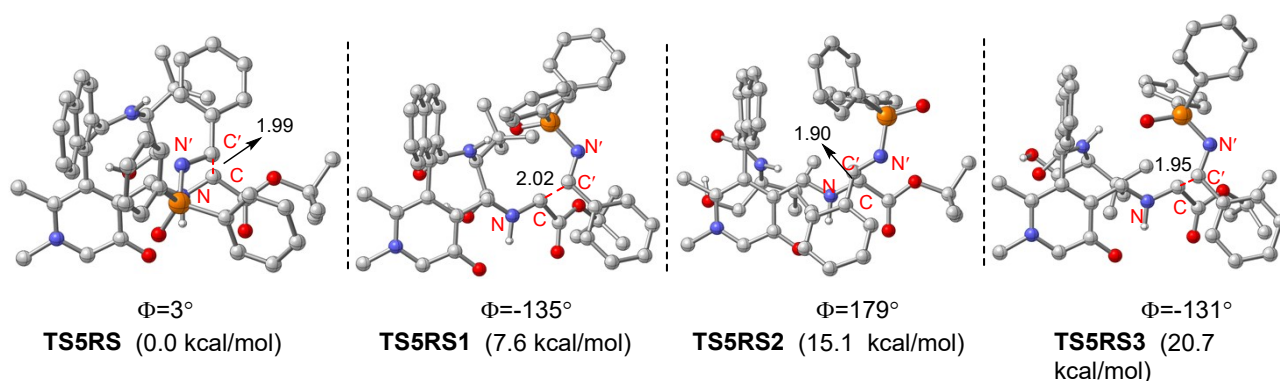
TS5RR (0.0 kcal/mol)			TS5SS (2.1 kcal/mol)			TS5SR (4.2 kcal/mol)			TS5RS (8.3 kcal/mol)		
type	$\nabla^2\rho$	distance(Å)	type	$\nabla^2\rho$	distance(Å)	Type	$\nabla^2\rho$	distance(Å)	type	$\nabla^2\rho$	distance(Å)
N-H...O	1.500	1.67	N-H...O	1.280	1.75	O-H...O	1.158	1.72	N-H...O	1.140	1.81
N-H...O	1.273	1.73	N-H...O	1.061	1.80	N-H...O	1.250	1.80	O-H...O	1.053	1.81
O-H...N	0.879	1.85	O-H...O	0.782	1.93	C-H...N	0.455	2.55	C-H...O	0.446	2.44
C-H... $\pi$	0.591	2.25	C-H...O	0.445	2.44	C-H...O	0.452	2.43	C-H...O	0.439	2.45
C-H...O	0.482	2.26	C-H...O	0.432	2.45	C-H...O	0.450	2.44	C-H...O	0.273	2.63
C-H...O	0.439	2.58	C-H...O	0.420	2.30	LP... $\pi$	0.450	3.34	C-H...O	0.211	2.90
C-H...O	0.439	2.44	C-H...N	0.383	2.54	C-H...O	0.320	2.46	C-H... $\pi$	0.188	2.94
C-H...O	0.424	2.47	C-H...O	0.373	2.45	C-H...N	0.296	3.23	C-H... $\pi$	0.181	3.17
C-H... $\pi$	0.349	2.55	C-H...O	0.343	2.49	C-H...N	0.205	2.70	C-H... $\pi$	0.163	3.00
C-H... $\pi$	0.269	2.73	$\pi$ ... $\pi$	0.198	3.38	LP... $\pi$	0.186	2.86	C-H... $\pi$	0.159	2.94
C-H...O	0.257	2.68	C-H... $\pi$	0.173	3.05	C-H... $\pi$	0.157	2.93	N-H... $\pi$	0.152	3.00
C-H... $\pi$	0.232	2.68	C-H... $\pi$	0.158	2.96	C-H... $\pi$	0.121	2.75	C-H... $\pi$	0.144	3.10
C-H... $\pi$	0.232	2.75	C-H... $\pi$	0.147	3.37	—	—	—	LP... $\pi$	0.127	3.48
C-H... $\pi$	0.171	3.16	—	—	—	—	—	C-H... $\pi$	0.120	3.20	

## Part 5: Comparison of different configurations of TS5s

To ensure the selected configuration of the stereochemical transition state with the lowest energy, we have searched multiple possible conformations in the fifth step. By rotating the dihedral angle  $\Phi(\text{N}-\text{C}-\text{C}'-\text{N}')$  depicted in Figs. S4-7 with  $90^\circ$  per time in stereo-controlling transition states **TS5RR**, **TS5RS**, **TS5SR**, and **TS5SS**, we have totally constructed  $4 \times 4 = 16$  conformations as the initial structures. Subsequently, B3LYP-D3 in conjunction with the standard 6-31G(d,p) basis set was employed for all geometry optimizations and (free) energy calculations. After the optimization, the corresponding dihedral  $\Phi$  angles change to  $50^\circ/25^\circ/-124^\circ/-176^\circ$ ,  $-72^\circ/-60^\circ/-167^\circ/77^\circ$ ,  $3^\circ/-135^\circ/-130^\circ/171^\circ$  and  $5^\circ/-8^\circ/171^\circ/-40^\circ$  in the **TS5RRs**, **TS5RSs**, **TS5SRs**, and **TS5SSs**, respectively. As revealed by Figs. S5-8, the most stable conformations with the lowest energies of the four diastereoselective transition states (denoted as **TS5RR**, **TS5RS**, **TS5SR**, and **TS5SS**) are associated with the dihedral angles  $\Phi(\text{N}-\text{C}-\text{C}'-\text{N}')$  of  $50^\circ/-72^\circ/3^\circ/6^\circ$ , separately.

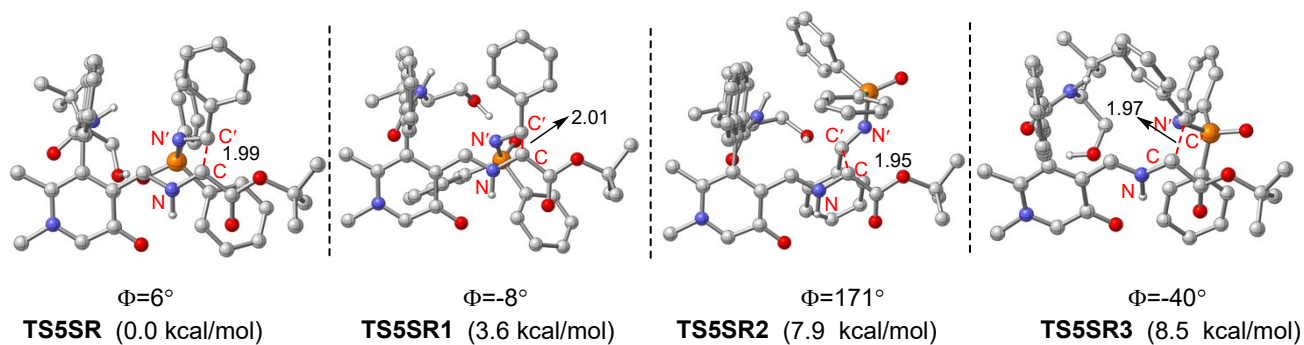


**Fig. S4** Different configurations of the transition states **TS5RRs** with different dihedral  $\Phi(\text{N}-\text{C}-\text{C}'-\text{N}')$  angles (distance in Å).

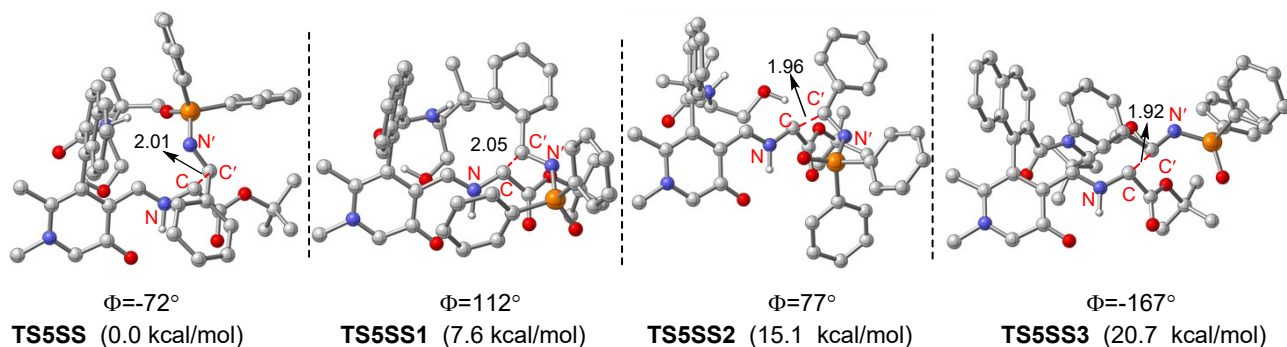


**Fig. S5** Different configurations of the transition states **TS5RSs** with different dihedral  $\Phi(\text{N}-\text{C}-\text{C}'-\text{N}')$  angles (distance in Å).





**Fig. S6** Different configurations of the transition states **TS5SRs** with different dihedral  $\Phi(\text{N}-\text{C}-\text{C}'-\text{N}')$  angles (distance in Å).



**Fig. S7** Different configurations of the transition states **TS5SSs** with different dihedral  $\Phi(\text{N}-\text{C}-\text{C}'-\text{N}')$  angles (distance in Å).

## Part 6: The Cartesian coordinates of all the stationary points

### R1

Zero-point correction= 0.192133

Thermal correction to Energy= 0.203037

Thermal correction to Enthalpy= 0.203981

Thermal correction to Gibbs Free Energy= 0.156340

Sum of electronic and zero-point Energies= -441.534489

Sum of electronic and thermal Energies= -441.523585

Sum of electronic and thermal Enthalpies= -441.522641

Sum of electronic and thermal Free Energies= -441.570282

Cartesian coordinates

C	0.974546	-0.088806	-0.027666
O	1.020761	-1.305382	-0.053681
O	-0.134624	0.659410	0.023201
C	2.204729	0.801151	-0.104955
H	2.190278	1.244166	-1.116817
H	2.076285	1.634059	0.594054
N	3.407232	0.041670	0.225498
H	3.422640	-0.799215	-0.347935
H	4.224369	0.585403	-0.040440
C	-1.490085	0.060427	0.012505
C	-2.395481	1.290773	0.058374
H	-2.218484	1.930319	-0.810910
H	-3.443971	0.980462	0.055354
H	-2.206833	1.873182	0.964590
C	-1.697756	-0.723370	-1.284929
H	-1.492421	-0.084414	-2.148998
H	-1.047531	-1.597320	-1.326744
H	-2.738580	-1.055501	-1.343461
C	-1.679075	-0.805412	1.259775
H	-1.031106	-1.681517	1.232986
H	-1.455500	-0.224641	2.159580
H	-2.720131	-1.137481	1.315471

#### Vibrational frequencies

67.7256	81.7137	124.1329
155.5106	212.1451	219.0605
258.6689	290.6835	296.1926
324.6220	352.0809	364.5025
437.3030	462.4889	500.5331
590.3930	702.4615	759.1393
855.1243	896.6366	928.1791

936.7461	941.1431	981.4900
1035.4710	1062.6603	1067.8688
1110.1887	1182.8827	1202.4356
1272.5362	1277.7015	1290.8620
1302.2678	1410.3720	1415.4104
1437.8661	1444.8388	1479.9216
1495.0157	1495.3768	1496.7058
1502.8468	1512.2614	1533.0656
1642.1648	1784.4982	2960.8604
3052.0268	3054.7067	3060.7166
3085.8507	3124.4916	3126.0515
3132.5426	3137.4191	3163.5588
3166.6532	3497.0219	3581.0318

## R2

Zero-point correction= 0.300788

Thermal correction to Energy= 0.319548

Thermal correction to Enthalpy= 0.320492

Thermal correction to Gibbs Free Energy= 0.250268

Sum of electronic and zero-point Energies= -1204.788125

Sum of electronic and thermal Energies= -1204.769365

Sum of electronic and thermal Enthalpies= -1204.768421

Sum of electronic and thermal Free Energies= -1204.838645

## Cartesian coordinates

P	-0.934097	-0.030906	1.085269
O	-1.283231	0.062371	2.546829
C	-1.848980	-1.328165	0.204151
C	-3.127802	-1.663940	0.671980
C	-1.333630	-1.970108	-0.931891
C	-3.886996	-2.625135	0.004092

H	-3.517305	-1.179205	1.561851
C	-2.097545	-2.928466	-1.599122
H	-0.336040	-1.731867	-1.287402
C	-3.373802	-3.254617	-1.132986
H	-4.875253	-2.884494	0.371276
H	-1.694923	-3.424037	-2.477154
H	-3.965565	-4.002396	-1.652294
C	-1.268061	1.535025	0.211892
C	-1.355752	1.609721	-1.187454
C	-1.399614	2.703102	0.976991
C	-1.571195	2.839155	-1.809977
H	-1.267575	0.711221	-1.790970
C	-1.617217	3.931033	0.350870
H	-1.340610	2.637963	2.058625
C	-1.701355	3.999693	-1.041797
H	-1.640862	2.891269	-2.892131
H	-1.722976	4.831436	0.948272
H	-1.871467	4.955207	-1.528736
N	0.687649	-0.490401	0.829683
C	1.550637	0.267012	0.252961
H	1.284342	1.253671	-0.150699
C	2.952189	-0.117779	0.071171
C	3.439179	-1.361429	0.513342
C	3.823574	0.780129	-0.567161
C	4.774438	-1.694999	0.318010
H	2.756722	-2.047705	1.003393
C	5.162292	0.443259	-0.761042
H	3.447473	1.740642	-0.909217
C	5.637541	-0.793687	-0.319126
H	5.148847	-2.655219	0.658883
H	5.831835	1.140500	-1.254442

H	6.679718	-1.058389	-0.470120
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Vibrational frequencies

19.1187	27.5002	30.8451
36.0757	45.1992	59.0480
100.5547	116.6679	166.8477
179.3673	195.7079	242.9288
250.9887	274.2935	298.1749
316.4935	372.1868	409.0791
409.5562	415.6094	420.7007
455.7787	471.7966	510.2360
529.3528	553.8650	621.9859
628.9230	629.2113	630.8296
701.5209	703.1126	710.0360
710.7729	733.7177	763.6541
767.1581	776.0722	817.5128
865.5921	866.9987	870.9206
873.6221	947.8827	948.9534
950.4913	991.0333	992.5663
993.1450	1011.6966	1012.6688
1013.1789	1016.2563	1016.4128
1017.3081	1038.5677	1049.8577
1050.0860	1051.1319	1105.7580
1106.7426	1113.3661	1120.7794
1134.4736	1192.8497	1193.7855
1194.0204	1198.1717	1204.3049
1211.5241	1215.4571	1255.9817
1327.7758	1330.6370	1340.8449
1359.0759	1361.8754	1367.1492
1434.5180	1474.0058	1476.3092
1492.1986	1524.2703	1524.7917

1534.5738	1625.3953	1626.3232
1628.3762	1644.0143	1645.0472
1651.1642	1682.5072	3042.1306
3184.1152	3185.8024	3186.4996
3191.6581	3192.1631	3193.5774
3200.0170	3200.2654	3201.9284
3207.1791	3207.9783	3211.9631
3213.9358	3214.3109	3218.0660

### **(R,S)-Cat**

Zero-point correction= 0.503657

Thermal correction to Energy= 0.532775

Thermal correction to Enthalpy= 0.533720

Thermal correction to Gibbs Free Energy= 0.445348

Sum of electronic and zero-point Energies= -1380.023824

Sum of electronic and thermal Energies= -1379.994706

Sum of electronic and thermal Enthalpies= -1379.993761

Sum of electronic and thermal Free Energies= -1380.082133

### Cartesian coordinates

C	0.803204	-3.571001	-0.350331
C	0.162701	-2.681642	-1.209509
C	0.405866	-1.297321	-1.041462
C	1.235026	-0.864794	0.007419
C	1.839144	-1.798559	0.863189
N	1.607405	-3.123933	0.635187
H	0.662833	-4.637595	-0.450206
C	1.429191	0.598462	0.251822
C	2.628594	1.246579	-0.173010
C	0.415297	1.325765	0.862465
C	3.683408	0.554727	-0.830285

C	2.773614	2.652792	0.073201
C	0.563448	2.717933	1.083441
C	4.829503	1.217985	-1.207206
H	3.580568	-0.504667	-1.039125
C	3.969591	3.304558	-0.330875
C	1.719047	3.360118	0.707028
H	-0.234187	3.265397	1.574988
C	4.976799	2.603922	-0.954495
H	5.627076	0.675764	-1.705024
H	4.072844	4.368559	-0.139406
H	1.837849	4.423271	0.892798
H	5.886504	3.111443	-1.258960
C	-0.227276	-0.344110	-1.977031
O	-0.995638	-0.710078	-2.862829
O	-0.636423	-3.187483	-2.144091
C	2.684376	-1.403774	2.034628
H	2.692566	-0.321449	2.136822
H	2.289376	-1.827851	2.961844
H	3.717644	-1.744680	1.917469
C	-0.834149	0.599122	1.289652
O	-0.757975	-0.437170	1.970139
N	-1.975029	1.126651	0.803295
H	-1.866378	1.967633	0.255174
C	-3.361439	0.659131	0.986415
C	-3.425047	-0.882913	1.145607
H	-3.181151	-1.132119	2.181864
H	-4.449211	-1.211452	0.960356
O	-2.575790	-1.600693	0.256792
H	-1.722990	-1.612600	0.720042
C	-4.258701	1.243837	-0.155444
C	-5.734032	0.908021	0.147293

H	-5.939628	-0.163593	0.084485
H	-6.027151	1.254927	1.144370
H	-6.380954	1.402971	-0.583324
C	-3.870188	0.668746	-1.529040
H	-4.531855	1.072562	-2.302529
H	-2.844018	0.929010	-1.801421
H	-3.945253	-0.420901	-1.541909
C	-4.138622	2.785064	-0.186355
H	-3.156276	3.137977	-0.520303
H	-4.863759	3.197316	-0.894406
H	-4.341156	3.221334	0.797713
C	2.231057	-4.137792	1.520621
H	2.007411	-5.127562	1.132341
H	3.309270	-3.986721	1.538713
H	1.821393	-4.035482	2.525804
H	0.030252	0.717857	-1.862339
H	-3.738711	1.082162	1.928905
H	-1.015397	-2.426278	-2.650627

#### Vibrational frequencies

34.2960	35.8302	42.7676
47.3688	51.9621	59.4142
62.9551	101.1639	111.0943
116.4650	126.3868	133.5580
144.3637	156.7941	183.3516
192.9345	207.0396	209.7680
228.6140	232.6868	251.9040
258.3712	261.2989	276.8394
287.7435	290.1568	298.3816
318.5535	327.3761	334.6036
359.1900	367.1189	382.5651



385.8870	393.2034	407.4663
413.3374	418.6441	438.3447
461.6023	478.4262	488.6993
497.2784	531.3486	541.8872
548.5503	576.5714	588.5402
602.2451	610.0133	632.2464
643.9567	654.4319	662.7834
693.2148	708.2253	739.1462
752.4186	761.3060	768.8162
777.2263	794.5253	798.8798
809.7719	842.1892	847.7403
853.1141	878.7809	884.4428
891.0119	898.3022	907.8354
940.9663	946.1777	961.6360
973.4666	974.3629	990.4291
1009.4498	1011.3205	1021.7866
1029.1923	1042.6222	1054.7306
1057.7631	1062.3338	1077.2577
1083.8151	1122.2808	1134.3371
1137.7195	1150.3406	1183.5858
1194.5059	1205.6794	1217.9789
1222.2692	1246.6919	1247.9761
1250.1487	1251.4806	1278.4384
1287.3611	1294.6499	1316.4021
1324.7176	1340.5446	1355.5293
1362.0462	1378.0823	1387.1013
1408.8546	1415.2129	1422.8619
1423.0620	1426.4339	1427.3215
1433.5437	1436.4335	1452.6376
1460.0442	1468.9381	1471.4577
1479.2092	1485.9195	1493.2589

1496.0323	1497.7863	1504.1293
1506.0223	1508.8347	1516.6073
1521.3549	1523.5731	1529.9466
1533.5423	1554.8659	1576.5513
1610.0478	1611.3149	1643.0425
1671.3032	1674.0014	1702.9814
1740.0464	3008.1784	3034.0511
3043.5144	3053.2772	3065.6811
3068.2728	3075.0782	3097.9962
3100.4787	3112.5538	3117.7763
3121.7125	3124.3006	3128.4714
3136.5402	3142.9084	3190.0665
3190.1063	3193.8800	3194.9274
3197.3066	3208.2178	3211.3782
3214.6672	3217.3894	3270.7726
3364.1250	3636.1320	3730.3195

### **(R,S)-Cat**

Zero-point correction= 0.461253

Thermal correction to Energy= 0.488950

Thermal correction to Enthalpy= 0.489894

Thermal correction to Gibbs Free Energy= 0.404259

Sum of electronic and zero-point Energies= -1340.304582

Sum of electronic and thermal Energies= -1340.276885

Sum of electronic and thermal Enthalpies= -1340.275941

Sum of electronic and thermal Free Energies= -1340.361576

### Cartesian coordinates

C	0.596844	3.807207	-0.277385
C	0.044569	3.018641	0.742258
C	0.383637	1.644616	0.771203

C	1.228300	1.133530	-0.239419
C	1.715110	2.008307	-1.223235
N	1.399520	3.318158	-1.219596
H	0.355829	4.867125	-0.311547
C	1.546836	-0.325913	-0.300828
C	2.809370	-0.812847	0.161036
C	0.599585	-1.220084	-0.783733
C	3.807874	0.049805	0.693736
C	3.082549	-2.219495	0.092172
C	0.870331	-2.611582	-0.828601
C	5.018247	-0.450527	1.118508
H	3.604867	1.113269	0.761639
C	4.342060	-2.701910	0.540878
C	2.086590	-3.096793	-0.411298
H	0.112360	-3.286374	-1.214020
C	5.290410	-1.838701	1.040674
H	5.770298	0.222300	1.518740
H	4.541397	-3.768278	0.483989
H	2.298287	-4.160890	-0.460272
H	6.248907	-2.218548	1.380428
C	-0.149457	0.795202	1.838047
O	-0.923271	1.205952	2.707758
O	-0.772089	3.591057	1.640088
C	2.561474	1.505387	-2.363265
H	2.000168	0.765138	-2.943346
H	2.834317	2.336824	-3.014745
H	3.474392	1.018886	-2.006148
C	-0.723763	-0.689666	-1.272801
O	-0.780433	0.185460	-2.149083
N	-1.795867	-1.206760	-0.635726
H	-1.594681	-1.900259	0.068877

C	-3.217502	-0.900967	-0.863963
C	-3.422324	0.596459	-1.222596
H	-3.212463	0.727175	-2.287302
H	-4.469804	0.856650	-1.056966
O	-2.636954	1.495240	-0.450256
H	-1.776520	1.520096	-0.896261
C	-4.059459	-1.406862	0.354096
C	-5.558648	-1.282678	0.010654
H	-5.876678	-0.243434	-0.105352
H	-5.802137	-1.819048	-0.913293
H	-6.158388	-1.715005	0.817545
C	-3.753237	-0.596609	1.626720
H	-4.356946	-0.970005	2.460790
H	-2.701349	-0.671648	1.914863
H	-3.974776	0.463967	1.486799
C	-3.775422	-2.904738	0.611091
H	-2.767487	-3.096388	0.996038
H	-4.466825	-3.286869	1.368269
H	-3.909494	-3.498010	-0.299977
H	0.182000	-0.254361	1.852730
H	-3.553646	-1.477361	-1.738619
H	-1.069066	2.874905	2.252653

#### Vibrational frequencies

32.9440	33.9070	42.1250
52.3704	54.8891	61.9911
74.9766	102.0935	108.9247
114.2789	135.6156	142.0001
153.5892	159.9712	166.6340
201.8997	206.2349	233.1750
237.8415	253.2168	259.7108

272.7403	280.5235	284.9299
296.7172	319.2246	327.3448
329.9772	350.4014	364.2700
370.4871	383.7948	408.3050
415.7710	429.2542	449.3932
461.4917	475.6576	480.1878
496.1147	513.3471	534.1053
541.9142	559.3341	566.0011
573.8049	593.1480	606.3605
652.7938	661.7114	688.9738
706.3260	716.9230	745.4288
750.3238	764.2912	772.7909
777.0195	796.7148	801.8800
817.3137	841.8409	846.4591
851.6521	888.9072	896.6603
907.4207	916.3969	942.0629
946.8021	949.0582	968.8867
972.6724	979.0683	984.2401
1007.7617	1011.1216	1023.0399
1033.2438	1042.0728	1054.9226
1060.7521	1062.9881	1082.1397
1106.5259	1127.1579	1179.3098
1189.6340	1197.0053	1211.8646
1219.8976	1228.5566	1244.7591
1246.2184	1247.5950	1277.1322
1282.8133	1290.9180	1307.1113
1318.7627	1341.6973	1345.4135
1352.7461	1370.3314	1381.0401
1407.9069	1411.6985	1415.0572
1418.7891	1422.8001	1424.4714
1427.9670	1433.5562	1454.1808

1465.3301	1472.3364	1476.8248
1488.1207	1490.3373	1492.5475
1499.2580	1502.4269	1503.6685
1508.6352	1514.7997	1523.0913
1532.5575	1553.5985	1566.3642
1600.5426	1610.5310	1635.2359
1643.8241	1672.0003	1710.4491
1720.5646	3005.6425	3034.4248
3037.2389	3042.5635	3049.8572
3051.8409	3076.5077	3098.1408
3111.3419	3112.7145	3116.3835
3120.3213	3123.4245	3132.5315
3141.0031	3154.0451	3178.3506
3185.1367	3188.9382	3194.0270
3205.3371	3205.8720	3214.7260
3384.3200	3642.2789	3758.2613

### **HCO<sub>3</sub><sup>-</sup>**

Zero-point correction= 0.026274

Thermal correction to Energy= 0.029799

Thermal correction to Enthalpy= 0.030744

Thermal correction to Gibbs Free Energy= 0.000502

Sum of electronic and zero-point Energies= -264.509353

Sum of electronic and thermal Energies= -264.505828

Sum of electronic and thermal Enthalpies= -264.504883

Sum of electronic and thermal Free Energies= -264.535125

### Cartesian coordinates

C	-1.497122	0.018185	0.000000
O	-0.810971	-1.229655	0.000000
O	-2.739632	-0.088994	0.000000
O	-0.758821	1.032415	0.000000

H	0.125423	-0.983614	0.000000
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Vibrational frequencies

521.4981	548.3324	648.1934
804.7084	905.8982	1192.8216
1336.0166	1784.4817	3790.9358

## **H<sub>2</sub>O**

Zero-point correction= 0.021323

Thermal correction to Energy= 0.024158

Thermal correction to Enthalpy= 0.025102

Thermal correction to Gibbs Free Energy= 0.003007

Sum of electronic and zero-point Energies= -76.405295

Sum of electronic and thermal Energies= -76.402460

Sum of electronic and thermal Enthalpies= -76.401515

Sum of electronic and thermal Free Energies= -76.423611

Cartesian coordinates

O	-0.820261	-1.200023	0.000000
H	0.081685	-1.546595	0.000000
H	-1.362286	-1.999958	0.000000

Vibrational frequencies

1662.7218	3799.4666	3897.6184
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## **H<sub>2</sub>CO<sub>3</sub>**

Zero-point correction= 0.039581

Thermal correction to Energy= 0.043300

Thermal correction to Enthalpy= 0.044244

Thermal correction to Gibbs Free Energy= 0.013679

Sum of electronic and zero-point Energies= -264.976093

Sum of electronic and thermal Energies= -264.972375

Sum of electronic and thermal Enthalpies= -264.971430

Sum of electronic and thermal Free Energies= -265.001995

Cartesian coordinates

C	-1.435725	0.018329	0.000000
O	-0.847196	-1.185085	0.000000
O	-2.763486	-0.159917	0.000000
O	-0.863624	1.088613	0.000000
H	0.111310	-1.035839	0.000000
H	-3.171708	0.720298	0.000000

Vibrational frequencies

508.9189	558.7239	592.4942
599.4911	781.7170	995.4075
1148.0089	1293.4485	1476.6894
1824.0414	3795.3449	3799.7366

TS1

Zero-point correction= 0.699366

Thermal correction to Energy= 0.739070

Thermal correction to Enthalpy= 0.740014

Thermal correction to Gibbs Free Energy= 0.628138

Sum of electronic and zero-point Energies= -1821.593252

Sum of electronic and thermal Energies= -1821.553548

Sum of electronic and thermal Enthalpies= -1821.552604

Sum of electronic and thermal Free Energies= -1821.664480

Cartesian coordinates

C	4.192984	0.570739	1.689551
C	3.016991	0.054171	2.215990
C	2.038375	-0.434258	1.318822



C	2.300454	-0.432038	-0.052356
C	3.530222	0.047150	-0.539371
N	4.419972	0.558578	0.354229
H	4.960344	0.983638	2.328359
C	1.263176	-0.924385	-1.015938
C	1.105848	-2.331148	-1.226075
C	0.417435	-0.028828	-1.657663
C	1.926672	-3.296422	-0.578744
C	0.074437	-2.790136	-2.110785
C	-0.596439	-0.496381	-2.533002
C	1.728096	-4.643006	-0.787794
H	2.716685	-2.964979	0.086103
C	-0.101162	-4.186213	-2.304790
C	-0.755859	-1.840203	-2.761297
H	-1.243202	0.223827	-3.022356
C	0.704325	-5.094343	-1.655783
H	2.362166	-5.365784	-0.284154
H	-0.888026	-4.523439	-2.973154
H	-1.530637	-2.193086	-3.435296
H	0.558808	-6.159125	-1.807782
C	0.763504	-0.977496	1.935093
O	0.833373	-1.401221	3.141789
O	2.827122	0.041805	3.534773
H	1.998094	-0.559657	3.655847
C	3.892434	0.035261	-1.992587
H	3.157751	-0.541981	-2.549983
H	3.887604	1.052031	-2.394329
H	4.877775	-0.407406	-2.158319
C	0.547087	1.446279	-1.398256
O	1.623972	2.051193	-1.521484
N	-0.591297	2.046252	-0.979094

H	-1.393922	1.454020	-0.788305
C	-0.650324	3.478726	-0.669932
C	-0.118574	3.750093	0.759458
H	0.108170	4.819304	0.849966
H	-0.877160	3.508494	1.510685
O	1.022943	2.960061	1.091019
H	1.603245	2.932250	0.310952
C	-2.073599	4.048962	-0.949046
C	-2.084688	5.553450	-0.611420
H	-1.975678	5.734323	0.461866
H	-1.279461	6.083182	-1.132124
H	-3.035470	5.996268	-0.924253
C	-3.161307	3.336452	-0.116843
H	-4.134489	3.792328	-0.323829
H	-3.248030	2.272170	-0.357136
H	-2.981398	3.422904	0.958746
C	-2.388595	3.873242	-2.447650
H	-2.394195	2.818501	-2.737473
H	-3.374486	4.289844	-2.677310
H	-1.649195	4.390863	-3.068378
C	-2.417794	-0.437639	1.314207
O	-2.264980	-0.087048	0.152565
O	-3.267037	-1.346169	1.754019
C	-1.611696	0.167739	2.456084
H	-2.154140	1.039033	2.837828
H	-1.482028	-0.550392	3.268273
N	-0.283171	0.543418	1.956727
H	0.192051	1.190930	2.584122
C	-4.152122	-2.114850	0.823074
C	-4.923824	-3.014291	1.784757
H	-5.509706	-2.415368	2.487354

H	-5.605930	-3.654714	1.219283
H	-4.237749	-3.649697	2.351209
C	-5.085965	-1.152346	0.090338
H	-5.612839	-0.515364	0.806588
H	-4.539948	-0.523529	-0.612947
H	-5.829175	-1.733406	-0.463155
C	-3.273586	-2.932580	-0.124481
H	-2.709940	-2.291119	-0.801525
H	-2.572758	-3.550742	0.444145
H	-3.910152	-3.594439	-0.718762
C	5.700466	1.126121	-0.128726
H	6.219632	1.582584	0.709874
H	6.315450	0.330829	-0.550713
H	5.498380	1.881489	-0.887179
H	0.135569	-1.529975	1.221447
H	-0.330270	1.009557	1.050245
H	0.044771	3.958181	-1.367909

Vibrational frequencies

-146.0402	15.6304	21.2011
27.5909	34.6261	45.9118
48.2865	52.4819	53.7113
56.5296	74.4059	86.6321
92.7481	112.0717	116.8073
125.2491	127.4915	130.5261
144.5864	150.5744	160.6235
166.6601	174.0304	187.4549
189.8755	208.8206	216.3557
223.8738	241.9577	244.5736
250.6051	252.2756	257.0352
260.0609	280.7116	283.2363

286.9903	299.5950	303.7053
317.9947	321.1394	332.8563
347.7663	354.9517	358.2164
361.3212	362.3570	370.6667
373.2608	386.5471	406.2826
408.8529	410.7443	438.5937
439.4086	446.5596	456.6246
462.0030	476.9974	479.3798
488.8679	503.9216	526.1209
533.6672	544.7745	552.5184
570.7943	574.5361	585.5978
595.0538	599.7680	618.3372
641.2309	658.6704	666.8823
681.0466	692.0218	699.7852
752.2357	759.0775	760.9345
762.6238	780.3091	786.1988
798.7384	805.9302	824.9113
836.3669	849.8146	855.9816
868.6220	880.3333	891.2169
901.2036	915.4292	935.2267
936.2930	940.8093	946.3457
949.2839	951.5637	972.9053
979.2956	983.1667	986.3447
987.3091	1003.3512	1008.7812
1009.6379	1020.2110	1024.7770
1050.6636	1056.4303	1060.5244
1060.9109	1068.0347	1074.6134
1084.3094	1086.3800	1103.1201
1125.7676	1129.4575	1134.9331
1148.9144	1178.7785	1183.9988
1190.9294	1192.3156	1202.4201

1206.4035	1213.4579	1215.5379
1242.2572	1248.2827	1254.8017
1256.0292	1269.5324	1277.9667
1278.2504	1279.4938	1290.3420
1294.1892	1313.0537	1317.8669
1319.3396	1324.6681	1346.6419
1351.4418	1360.6906	1381.9492
1395.7357	1410.0537	1411.2376
1412.7958	1413.8820	1415.8453
1418.1357	1419.0987	1421.1664
1425.1979	1439.8861	1442.9001
1449.0922	1450.4515	1467.9415
1468.6808	1471.3581	1479.3355
1479.7975	1480.5538	1491.9944
1495.2454	1495.3848	1495.6691
1495.7844	1499.6568	1502.2636
1502.4240	1508.0030	1511.5293
1513.2737	1518.5214	1524.2531
1530.0851	1531.4886	1531.8690
1536.4618	1554.3814	1571.4224
1583.4299	1601.0704	1613.1372
1631.5213	1647.0808	1672.1818
1679.5248	1696.4975	1762.7502
2624.0273	3024.8035	3037.9229
3040.3531	3042.9855	3051.9979
3055.2921	3058.3049	3063.7874
3065.0292	3070.3952	3076.0061
3096.7911	3100.4987	3110.4757
3113.9087	3117.1122	3120.6834
3122.4287	3126.4671	3129.1166
3130.3465	3136.1758	3137.8024

3141.3548	3144.1772	3165.0090
3170.7464	3183.4303	3184.3700
3187.7402	3193.0769	3197.4417
3209.4025	3209.6424	3213.5177
3218.8397	3266.9993	3482.1548
3542.1303	3562.1632	3699.7657

## M1

Zero-point correction= 0.701275

Thermal correction to Energy= 0.741591

Thermal correction to Enthalpy= 0.742535

Thermal correction to Gibbs Free Energy= 0.627788

Sum of electronic and zero-point Energies= -1821.595071

Sum of electronic and thermal Energies= -1821.554756

Sum of electronic and thermal Enthalpies= -1821.553811

Sum of electronic and thermal Free Energies= -1821.668558

## Cartesian coordinates

C	2.334236	2.960649	-2.029088
C	1.000376	2.607935	-2.358777
C	0.250293	2.029564	-1.284465
C	0.822465	1.790795	-0.039777
C	2.151100	2.172644	0.219144
N	2.855447	2.744057	-0.804004
H	2.981834	3.400135	-2.774946
C	0.041608	1.069827	1.016495
C	-0.865769	1.781565	1.859454
C	0.207314	-0.295773	1.181320
C	-1.082880	3.181966	1.733671
C	-1.595515	1.056583	2.860279
C	-0.487091	-0.999479	2.198022

C	-1.986664	3.828604	2.546784
H	-0.533270	3.738435	0.982119
C	-2.518117	1.757285	3.682838
C	-1.374281	-0.338062	3.010688
H	-0.326729	-2.068692	2.296997
C	-2.712317	3.111468	3.529466
H	-2.145548	4.896575	2.435123
H	-3.068752	1.202279	4.436922
H	-1.923394	-0.877360	3.776728
H	-3.421490	3.635505	4.162474
C	-1.155417	1.590429	-1.627458
O	-1.834137	2.468961	-2.445410
O	0.508568	2.761799	-3.531911
H	-1.142207	2.768982	-3.100081
C	2.823198	1.984007	1.549283
H	2.120893	1.548660	2.257387
H	3.687573	1.315314	1.481903
H	3.172041	2.934945	1.963662
C	1.093787	-1.075317	0.255960
O	0.915590	-1.101715	-0.978224
N	2.092129	-1.744489	0.852963
H	2.151480	-1.685650	1.860594
C	2.946949	-2.720568	0.176346
C	2.851559	-4.044693	0.956962
H	3.398696	-4.827287	0.418479
H	3.307225	-3.942027	1.946826
O	1.498947	-4.422924	1.194587
H	1.079320	-4.578313	0.336748
C	4.387034	-2.166404	-0.057841
C	5.233650	-3.227316	-0.787570
H	5.443726	-4.093656	-0.153561

H	4.730359	-3.580846	-1.694437
H	6.195544	-2.797188	-1.084270
C	5.068270	-1.785049	1.270175
H	6.062395	-1.371259	1.073291
H	4.497486	-1.023786	1.812332
H	5.196541	-2.648654	1.929936
C	4.286424	-0.913766	-0.951995
H	3.674444	-0.137762	-0.484205
H	5.283307	-0.498068	-1.131676
H	3.834676	-1.150851	-1.920234
C	-2.916330	-0.996622	-1.438556
O	-2.332962	-1.003059	-0.370850
O	-4.124890	-1.467655	-1.701335
C	-2.296060	-0.410699	-2.700327
H	-2.123484	-1.203612	-3.430681
H	-2.951123	0.340237	-3.144579
N	-1.000687	0.232304	-2.361331
H	-0.485415	0.443687	-3.222579
C	-4.965973	-2.088872	-0.632182
C	-6.235860	-2.459261	-1.393812
H	-6.009572	-3.158928	-2.202973
H	-6.947462	-2.932873	-0.712415
H	-6.702676	-1.567633	-1.821114
C	-4.258311	-3.330804	-0.090853
H	-4.003361	-4.010022	-0.909409
H	-3.349278	-3.064840	0.448714
H	-4.932555	-3.854527	0.592949
C	-5.250012	-1.048703	0.452113
H	-4.344263	-0.783054	0.997831
H	-5.678161	-0.145368	0.008353
H	-5.976225	-1.461652	1.158236



C	4.265932	3.134853	-0.578711
H	4.667428	3.546961	-1.500714
H	4.316860	3.886621	0.208876
H	4.844612	2.256935	-0.291165
H	-1.752952	1.369763	-0.744642
H	-0.380702	-0.390520	-1.768802
H	2.493441	-2.877700	-0.807787

Vibrational frequencies

13.7854	23.1432	24.3112
31.6821	34.8381	40.7974
43.5856	49.2055	60.3176
66.1922	68.3856	76.7529
88.3720	100.4323	106.7396
115.6136	119.1857	124.1317
135.3117	146.3397	148.2193
167.7826	180.1110	191.8681
211.7616	219.8861	231.0822
233.6842	244.6352	246.8889
251.6672	265.6605	274.5902
285.4218	287.1297	292.6001
295.9804	306.0266	309.5812
320.0934	327.8176	334.9706
336.8428	344.5622	349.1788
362.6069	363.8698	381.2348
385.8448	387.6032	406.5668
408.7928	415.7524	439.8608
440.9087	450.0213	459.9179
475.7877	483.1814	487.5328
521.4904	529.2741	537.6614
539.5246	551.1314	560.2578

574.3732	584.3858	593.1397
599.1767	606.4680	622.6173
644.9414	665.6329	676.0640
700.5942	710.8042	741.0280
752.3702	754.7692	770.3618
784.7095	789.7497	793.9166
806.2906	813.6938	824.1782
844.5169	853.4561	855.5542
882.3265	890.6618	897.8966
903.7002	904.9182	931.4292
933.9637	938.9058	944.1804
949.0781	950.0080	972.9540
974.4947	979.0746	986.5984
996.8336	1002.5423	1008.6427
1014.1776	1024.1106	1030.9704
1050.2173	1056.5778	1058.9889
1065.2310	1066.6163	1070.0090
1072.4885	1079.7157	1098.6384
1123.6936	1128.7728	1133.3897
1147.5493	1169.9880	1181.4307
1189.1285	1190.0547	1194.0561
1197.5267	1212.3885	1246.6741
1249.0723	1251.9792	1260.1159
1264.4590	1270.4302	1276.3407
1277.4660	1279.9678	1294.7384
1295.0632	1317.9022	1323.5375
1326.4161	1354.0223	1359.3148
1367.8530	1392.5754	1403.8757
1407.1505	1407.6656	1413.2319
1414.0512	1416.8176	1417.0417
1420.5199	1429.6574	1431.2246

1433.9377	1439.3693	1450.8705
1452.7493	1457.8752	1469.0060
1469.4912	1480.1413	1481.3459
1483.4358	1484.5896	1491.6240
1496.0506	1496.3442	1496.7850
1501.2475	1504.0590	1504.5190
1507.0416	1509.3863	1513.9576
1514.1984	1515.9144	1520.1118
1523.0865	1532.6034	1533.4376
1534.8882	1553.5657	1573.6750
1581.0155	1582.6414	1616.7772
1648.0442	1649.8133	1661.6051
1672.3761	1680.1398	1791.7852
2841.0284	3037.5890	3041.9297
3046.6658	3050.0790	3054.9704
3055.5752	3058.9675	3063.9081
3078.3891	3095.2947	3105.2470
3109.4193	3110.5427	3111.0668
3112.0891	3117.3190	3118.6240
3120.4558	3130.2466	3131.3116
3131.5311	3136.1267	3141.8060
3160.9640	3165.1048	3166.9911
3168.9742	3178.4155	3181.0840
3186.0355	3189.5227	3195.2009
3205.1799	3206.3336	3206.9985
3209.4458	3216.0029	3254.5805
3446.6284	3622.0602	3802.9963

**TS1'**

Zero-point correction= 0.698654

Thermal correction to Energy= 0.739028

Thermal correction to Enthalpy= 0.739973

Thermal correction to Gibbs Free Energy= 0.626507

Sum of electronic and zero-point Energies= -1821.586522

Sum of electronic and thermal Energies= -1821.546148

Sum of electronic and thermal Enthalpies= -1821.545204

Sum of electronic and thermal Free Energies= -1821.658669

#### Cartesian coordinates

C	1.152219	-1.606195	1.883350
C	0.888966	-1.612052	0.521501
C	0.238908	-0.493079	-0.048289
C	-0.150646	0.555447	0.790251
C	0.115578	0.512909	2.168334
N	0.782531	-0.564689	2.662355
H	1.660349	-2.434863	2.353468
C	-0.860637	1.743252	0.223299
C	-0.124861	2.928364	-0.080168
C	-2.220773	1.674187	-0.046741
C	1.267942	3.055240	0.191052
C	-0.814230	4.034609	-0.677979
C	-2.889526	2.770662	-0.647506
C	1.939449	4.217475	-0.118305
H	1.808470	2.221711	0.627556
C	-0.087848	5.218097	-0.982496
C	-2.201574	3.920968	-0.953527
H	-3.955003	2.700896	-0.841169
C	1.257919	5.309479	-0.710486
H	3.001154	4.297263	0.092771
H	-0.616944	6.050654	-1.436983
H	-2.718478	4.762470	-1.404931

H	1.802578	6.217381	-0.948936
C	-0.059163	-0.514381	-1.513161
O	0.116529	-1.553139	-2.175176
O	1.283201	-2.670579	-0.192717
H	0.927340	-2.524778	-1.115769
C	-0.342653	1.619687	3.070636
H	-1.365728	1.880110	2.793743
H	-0.334802	1.352253	4.124177
H	0.285451	2.506018	2.933964
C	-2.993005	0.451032	0.376339
O	-2.903334	0.027905	1.540524
N	-3.758205	-0.108513	-0.581427
H	-3.726910	0.328071	-1.491935
C	-4.605593	-1.312932	-0.488148
C	-5.219654	-1.508044	0.917220
H	-6.067623	-2.189474	0.811441
H	-4.494027	-1.973404	1.589508
O	-5.724540	-0.303492	1.474099
H	-4.949900	0.135587	1.858720
C	-3.863216	-2.578445	-1.036764
C	-2.630217	-2.928576	-0.182386
H	-1.963961	-2.071221	-0.075135
H	-2.905227	-3.262768	0.821683
H	-2.061706	-3.734032	-0.657983
C	-3.409144	-2.305571	-2.485370
H	-2.978270	-3.212913	-2.920502
H	-4.251550	-1.998043	-3.115476
H	-2.639057	-1.531140	-2.533008
C	-4.840168	-3.771464	-1.046885
H	-5.754625	-3.533020	-1.601794
H	-4.369838	-4.633069	-1.531520

H	-5.123864	-4.079507	-0.036408
C	3.563836	-0.335253	-1.023383
O	3.325919	0.299951	-0.009607
O	4.471561	-1.296504	-1.162699
C	2.841657	-0.109053	-2.343364
H	3.583896	0.238767	-3.074482
H	2.465011	-1.072077	-2.708278
N	1.725531	0.805810	-2.158042
H	1.405417	1.174646	-3.048994
C	5.365588	-1.711722	-0.048950
C	6.172097	-2.842205	-0.684776
H	6.717514	-2.479541	-1.560355
H	6.892943	-3.234260	0.037724
H	5.512279	-3.656779	-0.996219
C	6.262794	-0.537241	0.340358
H	6.809522	-0.170150	-0.532936
H	5.677166	0.279170	0.764483
H	6.989450	-0.871958	1.086347
C	4.526088	-2.225525	1.121495
H	4.002798	-1.408500	1.618253
H	3.792798	-2.954151	0.765065
H	5.181861	-2.714956	1.847278
C	1.126412	-0.643875	4.104201
H	1.752962	-1.517628	4.262281
H	1.674873	0.250892	4.394735
H	0.213377	-0.739548	4.691981
H	-0.666531	0.305963	-1.904242
H	1.983152	1.586695	-1.559697
H	-5.439278	-1.106926	-1.170145

Vibrational frequencies

-109.7496	18.7565	24.7697
28.0356	37.8064	42.5485
43.7446	48.5903	57.7163
61.8697	69.4500	85.4090
89.3586	93.4122	97.1836
105.4922	110.4743	121.3437
126.6170	147.8548	151.6129
166.4756	174.5409	177.4294
191.1795	199.3576	216.4641
225.2476	226.8000	231.5035
237.9581	252.7490	255.8467
263.6254	267.4478	278.9292
292.0283	294.1674	300.2287
309.7285	316.2157	329.5885
331.5658	338.7715	346.8132
358.5135	360.6863	361.6891
371.6731	375.5759	398.6443
401.4194	411.4957	419.6060
441.4348	445.3581	456.3273
461.7209	468.7868	470.6495
490.7613	509.4407	513.1714
525.1889	533.0014	543.0164
551.0953	568.8766	572.0202
591.9997	595.3245	601.5932
628.7983	643.2058	651.2802
663.4181	678.9403	696.6540
701.4036	752.7216	760.1385
760.5998	772.4761	781.2825
797.8158	801.1760	812.1908
827.1458	849.7823	851.9163
865.5574	867.2438	872.1279

879.2165	897.5093	902.0296
928.5461	930.8615	935.0197
939.8919	941.9426	944.5852
946.7483	955.5643	973.7030
981.7580	988.1384	993.5043
1017.2414	1023.4003	1028.9607
1030.8397	1043.6162	1051.2531
1056.8632	1059.4587	1065.4720
1071.3730	1072.3512	1083.5795
1090.8920	1115.5041	1117.4442
1132.6758	1135.6588	1147.5515
1183.5768	1189.2648	1196.3675
1198.8310	1205.7860	1211.8795
1217.7610	1247.4244	1252.4183
1254.7892	1263.0265	1267.9069
1271.5616	1278.9329	1285.0309
1291.6207	1299.0291	1304.7985
1326.6998	1329.6238	1343.6271
1358.6687	1373.9394	1388.0710
1399.8627	1409.2938	1414.2437
1415.4411	1415.6252	1416.2487
1418.4144	1419.0067	1429.9514
1431.2308	1438.5908	1439.8480
1441.8678	1450.2565	1458.2142
1468.8569	1473.5269	1476.2463
1480.1450	1489.4113	1492.1362
1494.0705	1494.7596	1495.4610
1498.2969	1502.0818	1502.7715
1504.6657	1508.8438	1511.2230
1515.4483	1516.2280	1521.2874
1523.3136	1532.2459	1533.1900



1537.7727	1554.9193	1583.3011
1612.6822	1615.8042	1627.2083
1642.2137	1645.2966	1671.9867
1698.6154	1701.1815	1775.9488
3034.4452	3036.1263	3040.7857
3045.5296	3053.6371	3057.5729
3058.1838	3063.1580	3068.6777
3071.5580	3079.8801	3095.4381
3105.4266	3108.8452	3109.8160
3114.7879	3121.7947	3126.2491
3129.5910	3131.9747	3132.0223
3134.6177	3139.5690	3142.6740
3159.7079	3161.4509	3164.8323
3166.0330	3186.5945	3188.8101
3193.1587	3196.9752	3197.5541
3208.4786	3209.1219	3210.1341
3216.9641	3273.0997	3509.3053
3603.4859	3631.7604	3749.1859

### **M1'**

Zero-point correction= 0.702202

Thermal correction to Energy= 0.742080

Thermal correction to Enthalpy= 0.743024

Thermal correction to Gibbs Free Energy= 0.631352

Sum of electronic and zero-point Energies= -1821.584163

Sum of electronic and thermal Energies= -1821.544285

Sum of electronic and thermal Enthalpies= -1821.543341

Sum of electronic and thermal Free Energies= -1821.655013

Cartesian coordinates

C	1.013850	-1.811060	1.731978
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C	0.983974	-1.609327	0.333832
C	0.372637	-0.386491	-0.093514
C	-0.155057	0.514367	0.830347
C	-0.059348	0.264739	2.209110
N	0.525928	-0.901744	2.601869
H	1.448604	-2.711221	2.141774
C	-0.850937	1.748476	0.344010
C	-0.094010	2.923698	0.051422
C	-2.214196	1.716826	0.083549
C	1.306328	3.005804	0.301569
C	-0.759099	4.055561	-0.525726
C	-2.864034	2.844684	-0.481384
C	2.012765	4.142286	-0.029400
H	1.818258	2.167472	0.761011
C	0.000472	5.214506	-0.841493
C	-2.153863	3.983974	-0.777111
H	-3.931999	2.800291	-0.669198
C	1.356424	5.256451	-0.607100
H	3.080200	4.186083	0.162374
H	-0.510063	6.067707	-1.278682
H	-2.655760	4.844294	-1.209690
H	1.926461	6.144660	-0.859903
C	0.281308	-0.155612	-1.588001
O	0.180163	-1.298499	-2.324577
O	1.476149	-2.463113	-0.492355
H	0.683629	-1.995121	-1.783333
C	-0.600335	1.198821	3.249296
H	-0.917965	2.127336	2.778792
H	-1.476098	0.764545	3.740672
H	0.145734	1.440491	4.010975
C	-3.014307	0.485086	0.429632

O	-3.012749	0.031103	1.584493
N	-3.712705	-0.041122	-0.596838
H	-3.610753	0.421170	-1.489422
C	-4.534047	-1.266357	-0.614420
C	-5.217293	-1.553157	0.741711
H	-6.039515	-2.248445	0.553894
H	-4.516329	-2.036994	1.427463
O	-5.785365	-0.394601	1.334323
H	-5.039555	0.045510	1.772685
C	-3.729778	-2.481344	-1.188932
C	-2.514835	-2.826067	-0.307646
H	-1.862595	-1.961080	-0.176060
H	-2.810047	-3.181551	0.683469
H	-1.922933	-3.615646	-0.781821
C	-3.231121	-2.128436	-2.605375
H	-2.768585	-3.005945	-3.068719
H	-4.056363	-1.804505	-3.250135
H	-2.469725	-1.344092	-2.585178
C	-4.664341	-3.703765	-1.288197
H	-5.568702	-3.469233	-1.861315
H	-4.149323	-4.524745	-1.797349
H	-4.969369	-4.070576	-0.303829
C	3.565260	-0.286825	-0.978470
O	3.321342	0.413820	-0.011720
O	4.493153	-1.215604	-1.096060
C	2.808196	-0.147250	-2.291809
H	3.440931	0.366260	-3.018978
H	2.530907	-1.119185	-2.693507
N	1.568994	0.657585	-2.086990
H	1.305710	1.086647	-2.976878
C	5.359769	-1.615528	0.055032

C	6.189917	-2.746241	-0.546442
H	6.764492	-2.388052	-1.404999
H	6.886486	-3.128794	0.204300
H	5.544097	-3.565815	-0.873075
C	6.235038	-0.431956	0.461785
H	6.807758	-0.067877	-0.395899
H	5.632943	0.383935	0.862754
H	6.939566	-0.758727	1.232127
C	4.468934	-2.122590	1.189175
H	3.927355	-1.304400	1.664743
H	3.743189	-2.839739	0.797393
H	5.091776	-2.615510	1.940824
C	0.635635	-1.206779	4.046917
H	1.060980	-2.199957	4.165057
H	1.285548	-0.473025	4.524547
H	-0.353358	-1.176727	4.503392
H	-0.524410	0.534190	-1.841463
H	1.764083	1.422981	-1.425025
H	-5.335749	-1.043459	-1.328973

#### Vibrational frequencies

23.1829	27.8185	32.0120
38.4653	49.1980	50.3966
55.6964	58.0767	64.0499
72.0707	81.0089	88.1164
92.2182	100.9803	108.6423
111.8027	130.5348	135.6617
140.0918	154.9545	163.0312
171.9471	182.0362	186.9137
212.7617	223.2169	237.7551
239.0141	243.7586	249.0377

255.1823	266.7560	269.7336
280.0596	280.9637	296.7507
301.5238	305.1042	310.0552
326.9290	331.4358	337.9327
339.1433	347.6446	357.6130
360.3659	367.1965	368.7873
389.0834	400.0276	410.1150
414.9865	439.3282	442.8069
453.2270	458.8235	466.5003
467.8604	476.1482	497.0592
519.2748	524.9243	537.9126
542.7415	557.4306	571.5436
582.5920	589.2117	598.4789
620.6638	624.3216	640.4813
646.2480	656.1136	674.9345
689.4479	698.1991	711.7287
752.9874	759.2436	769.4554
772.2537	781.4976	792.1866
802.3278	806.1113	826.8770
840.7887	849.6924	852.6736
867.3181	875.3214	895.9588
898.7306	908.9578	927.2182
940.8782	941.8905	944.5322
947.7060	955.7128	977.3672
980.1110	982.5558	991.1146
991.2151	998.1387	1013.2445
1014.3448	1019.3582	1030.7148
1043.0830	1045.7057	1055.5590
1058.0072	1067.4693	1073.8189
1074.2983	1084.4873	1090.5786
1117.3947	1131.1820	1135.7764

1148.8523	1178.6653	1189.7529
1191.1427	1195.0974	1199.5800
1212.4958	1214.0900	1246.5960
1248.1558	1252.2155	1253.6356
1261.1500	1268.9082	1275.1017
1281.3887	1289.3129	1295.1905
1296.1994	1318.6152	1324.9676
1332.0651	1344.3138	1345.5669
1366.8185	1383.1243	1399.1714
1401.9019	1410.1744	1414.8944
1417.2168	1418.1658	1418.6903
1425.0127	1428.8670	1430.2278
1431.9059	1436.7958	1440.2377
1445.1549	1450.5370	1451.2842
1469.0699	1477.3767	1480.6161
1481.5091	1482.6547	1489.0365
1489.7685	1493.9135	1495.5404
1498.9834	1500.7606	1502.9952
1504.2362	1507.5674	1508.0847
1511.3784	1517.0577	1517.2213
1521.9732	1531.6855	1535.9842
1538.1232	1553.2365	1581.4768
1585.6246	1591.1865	1609.5948
1613.5430	1643.9317	1656.1088
1670.7912	1704.2167	1786.0882
2871.9673	3034.6720	3039.1653
3045.6401	3055.4077	3055.7936
3059.9377	3062.4188	3065.2270
3069.8116	3094.3153	3103.3168
3107.5782	3113.2732	3113.8835
3119.6094	3124.2705	3126.2752

3130.9670	3131.2714	3133.5298
3136.0311	3138.3603	3143.4190
3155.1350	3161.5151	3165.2477
3178.3852	3180.6190	3188.8844
3192.6915	3197.1462	3199.0315
3204.4849	3209.2218	3212.3000
3221.4334	3260.9643	3356.5151
3504.1800	3629.8412	3736.9140

## TS2

Zero-point correction= 0.726316

Thermal correction to Energy= 0.769900

Thermal correction to Enthalpy= 0.770844

Thermal correction to Gibbs Free Energy= 0.649913

Sum of electronic and zero-point Energies= -2086.151418

Sum of electronic and thermal Energies= -2086.107834

Sum of electronic and thermal Enthalpies= -2086.106890

Sum of electronic and thermal Free Energies= -2086.227822

## Cartesian coordinates

C	0.516880	1.999027	3.423232
C	1.405801	1.546779	2.416598
C	0.843519	1.480764	1.097666
C	-0.489028	1.822357	0.873307
C	-1.314156	2.264107	1.921237
N	-0.769496	2.324609	3.169586
H	0.856100	2.079007	4.446709
C	-1.039343	1.760497	-0.522725
C	-0.833663	2.901144	-1.366626
C	-1.708536	0.643729	-1.018044
C	-0.182009	4.079752	-0.903951

C	-1.291562	2.865493	-2.724426
C	-2.132591	0.618541	-2.377002
C	0.001799	5.159512	-1.738652
H	0.175191	4.121810	0.118268
C	-1.083919	3.994816	-3.559928
C	-1.926651	1.691415	-3.204352
H	-2.561730	-0.289170	-2.783687
C	-0.452461	5.119506	-3.079048
H	0.500245	6.049341	-1.367025
H	-1.433315	3.953466	-4.587581
H	-2.239817	1.647901	-4.243220
H	-0.299226	5.978103	-3.725352
C	1.713693	0.916214	-0.018523
O	3.065112	1.207261	0.155742
O	2.616624	1.215876	2.687593
H	3.195031	1.197401	1.148904
C	-2.753117	2.651637	1.737507
H	-3.026691	2.573510	0.686850
H	-3.423913	1.997802	2.304756
H	-2.942749	3.681061	2.057902
C	-1.985722	-0.536039	-0.126819
O	-1.264200	-0.810763	0.845471
N	-3.067063	-1.286837	-0.446375
H	-3.693562	-0.960129	-1.167651
C	-3.436300	-2.500207	0.282429
C	-3.701895	-3.630680	-0.724654
H	-4.031610	-4.522972	-0.180944
H	-4.505332	-3.350394	-1.413510
O	-2.568743	-3.953870	-1.530344
H	-1.735138	-3.808366	-1.030160
C	-4.604257	-2.257188	1.297030



C	-4.733294	-3.478410	2.229763
H	-5.038297	-4.382633	1.695420
H	-3.785818	-3.686980	2.738970
H	-5.489446	-3.283060	2.997032
C	-5.941710	-2.013840	0.572604
H	-6.720991	-1.766637	1.300838
H	-5.873648	-1.175072	-0.129157
H	-6.278078	-2.896116	0.019397
C	-4.268810	-1.021719	2.156938
H	-4.263442	-0.110752	1.552450
H	-5.020781	-0.896936	2.942710
H	-3.285775	-1.118773	2.626568
C	3.773263	-1.440879	-0.122730
O	3.861538	-1.475287	-1.335056
O	4.786161	-1.488319	0.749968
C	2.446451	-1.401825	0.621453
H	2.045347	-2.420322	0.638419
H	2.595939	-1.055359	1.645970
N	1.470493	-0.580139	-0.107695
H	0.541523	-0.770628	0.293177
C	6.198131	-1.526637	0.307298
C	6.958912	-1.534034	1.632757
H	6.686585	-2.410672	2.227404
H	8.035705	-1.561877	1.444234
H	6.729163	-0.634958	2.211620
C	6.459160	-2.810066	-0.483053
H	6.161330	-3.683210	0.105258
H	5.907498	-2.810348	-1.423152
H	7.528668	-2.890490	-0.699597
C	6.512103	-0.263580	-0.497242
H	5.981854	-0.262258	-1.449476

H	6.218588	0.624383	0.069963
H	7.588071	-0.214335	-0.689045
C	-1.606576	2.764974	4.307122
H	-1.013098	2.725860	5.217119
H	-1.947325	3.787307	4.140172
H	-2.467361	2.103417	4.407025
H	1.400032	1.318577	-0.985221
H	1.261136	-1.010021	-1.382210
C	-0.095795	-2.228057	-2.124028
O	0.781442	-1.313531	-2.389685
O	-1.027786	-2.363071	-3.089635
H	-1.727992	-2.964138	-2.735116
O	-0.122696	-2.913826	-1.085493
H	-2.549941	-2.764144	0.867047

Vibrational frequencies

-563.7370	15.8300	21.1550
27.7392	32.4439	35.6348
42.2360	45.6900	52.2487
59.5575	62.5002	66.8777
80.8457	91.2788	94.2870
100.1266	112.5369	119.0337
119.6339	133.1947	140.3793
143.9506	145.9917	157.8473
160.4300	173.9726	184.1094
189.2867	194.4617	218.1945
221.8413	224.0297	226.5842
240.0335	249.7077	258.0126
259.1514	272.5835	278.1552
283.4908	287.7732	288.6638
298.4321	311.8313	318.2093

322.2597	331.0377	336.3124
343.9131	348.7638	361.4349
363.5006	381.0890	381.6461
389.4907	403.0880	406.3252
411.8462	426.9558	439.9094
441.8372	467.3968	468.9349
480.2424	486.5829	487.1247
515.4485	523.0476	534.5857
547.7448	557.1433	564.9574
574.9334	582.6014	586.9237
600.6287	619.8708	625.1908
641.3652	665.0781	666.0296
680.0475	687.0847	689.7766
732.9340	751.5239	756.8802
762.3902	775.5257	785.1238
788.1659	793.8805	801.1430
806.9955	812.3301	822.2230
832.5594	841.1769	845.5274
866.8157	871.0094	892.2828
895.1356	912.6281	919.0012
926.1452	937.4174	937.9334
943.5117	947.1782	950.0243
950.9195	965.2178	972.6662
980.4415	983.0922	985.3895
1008.7256	1019.2448	1029.3947
1033.2444	1034.6610	1053.6656
1056.6107	1059.8694	1064.5549
1068.6228	1080.3132	1083.9422
1105.8984	1111.0288	1124.9329
1133.9078	1140.2113	1142.6889
1149.1739	1176.1511	1184.6005

1190.7374	1196.4908	1205.2528
1210.2933	1216.3306	1246.6466
1250.5707	1256.0102	1267.1883
1268.6911	1271.3705	1273.6820
1276.8308	1283.9530	1290.6155
1292.8666	1310.3819	1323.2309
1339.1457	1349.5304	1357.9299
1372.6927	1375.6481	1391.8043
1401.4891	1407.3898	1411.3549
1412.0018	1414.9123	1417.1033
1420.2952	1421.6861	1429.7573
1433.6512	1437.8495	1445.5771
1449.6642	1453.4105	1467.4328
1469.6308	1478.7589	1480.1170
1483.0003	1484.1440	1485.3167
1491.0384	1493.0880	1494.5921
1495.1779	1496.0879	1502.6857
1502.9730	1505.0618	1509.6239
1511.7068	1515.1004	1519.8882
1522.1633	1525.0083	1526.5087
1531.8139	1531.9167	1543.7650
1554.6117	1563.2749	1579.1001
1583.1533	1609.7279	1642.0271
1647.8481	1670.1258	1693.9441
1723.1314	1763.8646	1795.5141
3037.6460	3040.1714	3047.9812
3051.0185	3051.1756	3052.4476
3054.7705	3060.8957	3074.3981
3079.7075	3084.8762	3091.3870
3100.5171	3107.3131	3107.6643
3108.9410	3116.1866	3119.7280

3121.3433	3123.7506	3124.1290
3127.8268	3130.9222	3131.3051
3136.5121	3138.7848	3164.2656
3167.3920	3174.6454	3175.4575
3186.1470	3193.5455	3196.4399
3201.8982	3209.7139	3223.1089
3228.3609	3252.4778	3319.8841
3387.9686	3517.9326	3639.6199

## M2

Zero-point correction= 0.727231

Thermal correction to Energy= 0.771516

Thermal correction to Enthalpy= 0.772460

Thermal correction to Gibbs Free Energy= 0.648993

Sum of electronic and zero-point Energies= -2086.138119

Sum of electronic and thermal Energies= -2086.093834

Sum of electronic and thermal Enthalpies= -2086.092890

Sum of electronic and thermal Free Energies= -2086.216357

## Cartesian coordinates

C	0.330594	-0.768424	3.732770
C	1.284951	-0.482706	2.724861
C	0.799206	0.323344	1.638802
C	-0.526791	0.755374	1.614808
C	-1.414808	0.447675	2.661724
N	-0.942550	-0.320670	3.684477
H	0.610838	-1.374773	4.583106
C	-1.032201	1.560951	0.452839
C	-0.790556	2.972021	0.414869
C	-1.751701	0.961123	-0.571913
C	-0.085968	3.649139	1.449147

C	-1.263733	3.734430	-0.703800
C	-2.229011	1.729112	-1.667938
C	0.146182	5.004640	1.374143
H	0.274630	3.083651	2.301315
C	-1.005847	5.130535	-0.750121
C	-1.978632	3.075991	-1.738549
H	-2.749676	1.225581	-2.474731
C	-0.315770	5.753943	0.264877
H	0.687974	5.504126	2.171265
H	-1.364928	5.697933	-1.604045
H	-2.321660	3.652760	-2.592110
H	-0.123916	6.821394	0.218913
C	1.754164	0.653222	0.494473
O	3.082939	0.738204	0.921135
O	2.485269	-0.930263	2.795185
H	3.156869	0.061495	1.653155
C	-2.830975	0.943852	2.730260
H	-3.062940	1.536966	1.848054
H	-3.551671	0.122828	2.780888
H	-2.989857	1.578166	3.609046
C	-2.024085	-0.515103	-0.557112
O	-1.126189	-1.353448	-0.352765
N	-3.305649	-0.875636	-0.770996
H	-3.988254	-0.150035	-0.935652
C	-3.734251	-2.278571	-0.795998
C	-3.558408	-2.859906	-2.212845
H	-3.724293	-3.945059	-2.166754
H	-4.304894	-2.438731	-2.895031
O	-2.286899	-2.564828	-2.776132
H	-1.635467	-2.522683	-2.058696
C	-5.152538	-2.449542	-0.174192

C	-5.499126	-3.951745	-0.118233
H	-5.646830	-4.378562	-1.114157
H	-4.711154	-4.522292	0.385489
H	-6.428726	-4.096799	0.441053
C	-6.240381	-1.711935	-0.981308
H	-7.213768	-1.853566	-0.501030
H	-6.065940	-0.631157	-1.030087
H	-6.319595	-2.088315	-2.004887
C	-5.132367	-1.896742	1.265423
H	-4.955516	-0.818156	1.279040
H	-6.093656	-2.082549	1.754688
H	-4.349007	-2.376908	1.862770
C	3.877049	-1.261071	-0.848670
O	4.199199	-0.608530	-1.823498
O	4.709308	-1.871480	0.004377
C	2.429058	-1.542501	-0.465379
H	2.049522	-2.294231	-1.165335
H	2.386514	-1.953495	0.546514
N	1.612054	-0.334197	-0.628475
H	0.628613	-0.624930	-0.685296
C	6.177462	-1.726522	-0.095851
C	6.669785	-2.529213	1.108126
H	6.348644	-3.572002	1.031828
H	7.762049	-2.503240	1.152864
H	6.271575	-2.109401	2.036283
C	6.672575	-2.340957	-1.406393
H	6.329085	-3.376214	-1.492639
H	6.311244	-1.774335	-2.264661
H	7.766746	-2.340351	-1.416531
C	6.553479	-0.249460	0.041355
H	6.220672	0.321923	-0.824859

H	6.091567	0.172932	0.938220
H	7.639962	-0.158442	0.132140
C	-1.848937	-0.694982	4.792089
H	-1.296389	-1.294027	5.511449
H	-2.224872	0.203209	5.282258
H	-2.684843	-1.276183	4.400728
H	1.480429	1.619577	0.061980
H	1.770298	0.502942	-1.899918
C	0.565415	1.001305	-3.320065
O	1.660231	1.252031	-2.644506
O	0.287138	2.028972	-4.160307
H	-0.531992	1.788797	-4.619826
O	-0.139463	0.003984	-3.238837
H	-3.029650	-2.805128	-0.142230

Vibrational frequencies

-13.3361	17.7008	21.8304
26.2647	31.3106	31.5162
38.5012	42.3200	46.2356
52.2063	59.6792	66.6075
69.9099	81.7915	89.2028
91.0061	97.1510	109.3704
118.2367	121.9470	123.5711
125.0434	132.8626	141.8391
144.5894	150.3884	165.0475
174.2194	177.8187	198.9664
214.1728	221.1612	228.9508
239.6949	242.7209	251.1053
258.6150	260.8948	275.6045
284.9873	288.9410	289.6818
300.5972	316.5025	318.9799



325.4599	328.3002	335.9225
350.2130	353.8730	358.0196
367.0606	373.2389	386.2764
390.7200	401.1559	415.2264
418.2817	435.3150	439.5179
443.3664	460.5962	467.4343
474.4198	478.9699	482.0969
511.2488	529.0228	531.7256
536.1679	552.9144	553.2041
556.7909	557.4272	564.7760
578.8072	583.2549	597.7725
615.8183	630.0120	643.3605
661.0772	666.1774	677.9221
694.3377	740.2922	752.4473
756.8895	764.1136	764.6299
781.3741	793.9287	795.6489
797.2993	811.2887	823.6307
841.4992	846.2667	854.8116
869.3544	888.8336	890.6090
896.9037	916.9306	920.9908
934.9899	935.8371	938.6166
947.4215	948.2279	950.5839
969.9579	979.8505	981.7920
982.3989	987.5055	1005.2320
1007.5251	1015.7172	1020.0527
1033.7148	1050.0909	1054.9736
1058.8156	1059.4216	1064.1393
1069.0911	1076.4988	1083.4433
1108.0005	1113.4023	1120.8695
1129.7235	1134.8940	1147.4062
1165.3594	1179.0045	1186.8667

1193.0632	1199.1549	1207.0137
1210.9774	1211.6852	1237.1918
1246.1407	1250.7878	1256.2320
1271.2564	1273.3755	1274.6088
1276.2834	1277.2312	1285.6212
1289.4942	1292.8361	1309.2318
1324.7579	1349.1454	1349.5706
1362.2261	1379.6238	1395.5585
1402.8175	1409.2628	1410.4754
1410.8036	1413.5800	1419.2007
1420.5868	1423.3924	1424.3693
1427.8924	1431.3536	1435.9870
1448.7204	1449.0584	1460.8501
1467.2610	1478.6464	1478.8071
1481.9099	1484.3376	1487.0291
1490.8400	1494.7039	1496.0250
1496.6653	1500.3529	1500.6221
1504.2608	1507.3440	1512.5908
1513.0823	1518.0838	1521.3238
1522.0248	1527.3717	1530.1427
1532.5568	1548.2510	1553.3595
1557.5747	1576.8891	1579.5332
1603.2262	1613.4813	1638.8987
1648.0346	1670.9864	1680.3645
1773.1917	1791.5895	2135.7354
3018.1438	3038.9241	3039.6060
3046.3395	3050.8164	3054.7068
3055.1983	3060.6478	3060.8890
3066.1580	3080.3273	3081.8304
3090.5750	3104.8697	3108.5912
3113.0172	3114.6092	3123.3313

3123.6982	3124.8569	3126.8556
3128.1628	3128.3661	3130.6703
3136.5002	3156.3454	3164.4465
3167.4300	3173.7656	3180.1674
3185.2150	3193.5102	3194.9269
3202.1703	3207.6287	3216.6245
3217.2424	3249.3538	3367.7972
3641.7012	3747.5857	3799.1787

### TS3

Zero-point correction= 0.723236

Thermal correction to Energy= 0.768405

Thermal correction to Enthalpy= 0.769350

Thermal correction to Gibbs Free Energy= 0.644822

Sum of electronic and zero-point Energies= -2086.133299

Sum of electronic and thermal Energies= -2086.088129

Sum of electronic and thermal Enthalpies= -2086.087184

Sum of electronic and thermal Free Energies= -2086.211713

### Cartesian coordinates

C	-1.923944	3.994100	0.086964
C	-1.016213	3.157631	-0.630457
C	-1.252184	1.741913	-0.457072
C	-2.340557	1.285688	0.300886
C	-3.187249	2.179756	0.971304
N	-2.932343	3.516913	0.835948
H	-1.807591	5.067808	0.032493
C	-2.640901	-0.180847	0.389622
C	-3.628065	-0.752456	-0.475016
C	-1.949027	-0.990184	1.274185
C	-4.346815	0.019491	-1.428522

C	-3.898979	-2.157424	-0.386351
C	-2.211521	-2.382243	1.341634
C	-5.291799	-0.564735	-2.241864
H	-4.132258	1.078146	-1.519606
C	-4.880742	-2.728137	-1.239750
C	-3.171233	-2.949169	0.540854
H	-1.640425	-2.991337	2.034721
C	-5.564882	-1.951318	-2.146942
H	-5.829791	0.039948	-2.965577
H	-5.078180	-3.793908	-1.165202
H	-3.373711	-4.014652	0.595748
H	-6.311838	-2.398744	-2.795455
C	-0.328260	0.757584	-1.068464
O	-1.240286	0.176867	-2.503313
O	-0.092098	3.664701	-1.336934
C	-4.332805	1.745022	1.839139
H	-4.356064	0.659137	1.899308
H	-4.234091	2.130292	2.858630
H	-5.297244	2.082706	1.444617
C	-0.892444	-0.399044	2.172623
O	-1.169558	0.425473	3.051461
N	0.357629	-0.852406	1.922373
H	0.476334	-1.479224	1.129706
C	1.509943	-0.462510	2.742299
C	1.928438	0.989396	2.436867
H	1.046897	1.620364	2.603604
H	2.690965	1.296574	3.158318
O	2.474240	1.209326	1.141993
H	1.746412	1.293618	0.506352
C	2.625681	-1.549977	2.684195
C	2.067184	-2.852348	3.295423

H	1.757696	-2.702137	4.335966
H	1.201458	-3.218863	2.735103
H	2.831300	-3.636733	3.279633
C	3.825893	-1.081805	3.529976
H	4.552015	-1.895482	3.626926
H	4.341358	-0.234811	3.067265
H	3.517134	-0.785621	4.539172
C	3.115146	-1.839429	1.249304
H	3.462343	-0.930726	0.758268
H	3.943893	-2.556139	1.287462
H	2.335058	-2.286186	0.625793
C	3.292215	0.935003	-1.726858
O	3.457253	2.140289	-1.747866
O	4.231043	-0.001143	-1.597732
C	1.926302	0.285626	-1.887518
H	1.798256	0.039134	-2.952024
H	1.868577	-0.649689	-1.330938
N	0.900093	1.203291	-1.420564
H	0.946288	2.195276	-1.682472
C	5.662398	0.340215	-1.399382
C	6.301278	-1.036039	-1.220583
H	6.124437	-1.658954	-2.101882
H	7.380253	-0.928846	-1.079748
H	5.881584	-1.540281	-0.345743
C	6.191688	1.042708	-2.649824
H	6.016033	0.425257	-3.535715
H	5.708138	2.010363	-2.788444
H	7.269707	1.199432	-2.548042
C	5.821473	1.186160	-0.134355
H	5.402101	2.182878	-0.268499
H	5.314954	0.706801	0.707050

H	6.886086	1.277557	0.100760
C	-3.789828	4.493094	1.544701
H	-3.469827	5.498482	1.283072
H	-4.828882	4.352484	1.247473
H	-3.693345	4.348981	2.621294
H	-0.318125	-0.230413	-0.628564
C	-0.463877	-2.794613	-1.497735
O	-1.139804	-2.252363	-2.430094
O	-0.629411	-4.148267	-1.438639
O	0.300964	-2.244718	-0.676769
H	-1.147998	-0.945229	-2.486673
H	-0.089108	-4.453851	-0.694362
H	-0.793322	0.534244	-3.285999
H	1.148254	-0.430208	3.779346

Vibrational frequencies

-427.6390	19.1976	21.3179
30.5674	34.2784	38.4483
43.7869	48.0887	53.5321
53.8777	60.9718	68.8743
72.9811	79.2416	81.3644
95.5930	95.7592	103.5673
108.0292	109.4231	116.2192
120.6195	127.6836	138.2403
146.3116	151.7902	158.4466
164.7097	166.5876	178.5609
191.2295	203.0841	213.2957
219.5035	227.3731	234.1550
244.2889	249.5331	253.9351
268.0519	275.4517	282.5400
289.9487	301.2170	304.7085

310.3242	321.9302	333.1705
335.6944	341.3474	360.1453
365.5177	372.2244	383.8982
388.0951	403.4141	408.6117
412.0589	416.0677	431.7824
440.9448	444.2504	455.9609
463.9968	476.6896	479.5393
487.8457	494.6196	501.6320
508.0632	534.2761	535.2815
548.5234	554.7285	569.3862
579.4532	583.5440	604.4199
611.6726	615.6440	643.8668
661.3723	672.1121	688.2057
697.5693	704.1800	711.7968
741.2288	750.1735	754.2287
761.6002	767.0550	785.7915
791.2801	801.1724	805.8589
807.4545	822.1503	830.9404
842.8588	844.7779	851.8672
855.9045	871.4176	881.2701
889.5905	901.4493	922.7839
937.4392	938.5589	940.8673
953.9009	962.2786	967.1535
972.1746	972.3957	982.3758
983.7422	1000.5471	1001.7292
1016.6794	1025.9603	1028.5001
1049.3404	1055.2675	1058.1443
1064.6155	1071.2218	1075.7265
1084.6670	1090.6793	1104.5051
1126.8926	1135.9756	1139.0124
1145.2930	1145.7073	1179.0622

1187.5424	1194.1361	1195.1286
1208.4979	1223.4467	1238.9874
1244.4370	1248.1456	1252.5697
1256.3250	1260.9975	1268.6806
1278.8170	1281.4525	1293.3033
1294.0414	1295.6660	1316.1988
1319.5312	1327.4940	1338.0338
1352.4920	1356.9288	1365.6321
1388.6609	1393.2782	1405.5671
1410.7564	1412.1403	1415.9461
1416.0513	1418.0997	1422.0102
1424.7502	1426.9801	1432.6985
1438.1057	1438.6314	1445.8987
1452.1782	1463.6947	1467.7662
1477.1599	1478.9190	1480.3837
1487.8690	1493.2350	1494.9509
1496.9724	1497.2824	1500.6526
1501.2750	1502.6817	1506.5289
1506.9276	1508.8990	1512.2209
1513.9705	1521.4559	1529.4996
1531.2671	1547.5276	1552.3282
1556.8063	1578.4878	1579.2963
1593.3634	1617.6799	1647.6507
1649.7404	1652.5350	1673.9000
1719.5997	1789.6168	1800.0193
3014.8384	3026.8046	3032.7789
3036.5233	3043.9998	3047.3536
3051.2714	3053.2485	3056.6702
3064.5058	3091.2252	3102.6428
3104.2740	3106.5031	3107.6250
3111.5756	3116.0817	3117.7298



3126.1268	3134.3713	3134.7380
3140.4419	3157.7864	3160.7076
3171.1796	3175.5533	3175.9761
3182.4843	3182.7150	3188.5641
3192.1555	3201.9911	3205.9464
3206.7925	3218.2711	3231.5614
3250.7389	3347.4030	3503.4429
3728.4699	3796.2274	3800.5176

### M3

Zero-point correction= 0.699911

Thermal correction to Energy= 0.743566

Thermal correction to Enthalpy= 0.744510

Thermal correction to Gibbs Free Energy= 0.623749

Sum of electronic and zero-point Energies= -2009.710726

Sum of electronic and thermal Energies= -2009.667071

Sum of electronic and thermal Enthalpies= -2009.666126

Sum of electronic and thermal Free Energies= -2009.786888

### Cartesian coordinates

C	1.484940	-3.489569	0.593538
C	0.880262	-2.703931	-0.435761
C	1.370722	-1.348148	-0.528821
C	2.475003	-0.929658	0.254324
C	3.042390	-1.780598	1.195477
N	2.489766	-3.036674	1.346426
H	1.120690	-4.490559	0.778984
C	3.063349	0.431132	0.039023
C	4.123122	0.585334	-0.910472
C	2.559310	1.538120	0.704155
C	4.669094	-0.511499	-1.634057

C	4.662443	1.895079	-1.138525
C	3.084518	2.831993	0.452182
C	5.698112	-0.321952	-2.529159
H	4.268146	-1.506593	-1.475719
C	5.724687	2.053637	-2.069020
C	4.117345	3.002540	-0.437538
H	2.667335	3.681735	0.982687
C	6.233408	0.970787	-2.749231
H	6.103821	-1.170206	-3.071573
H	6.127449	3.048857	-2.233929
H	4.527698	3.991844	-0.617637
H	7.044886	1.103367	-3.457841
C	0.633869	-0.404050	-1.314178
O	-0.042263	-3.184777	-1.161288
C	4.172145	-1.376863	2.095597
H	4.593034	-0.433819	1.752999
H	3.813934	-1.223506	3.118769
H	4.974108	-2.118752	2.114240
C	1.427310	1.364253	1.684931
O	1.518465	0.620208	2.666017
N	0.321381	2.076254	1.369500
H	0.321581	2.549671	0.478539
C	-0.970845	1.925569	2.050405
C	-1.499274	0.498939	1.861544
H	-0.790078	-0.180947	2.347316
H	-2.457619	0.376172	2.377401
O	-1.614078	0.171567	0.482018
H	-1.778617	-0.800273	0.479188
C	-1.922042	3.093702	1.643310
C	-2.138099	3.179534	0.116872
H	-1.222502	3.451408	-0.423202

H	-2.503039	2.234633	-0.285888
H	-2.867664	3.965833	-0.105254
C	-1.316214	4.419722	2.148751
H	-1.960166	5.261310	1.872911
H	-1.214907	4.415062	3.239841
H	-0.325627	4.602432	1.720633
C	-3.291024	2.888839	2.319826
H	-3.184217	2.722125	3.397597
H	-3.911623	3.779438	2.177520
H	-3.831349	2.038470	1.894874
C	-2.733588	-0.331669	-2.216684
O	-2.965671	-1.515051	-2.062665
O	-3.578634	0.680377	-2.105973
C	-1.341437	0.165869	-2.619014
H	-1.276943	0.164415	-3.712638
H	-1.163760	1.174001	-2.247597
N	-0.368455	-0.759119	-2.062105
H	-0.590188	-1.775416	-2.035776
C	-4.983362	0.466005	-1.637536
C	-5.492438	1.897418	-1.485067
H	-5.394268	2.444600	-2.426914
H	-6.547649	1.881788	-1.199283
H	-4.929904	2.426575	-0.711946
C	-5.748451	-0.289235	-2.722365
H	-5.711929	0.255337	-3.670520
H	-5.332249	-1.287312	-2.865714
H	-6.795706	-0.387643	-2.421309
C	-4.971046	-0.265658	-0.294278
H	-4.780922	-1.332271	-0.407514
H	-4.193198	0.146161	0.352053
H	-5.943115	-0.130903	0.190127

C	3.030400	-3.939105	2.390670
H	2.417839	-4.835828	2.430866
H	4.057624	-4.206497	2.141945
H	3.002605	-3.432526	3.354551
H	0.874218	0.651303	-1.254842
H	-1.760637	-3.016493	0.058805
C	-3.259107	-2.732424	1.304378
O	-3.871397	-3.614116	0.667565
O	-3.591899	-2.019054	2.267645
O	-1.914873	-2.480877	0.854335
H	-0.776170	2.028885	3.125604

#### Vibrational frequencies

18.9596	27.3266	33.0821
39.9857	42.9283	50.2312
51.1273	56.9578	60.4750
65.6098	73.6799	75.1485
83.5894	85.7385	93.0725
94.4011	101.0330	105.8744
119.8618	123.6746	128.6331
131.3361	139.2697	142.4675
145.1754	159.0089	185.3809
188.0039	199.0407	208.5160
225.8986	230.5977	231.1526
237.2912	250.9081	255.6613
265.6452	275.6925	281.2700
296.3329	300.6668	302.2962
305.6533	315.5505	319.2810
334.5502	340.8988	342.9774
357.6852	360.0723	377.2507
384.0327	393.2421	399.8082

402.4343	412.5238	413.5420
434.1593	438.9601	446.7412
455.7727	463.5456	478.2076
484.4856	498.8208	503.0693
525.1184	534.1004	552.5008
563.6305	567.8264	571.3530
584.8316	603.0077	611.6500
634.8653	641.1804	654.6478
662.5331	672.9772	687.2895
708.6870	740.7217	743.7088
750.5719	756.9615	765.5639
774.6534	780.8287	790.2567
797.1816	807.4539	824.3255
834.1498	840.5145	851.2546
869.8336	872.4803	875.9083
883.1301	890.0643	905.4040
916.8769	934.0735	939.2808
940.6520	942.6598	952.9459
959.5279	969.3489	971.2495
977.6202	987.1225	988.8315
996.9199	1007.8898	1019.2388
1027.1609	1039.5094	1048.9489
1056.1707	1059.6110	1064.8557
1068.2578	1077.4140	1086.5406
1108.7718	1117.6726	1135.9700
1141.6704	1148.5143	1152.8276
1161.7523	1182.1357	1187.7394
1190.4877	1198.5624	1210.4013
1224.0171	1236.1298	1246.1579
1251.5446	1256.2114	1259.4345
1268.5075	1277.2334	1285.6817

1287.7782	1296.6350	1298.6275
1306.1785	1327.6438	1337.5065
1341.7617	1359.3458	1364.7563
1376.4361	1397.6850	1401.8166
1407.5223	1409.2102	1413.4577
1415.6787	1418.7106	1419.6020
1422.8923	1430.3070	1440.0842
1441.9131	1449.9988	1455.8636
1467.4698	1473.9863	1478.7797
1481.2038	1485.8325	1489.8938
1493.9327	1495.9729	1496.7240
1498.4113	1502.2315	1503.0406
1505.9862	1506.8461	1507.3515
1510.6239	1514.6955	1517.6856
1521.3491	1533.5776	1538.7511
1543.6065	1548.5967	1553.8781
1558.1178	1596.2661	1614.8929
1645.7098	1660.8654	1672.3342
1710.7615	1727.4628	1792.6214
1801.0449	3028.6528	3034.9039
3038.9107	3041.6893	3052.3499
3053.8499	3057.1602	3061.1332
3065.2008	3071.4327	3086.0961
3087.0367	3095.2548	3105.1875
3108.9143	3114.0853	3124.4559
3125.9356	3126.0232	3135.0030
3136.1147	3141.8850	3146.3811
3157.2241	3168.4447	3171.6871
3175.7274	3182.2684	3183.0173
3187.0871	3191.4690	3195.8371
3208.1505	3210.1798	3210.4409

3217.2938	3228.2563	3259.1404
3428.1884	3644.9356	3744.8456

#### TS4

Zero-point correction= 0.694577

Thermal correction to Energy= 0.737850

Thermal correction to Enthalpy= 0.738794

Thermal correction to Gibbs Free Energy= 0.617269

Sum of electronic and zero-point Energies= -2009.709134

Sum of electronic and thermal Energies= -2009.665861

Sum of electronic and thermal Enthalpies= -2009.664916

Sum of electronic and thermal Free Energies= -2009.786442

#### Cartesian coordinates

C	1.543344	-1.180533	3.631710
C	0.453105	-1.036344	2.729446
C	0.810132	-1.106684	1.326239
C	2.167522	-1.202956	0.948522
C	3.178555	-1.319128	1.900980
N	2.818096	-1.311917	3.224328
H	1.356076	-1.169768	4.696508
C	2.529871	-1.061679	-0.498226
C	2.613703	-2.202257	-1.352497
C	2.708865	0.212527	-1.017835
C	2.430848	-3.528049	-0.870161
C	2.888505	-2.005736	-2.746871
C	2.959359	0.398636	-2.400072
C	2.522942	-4.605099	-1.723009
H	2.220558	-3.681880	0.183193
C	2.976485	-3.140614	-3.597946
C	3.053798	-0.684926	-3.241255

H	3.079635	1.407017	-2.782973
C	2.798771	-4.411433	-3.099349
H	2.383828	-5.611371	-1.340080
H	3.185819	-2.985649	-4.652640
H	3.253173	-0.541562	-4.299326
H	2.867945	-5.270589	-3.759278
C	-0.229480	-1.093074	0.332114
O	-0.732035	-0.856594	3.152205
C	4.635388	-1.381855	1.547626
H	4.746846	-1.533196	0.475485
H	5.131618	-0.439495	1.800456
H	5.151997	-2.198327	2.058366
C	2.618301	1.398397	-0.087986
O	3.403088	1.544055	0.855181
N	1.594853	2.241745	-0.364463
H	0.931596	1.938014	-1.074268
C	1.143463	3.251362	0.600834
C	0.078784	2.609818	1.516424
H	0.557864	1.752384	2.012229
H	-0.212816	3.314196	2.299549
O	-1.121626	2.209604	0.865819
H	-0.890471	1.622210	0.126033
C	0.777137	4.593212	-0.100868
C	0.239980	5.584406	0.948353
H	-0.739264	5.279943	1.329608
H	0.925363	5.676686	1.798832
H	0.126265	6.577456	0.501260
C	-0.277429	4.413617	-1.210074
H	-0.525068	5.385994	-1.648816
H	0.101452	3.782174	-2.018676
H	-1.191158	3.963217	-0.819236



C	2.063594	5.171794	-0.723546
H	2.499941	4.472809	-1.443586
H	1.847519	6.109096	-1.247334
H	2.815940	5.381229	0.045338
C	-3.868991	-1.066538	0.539609
O	-3.990014	-0.825999	1.737107
O	-4.876343	-1.365838	-0.306466
C	-2.600959	-0.980863	-0.195485
H	-2.734394	0.241088	-0.970255
N	-1.485322	-0.960879	0.664252
H	-0.843764	2.308236	-3.639591
C	-6.286944	-1.341397	0.122443
C	-7.031942	-1.686548	-1.167592
H	-6.725588	-2.669664	-1.536474
H	-8.109661	-1.703750	-0.982993
H	-6.822088	-0.943374	-1.942160
C	-6.527177	-2.409350	1.192404
H	-6.195496	-3.387108	0.830022
H	-5.988999	-2.170418	2.109419
H	-7.597289	-2.469604	1.413212
C	-6.657296	0.063931	0.603665
H	-6.132355	0.314568	1.525529
H	-6.400620	0.801657	-0.162681
H	-7.735253	0.115028	0.784420
C	-1.698879	1.387374	-2.241044
O	-2.862815	1.101873	-1.771375
O	-0.607983	1.029904	-1.759809
O	-1.756833	2.149423	-3.353149
C	3.866401	-1.428521	4.262127
H	3.403793	-1.336466	5.241525
H	4.355327	-2.399810	4.180571

H	4.601445	-0.634473	4.130935
H	0.007564	-1.213393	-0.718072
H	-2.492117	-1.661947	-1.038568
H	-1.634910	-0.812393	1.689653
H	2.004305	3.448224	1.247868

Vibrational frequencies

-1251.4982	15.6478	23.9644
25.2496	29.6622	33.6671
38.5861	44.8894	51.3282
54.3045	56.9589	63.2100
67.6539	77.8493	82.3159
89.6756	103.0277	112.7302
121.1228	123.6620	129.4972
140.6332	141.7383	149.6634
155.8025	162.4499	178.6110
179.8424	193.0703	197.5477
212.9323	218.9379	233.0072
237.0694	245.9175	250.2883
259.7177	268.0348	277.2306
287.2923	289.4210	297.0341
314.7732	318.2485	323.8104
325.8635	332.3080	342.6590
362.0261	367.2498	381.4719
384.6458	391.5843	401.0084
405.5303	410.7844	414.3907
432.7722	438.7080	442.9838
446.6657	457.4595	470.4941
478.9553	486.1103	511.9980
518.8181	534.3909	555.2525
564.6056	570.1831	573.5279

584.8459	604.4745	609.5067
626.2886	643.5332	661.0526
670.1007	681.4377	688.8463
709.4464	717.5316	737.3944
741.8228	748.0870	760.6083
763.8136	767.4258	778.8995
792.0295	797.3294	810.1576
811.5149	827.1757	849.1569
850.2954	866.8321	878.3832
886.5587	892.3009	911.1211
913.0035	925.7026	935.8904
937.3117	942.7840	955.6265
962.8195	968.9414	970.0496
980.5162	980.7574	981.0901
1005.7571	1012.6653	1020.6952
1032.6926	1051.4142	1052.5013
1055.4759	1058.0499	1061.7625
1063.6177	1070.2856	1081.3579
1085.0093	1097.0287	1126.0951
1132.3850	1145.2203	1153.2711
1178.0685	1181.6631	1189.3594
1196.7168	1205.1591	1213.8351
1229.3389	1231.5162	1244.8059
1246.4595	1249.5951	1257.4621
1259.6171	1265.0430	1275.1579
1286.7159	1292.2203	1293.9473
1313.1653	1323.2284	1333.1992
1351.2058	1355.8819	1366.2984
1378.2200	1397.8484	1404.8996
1409.0190	1409.8224	1410.6519
1413.7848	1416.4167	1417.2609

1419.8294	1428.2502	1435.2521
1438.0901	1440.2266	1447.1767
1450.1904	1458.0786	1469.8792
1479.5792	1480.2099	1484.4068
1487.5932	1492.5761	1494.8097
1496.7940	1498.4414	1500.6877
1501.3924	1502.0180	1507.7673
1510.2679	1512.0879	1513.7144
1515.4961	1528.6922	1532.6962
1536.4710	1550.1686	1555.1918
1578.9386	1586.4954	1588.5350
1612.9242	1641.1307	1644.6432
1673.0263	1685.6232	1721.3491
1731.1418	1739.7261	3011.2122
3032.5843	3036.1628	3036.6793
3049.8948	3051.8237	3053.0273
3058.9020	3060.6959	3082.1080
3090.8438	3102.0448	3105.7186
3106.3890	3114.5403	3117.3066
3118.6116	3122.4656	3123.5620
3125.2072	3129.9639	3135.0845
3148.2054	3154.0960	3164.7622
3167.6464	3175.7907	3176.4821
3184.2872	3188.4973	3192.5651
3202.2895	3203.8305	3207.0061
3213.2461	3237.4081	3254.2661
3489.1706	3692.3766	3789.6823

#### **M4**

Zero-point correction= 0.657782

Thermal correction to Energy= 0.696251

Thermal correction to Enthalpy= 0.697195

Thermal correction to Gibbs Free Energy= 0.587507

Sum of electronic and zero-point Energies= -1744.714732

Sum of electronic and thermal Energies= -1744.676263

Sum of electronic and thermal Enthalpies= -1744.675319

Sum of electronic and thermal Free Energies= -1744.785007

Cartesian coordinates

C	-1.421699	0.493512	-3.471398
C	-0.437687	-0.074901	-2.644567
C	-0.891293	-0.502159	-1.327974
C	-2.221381	-0.216116	-0.938445
C	-3.126636	0.389549	-1.808037
N	-2.702814	0.709781	-3.066187
H	-1.165088	0.799840	-4.476079
C	-2.627913	-0.503305	0.472829
C	-3.338710	-1.703899	0.786041
C	-2.250299	0.359229	1.496045
C	-3.721330	-2.638288	-0.217211
C	-3.681591	-1.984042	2.150477
C	-2.584859	0.066428	2.845077
C	-4.415392	-3.780885	0.111101
H	-3.457217	-2.437627	-1.249827
C	-4.400230	-3.172140	2.454376
C	-3.289434	-1.069921	3.162183
H	-2.296943	0.764404	3.624969
C	-4.760901	-4.051139	1.458614
H	-4.700465	-4.482586	-0.666719
H	-4.658345	-3.374529	3.490066
H	-3.554678	-1.279687	4.194283
H	-5.309145	-4.956027	1.701921

C	0.019600	-1.141354	-0.439006
O	0.780545	-0.200518	-3.033785
C	-4.527910	0.755804	-1.410267
H	-4.720258	0.438233	-0.387542
H	-4.681735	1.839041	-1.456199
H	-5.275074	0.283470	-2.055804
C	-1.499409	1.628947	1.181559
O	-1.913545	2.411370	0.310539
N	-0.389880	1.824461	1.928615
H	-0.135745	1.063038	2.541794
C	0.578513	2.942369	1.874000
C	-0.099261	4.313623	1.670461
H	-0.973258	4.351562	2.340688
H	0.602577	5.076265	2.018998
O	-0.444525	4.655129	0.342223
H	-1.050093	3.935600	0.064876
C	1.797976	2.622221	0.944865
C	1.374210	2.316307	-0.503138
H	0.621393	1.529093	-0.533034
H	0.961644	3.201343	-0.988065
H	2.236331	1.963238	-1.079001
C	2.533434	1.391873	1.516621
H	3.414294	1.160724	0.909187
H	2.869278	1.566815	2.545587
H	1.900091	0.500542	1.507224
C	2.763280	3.822250	0.955945
H	3.052381	4.097207	1.977265
H	3.677116	3.568479	0.408535
H	2.316196	4.696485	0.475012
C	3.656130	-1.516014	-0.550838
O	3.922831	-0.922381	-1.600529

O	4.575968	-2.024571	0.312097
C	2.326003	-1.743497	-0.057494
N	1.309948	-1.234704	-0.762299
H	1.488850	-0.812135	-1.724555
C	6.013978	-1.793102	0.126623
C	6.626213	-2.491013	1.342745
H	6.380460	-3.556953	1.337166
H	7.714611	-2.384329	1.327860
H	6.245434	-2.051432	2.269200
C	6.495008	-2.449219	-1.171216
H	6.212674	-3.506461	-1.184143
H	6.059800	-1.956048	-2.039872
H	7.585935	-2.384571	-1.231784
C	6.308002	-0.289600	0.162860
H	5.867536	0.215912	-0.696758
H	5.901273	0.150086	1.079018
H	7.390096	-0.126845	0.154462
C	-3.635819	1.336937	-4.020400
H	-3.117093	1.502643	-4.961758
H	-4.491346	0.682424	-4.193447
H	-3.985222	2.294629	-3.630866
H	-0.293858	-1.523226	0.525462
H	0.976547	2.989854	2.896026
H	2.136525	-2.198193	0.906022

Vibrational frequencies

20.7799	22.9238	28.2622
33.7864	38.7235	46.8713
58.1797	62.7924	64.5761
71.0905	82.5117	86.7084
97.6787	107.4673	112.6209

124.0693	128.4936	144.6944
149.3534	169.9240	175.5887
183.0833	195.8820	202.3900
217.7128	230.7042	235.3258
240.4097	251.2108	255.1866
263.7878	264.1058	286.1288
287.0114	296.8397	313.0111
323.9967	327.3763	333.2122
343.5269	347.7678	362.3024
367.5433	378.7366	379.6636
382.0664	389.2735	401.2968
403.9942	419.1370	423.2046
436.5590	443.2703	452.9180
459.5298	466.5048	482.5744
486.8125	511.4702	522.8887
535.5580	554.1295	567.0879
570.3520	585.8920	596.8559
604.8529	644.4491	658.3666
661.9029	691.3029	698.3318
706.7684	735.7914	739.5227
744.3500	751.8195	759.6304
764.7570	765.4537	776.0868
791.5732	795.4620	810.0962
819.4241	826.5203	839.0842
851.3790	854.7910	875.2257
889.5183	893.7991	913.7224
923.6925	932.7317	935.5924
943.6958	951.1100	956.6671
971.8681	974.2967	977.6945
985.7016	1006.8118	1009.9638
1028.6024	1035.0815	1049.6055



1054.3859	1056.8616	1059.6839
1068.6997	1074.3772	1079.0015
1094.7589	1122.6079	1134.5292
1140.9483	1142.9749	1155.0779
1165.4725	1185.2500	1191.3456
1206.3351	1223.9753	1225.7685
1236.1678	1248.0759	1251.1543
1261.3995	1266.6410	1272.2494
1275.4664	1285.6472	1288.9827
1291.3521	1297.7302	1314.5144
1331.1416	1352.5419	1360.2490
1368.0086	1387.1118	1397.8324
1402.8804	1405.7404	1409.8559
1410.8049	1411.3884	1414.8126
1417.7323	1424.8016	1429.1026
1432.4582	1440.6711	1448.1080
1465.1076	1469.9568	1478.4363
1481.4047	1485.1266	1489.0360
1494.4670	1495.1155	1495.6687
1498.0561	1500.4646	1500.9327
1501.5724	1506.0873	1508.5202
1509.4297	1511.7627	1516.3872
1519.3919	1527.0095	1532.7389
1539.1352	1548.4691	1552.9115
1568.4392	1569.9952	1580.6592
1611.4341	1644.2339	1672.0271
1675.5766	1705.3176	1706.6542
2740.5065	2985.4587	3032.7514
3034.1483	3039.2862	3048.1860
3050.2320	3052.2144	3056.6168
3062.6616	3081.8741	3098.2683

3100.6218	3107.3830	3108.0815
3118.8967	3120.6509	3124.1812
3125.9438	3127.8476	3133.1900
3144.7367	3159.4255	3162.9862
3168.8516	3179.6955	3182.2497
3183.7019	3187.9260	3193.2271
3194.5909	3205.0561	3205.7603
3214.8110	3218.4712	3236.9450
3247.8221	3536.6932	3630.3125

### TS5RR

Zero-point correction= 0.961467

Thermal correction to Energy= 1.018758

Thermal correction to Enthalpy= 1.019703

Thermal correction to Gibbs Free Energy= 0.868939

Sum of electronic and zero-point Energies= -2949.539480

Sum of electronic and thermal Energies= -2949.482189

Sum of electronic and thermal Enthalpies= -2949.481245

Sum of electronic and thermal Free Energies= -2949.632009

### Cartesian coordinates

C	-2.453994	-2.585058	-3.413056
C	-1.276206	-2.294299	-2.679767
C	-1.490055	-1.933588	-1.290742
C	-2.797901	-1.929174	-0.757074
C	-3.895720	-2.304248	-1.533465
N	-3.679371	-2.599291	-2.853623
H	-2.380877	-2.831327	-4.463282
C	-3.020667	-1.506588	0.663505
C	-2.772583	-2.433246	1.727273
C	-3.421801	-0.209128	0.953309

C	-2.329036	-3.764844	1.490172
C	-2.968453	-2.010104	3.083587
C	-3.593554	0.199924	2.301873
C	-2.085697	-4.626188	2.536736
H	-2.181167	-4.098430	0.468909
C	-2.714792	-2.926597	4.140052
C	-3.388453	-0.678036	3.337448
H	-3.892102	1.223453	2.500888
C	-2.279542	-4.205885	3.875488
H	-1.744110	-5.636835	2.335660
H	-2.865070	-2.594599	5.163477
H	-3.529634	-0.357820	4.365704
H	-2.084151	-4.895785	4.690505
C	-0.354261	-1.631639	-0.466311
H	-0.473633	-1.347999	0.570279
O	-0.127113	-2.353616	-3.231623
C	-5.294715	-2.396602	-0.998414
H	-5.279991	-2.277659	0.083152
H	-5.921706	-1.598735	-1.404249
H	-5.752733	-3.362845	-1.228267
C	-3.699962	0.786758	-0.151113
O	-4.528853	0.546201	-1.038856
N	-2.999629	1.935484	-0.041093
H	-2.213972	1.934045	0.623085
C	-2.928106	2.892019	-1.139417
C	-1.574746	2.703875	-1.872713
H	-1.632126	3.185829	-2.855286
H	-0.767722	3.193541	-1.312857
O	-1.276882	1.329954	-2.054177
H	-0.616716	1.105475	-1.356541
C	-3.213248	4.346622	-0.661321

C	-3.121978	5.306373	-1.863972
H	-2.100720	5.383140	-2.249850
H	-3.771272	4.977898	-2.683866
H	-3.437805	6.312753	-1.568671
C	-2.221326	4.799052	0.429511
H	-2.477806	5.808792	0.768580
H	-2.242672	4.133443	1.296300
H	-1.190248	4.827645	0.063201
C	-4.642886	4.397595	-0.089815
H	-4.747767	3.718666	0.761606
H	-4.887066	5.410727	0.248220
H	-5.380388	4.106807	-0.846710
N	0.868171	-1.803268	-0.926403
C	2.023230	-1.449264	-0.270927
C	3.257725	-1.994911	-0.845571
O	3.328600	-2.541702	-1.939031
O	4.286576	-1.742196	-0.013833
C	5.639844	-2.284795	-0.244835
C	6.242036	-1.703681	-1.525336
H	5.658704	-1.995386	-2.398161
H	6.275619	-0.612864	-1.473164
H	7.265697	-2.073459	-1.639208
C	6.399098	-1.798076	0.989484
H	5.940664	-2.192454	1.900941
H	7.439180	-2.132961	0.946447
H	6.385471	-0.705421	1.038997
C	5.571049	-3.813526	-0.280122
H	6.584975	-4.222967	-0.310937
H	5.074290	-4.188613	0.619651
H	5.025109	-4.161104	-1.157889
P	0.614338	1.608081	1.353523

O	-0.839845	1.888034	1.678830
C	1.656398	3.095100	1.535098
C	1.980099	3.572654	2.814886
C	2.063162	3.821913	0.405845
C	2.703719	4.755866	2.962029
H	1.675534	3.014626	3.695736
C	2.782793	5.008379	0.556023
H	1.821709	3.454277	-0.586127
C	3.104434	5.475279	1.832552
H	2.956177	5.115372	3.954948
H	3.095431	5.564531	-0.322541
H	3.668111	6.396174	1.948055
C	1.269798	0.366295	2.518349
C	0.359822	-0.587590	3.002681
C	2.636505	0.220471	2.802502
C	0.811607	-1.691021	3.726176
H	-0.699087	-0.456612	2.806124
C	3.086848	-0.883570	3.529462
H	3.349690	0.963006	2.458312
C	2.178026	-1.844362	3.980837
H	0.097889	-2.427017	4.083162
H	4.146436	-0.994802	3.738265
H	2.533414	-2.707024	4.536233
N	0.834482	1.059739	-0.211688
C	2.061087	0.622299	-0.569789
C	2.517822	0.712138	-1.980547
C	1.653964	0.569248	-3.077896
C	3.884321	0.933091	-2.215231
C	2.158003	0.637623	-4.376243
H	0.595120	0.416656	-2.922737
C	4.383520	1.009938	-3.514511

H	4.556021	1.046443	-1.369359
C	3.519897	0.858247	-4.601685
H	1.481590	0.518603	-5.217799
H	5.442835	1.185644	-3.676312
H	3.904092	0.912949	-5.615985
H	1.962102	-1.406824	0.808319
C	-4.827036	-2.949340	-3.717908
H	-5.252776	-3.901356	-3.398198
H	-5.584824	-2.168875	-3.654210
H	-4.480176	-3.033973	-4.744829
H	2.892998	0.729846	0.132910
H	0.892137	-2.079420	-1.940451
H	-3.721713	2.607147	-1.836423

Vibrational frequencies

-301.5776	15.8645	19.1598
23.7559	29.0894	32.9018
35.0090	38.1706	39.0499
40.7108	45.9385	49.4724
52.4620	55.0915	59.7682
64.3326	65.9462	75.1973
76.8024	82.0617	88.8087
92.3256	95.8026	103.3567
116.7063	119.2398	125.9324
131.5867	135.2770	145.0118
146.4136	153.8792	156.2928
162.5641	179.4838	183.7778
189.5547	197.6948	201.2701
208.6376	216.7988	223.7320
232.6546	234.2621	239.3863
246.4016	250.3291	259.0812

263.7664	273.3144	280.0728
284.2357	292.3954	295.7945
298.8131	301.2027	310.9374
313.3464	320.1276	332.8026
343.4400	349.0940	361.5638
366.1509	375.5143	380.6353
383.3147	387.9853	391.5458
399.1901	406.0962	407.5745
410.6366	411.2530	418.9507
419.6039	422.5365	435.8934
441.3575	443.6670	451.5301
459.9211	469.8300	482.1899
485.3236	501.6572	519.3283
521.9198	527.8621	532.1786
535.2283	545.4030	554.6626
557.2703	566.5046	569.3421
574.3673	591.0734	612.1691
628.6162	630.9694	631.3817
639.7989	647.9872	662.4703
673.8379	697.0823	697.7823
702.3634	711.9917	721.1153
732.3402	736.2596	738.0996
745.5865	749.0418	759.6374
766.6008	768.0674	768.6515
769.8119	775.5931	776.2016
793.5889	796.2716	812.1738
818.5572	834.0309	844.1820
847.9104	849.5600	864.9166
869.5201	871.3180	882.3819
884.9550	886.8945	889.2624
892.8795	912.0839	920.0381

922.9261	925.6742	934.9800
936.6725	939.3598	947.2794
949.0491	949.9763	957.4246
967.8288	971.3575	973.7404
977.5935	980.2749	981.3525
992.5219	998.4070	1003.4794
1003.9359	1012.2978	1013.9386
1014.3167	1015.3084	1019.1554
1024.9804	1030.6865	1034.8236
1049.9547	1050.8865	1051.6508
1055.9615	1057.7846	1058.1226
1058.9705	1063.4926	1072.3299
1081.6345	1089.9857	1092.0330
1096.7460	1106.0817	1111.0422
1117.0130	1121.4393	1131.3226
1134.3831	1138.6711	1145.3555
1155.0892	1164.7561	1179.2074
1182.3145	1188.6104	1192.5761
1193.9951	1195.0319	1204.1251
1213.0713	1214.6815	1215.6923
1222.7414	1224.2994	1226.7730
1239.9849	1246.5546	1247.9377
1254.1067	1263.8601	1273.5272
1276.0277	1279.9454	1285.3051
1289.1692	1295.0050	1314.8812
1324.9349	1328.4719	1332.0581
1333.6004	1347.1404	1352.2747
1358.6525	1360.5600	1361.7773
1364.3469	1373.5053	1383.7024
1402.8195	1408.5696	1410.2909
1412.0525	1412.6778	1413.7334



1417.7017	1422.9560	1424.5822
1427.4175	1436.3788	1439.0244
1447.5620	1459.9391	1461.1659
1466.8738	1472.9304	1476.6139
1479.3655	1481.7572	1482.0057
1486.1348	1493.0658	1494.7521
1495.3219	1496.1227	1499.4129
1501.4216	1501.8489	1504.1954
1507.3849	1509.6836	1509.7657
1512.1382	1518.1281	1520.3847
1521.8702	1524.2128	1525.6158
1529.0987	1532.5649	1544.2413
1550.1551	1552.8440	1577.4742
1609.0546	1620.7123	1622.4170
1624.6710	1626.1110	1636.0479
1642.2386	1644.7612	1646.7843
1655.5474	1670.8264	1672.5135
1716.1230	1743.0358	2955.0127
3025.8657	3030.7977	3033.9564
3044.2821	3050.2603	3055.7852
3063.8495	3064.1030	3069.2598
3070.6819	3089.6988	3090.1914
3099.1172	3103.1698	3107.3226
3111.4821	3118.2096	3126.0635
3128.3889	3130.7692	3131.5471
3132.7442	3137.4443	3159.6767
3172.9009	3175.0955	3178.5960
3179.7461	3183.0736	3184.0059
3186.1330	3186.5768	3188.6780
3189.1764	3193.6582	3194.2194
3195.6261	3197.9396	3200.1851

3202.9234	3206.3228	3206.4297
3207.0553	3210.4227	3211.7953
3212.9223	3215.9013	3218.2272
3237.2666	3252.4657	3254.9733
3260.4524	3272.1656	3391.6430

### TS5RR1

Zero-point correction= 0.961394

Thermal correction to Energy= 1.018873

Thermal correction to Enthalpy= 1.019817

Thermal correction to Gibbs Free Energy= 0.868725

Sum of electronic and zero-point Energies= -2949.512395

Sum of electronic and thermal Energies= -2949.454917

Sum of electronic and thermal Enthalpies= -2949.453972

Sum of electronic and thermal Free Energies= -2949.605065

### Cartesian coordinates

C	-0.134126	-2.668295	-3.818800
C	0.713508	-2.117722	-2.822526
C	0.120396	-2.028477	-1.503843
C	-1.166241	-2.565831	-1.259392
C	-1.867723	-3.225123	-2.273009
N	-1.333507	-3.212810	-3.535230
H	0.204671	-2.711983	-4.844650
C	-1.715887	-2.521379	0.136485
C	-1.089373	-3.356309	1.125316
C	-2.733416	-1.646268	0.517851
C	-0.086996	-4.313595	0.791821
C	-1.468228	-3.234313	2.502017
C	-3.104947	-1.561380	1.889529
C	0.517018	-5.079485	1.763289

H	0.199572	-4.442867	-0.245064
C	-0.819934	-4.033368	3.482368
C	-2.485020	-2.314055	2.852859
H	-3.901333	-0.885191	2.175258
C	0.156628	-4.933856	3.125184
H	1.275711	-5.803562	1.482748
H	-1.114466	-3.918819	4.521754
H	-2.773639	-2.214750	3.894615
H	0.647522	-5.538753	3.881204
C	0.909639	-1.481585	-0.429621
H	0.464213	-1.312548	0.539557
O	1.902418	-1.747620	-3.097807
C	-3.115462	-4.025846	-2.039077
H	-3.387224	-3.977268	-0.987402
H	-3.962347	-3.641346	-2.609840
H	-2.956106	-5.076423	-2.306675
C	-3.564691	-0.847630	-0.465471
O	-3.935660	-1.323381	-1.542250
N	-3.982223	0.360539	-0.005299
H	-3.406830	0.789281	0.706323
C	-4.957669	1.208794	-0.687988
C	-4.261110	2.452231	-1.272221
H	-5.006779	3.099052	-1.742276
H	-3.791412	3.035484	-0.464047
O	-3.318230	2.112167	-2.270915
H	-2.556539	1.692638	-1.802679
C	-6.175822	1.501519	0.247165
C	-5.743067	2.236916	1.531411
H	-5.030011	1.647137	2.116881
H	-5.284904	3.206788	1.312801
H	-6.613293	2.420682	2.170262

C	-6.833630	0.160974	0.628769
H	-7.697580	0.332190	1.279802
H	-7.182494	-0.372559	-0.262525
H	-6.135107	-0.491518	1.159460
C	-7.217318	2.356930	-0.501879
H	-7.469592	1.913675	-1.471942
H	-8.139291	2.424089	0.085267
H	-6.867262	3.378500	-0.675387
N	2.220622	-1.387182	-0.529926
C	3.021639	-0.758872	0.397550
C	4.465518	-0.926335	0.153601
O	4.929134	-1.345217	-0.898959
O	5.165669	-0.515543	1.222909
C	6.635006	-0.675076	1.304408
C	7.327833	0.130106	0.204413
H	7.087574	-0.264168	-0.782431
H	7.017085	1.175691	0.245903
H	8.410733	0.080637	0.354844
C	6.950306	-0.095932	2.683161
H	6.419263	-0.648127	3.463725
H	8.024276	-0.161577	2.877937
H	6.650634	0.954852	2.733428
C	6.978743	-2.164881	1.239714
H	8.048748	-2.299012	1.423395
H	6.425332	-2.715117	2.006546
H	6.736081	-2.578851	0.260323
P	-0.216817	1.698644	0.057722
O	-1.327906	1.151991	-0.817166
C	-0.144275	3.522381	-0.040422
C	0.738938	4.244951	0.776694
C	-0.949115	4.205996	-0.961334

C	0.815804	5.633052	0.675500
H	1.365738	3.726107	1.497625
C	-0.870597	5.598025	-1.059533
H	-1.634466	3.651747	-1.594728
C	0.009536	6.311871	-0.244292
H	1.500881	6.185494	1.311742
H	-1.498174	6.123700	-1.773414
H	0.068570	7.393456	-0.322623
C	-0.639241	1.374405	1.813620
C	0.081205	0.478629	2.610836
C	-1.786930	1.985077	2.350443
C	-0.342817	0.177100	3.907469
H	0.978534	0.011396	2.225519
C	-2.216082	1.681567	3.641503
H	-2.339246	2.710339	1.758517
C	-1.494612	0.772090	4.421714
H	0.222382	-0.528764	4.508025
H	-3.108186	2.155648	4.039636
H	-1.829379	0.532027	5.426144
N	1.234773	1.138917	-0.395807
C	2.473090	1.232063	0.105232
C	3.547299	1.716462	-0.810058
C	3.530301	1.395599	-2.176854
C	4.571584	2.529047	-0.309755
C	4.523383	1.884524	-3.022208
H	2.744298	0.750818	-2.557921
C	5.554235	3.035998	-1.163470
H	4.591919	2.773844	0.748971
C	5.534859	2.712411	-2.521046
H	4.509661	1.623554	-4.076643
H	6.334802	3.678520	-0.766462

H	6.301283	3.100747	-3.185271
H	2.702951	-0.848734	1.430166
C	-2.087972	-3.833576	-4.645779
H	-2.185626	-4.905792	-4.472297
H	-3.077590	-3.381979	-4.712316
H	-1.548850	-3.665002	-5.574678
H	2.633219	1.519485	1.151954
H	2.575853	-1.537404	-1.497844
H	-5.317591	0.622284	-1.537804

Vibrational frequencies

-280.6017	12.9814	18.1083
24.5164	31.4198	33.6253
36.7530	39.0869	39.6691
44.2219	48.6457	50.1641
53.3391	60.2444	63.2260
67.1511	72.4780	74.3386
78.5263	82.2218	87.1189
89.3105	91.5169	100.8382
102.0779	111.8013	120.6974
129.1663	134.6813	136.9205
143.3056	151.0558	157.7163
165.1764	179.5439	192.0822
200.5381	201.4714	205.0140
208.2274	218.6320	221.8935
224.0728	237.5606	241.3370
244.8445	253.9025	261.5466
264.7931	266.6381	273.6653
274.3211	278.8774	291.6758
293.6432	297.2265	312.7629
317.3329	323.1338	332.3387

337.5922	344.8597	355.1011
357.0177	365.1850	374.4423
377.8460	384.2931	389.1414
399.5865	405.7974	407.9013
411.9748	413.4931	418.3536
422.7607	432.7319	438.9628
443.3512	447.8519	455.1465
464.0469	470.5919	485.9281
491.3236	493.4872	500.4917
516.5996	523.0305	531.6134
535.4934	540.6229	547.3752
555.5315	559.5321	568.1407
575.7282	584.8736	591.0886
616.8672	628.9343	630.2102
630.9983	637.2782	643.0541
664.5367	674.5045	690.1152
703.7853	714.8688	716.8866
718.6231	726.4829	737.6280
745.7683	750.0742	752.1542
760.1833	764.5979	765.5705
773.2545	777.7544	778.4987
793.2429	797.2459	810.0990
812.1819	829.7169	831.1110
843.3432	847.0772	862.3065
867.5373	869.6991	879.5376
883.0103	887.4311	891.7754
906.2805	909.8666	914.9197
917.4760	922.5117	936.4110
938.7832	940.5527	942.5928
943.4625	945.8408	955.0265
967.4192	971.2388	974.0130

982.3497	982.6163	987.5825
989.8110	1001.5672	1004.7628
1007.9852	1010.2622	1012.5931
1013.6684	1014.6177	1024.4427
1027.5381	1032.1176	1041.4597
1048.5847	1050.3230	1051.1116
1051.4181	1056.0437	1059.0886
1060.4392	1065.5495	1068.1345
1080.2612	1082.0033	1094.4674
1109.0619	1109.2908	1111.2587
1114.9432	1121.0181	1127.0818
1131.0653	1133.1705	1144.1705
1153.8226	1170.0825	1181.3506
1182.0975	1188.3827	1190.2691
1192.9722	1193.2321	1203.4900
1210.3942	1214.5136	1215.3345
1218.1128	1224.5082	1230.9201
1243.6444	1246.4543	1249.9622
1252.7411	1262.5225	1267.8759
1274.4885	1274.9168	1278.0436
1290.9191	1291.7374	1307.2556
1326.6595	1328.5849	1331.5950
1334.9068	1341.4725	1344.3478
1352.6164	1360.2865	1364.7363
1366.0891	1375.6026	1383.0912
1400.2201	1408.8445	1412.1951
1412.4988	1413.8342	1414.8918
1416.6886	1422.6814	1429.6653
1432.4072	1436.8462	1437.3211
1446.5225	1458.5328	1461.7941
1464.4205	1473.8757	1475.4556



1475.8495	1479.4842	1479.9244
1485.5946	1490.2678	1493.1689
1495.5948	1496.8838	1497.2504
1498.0105	1502.2499	1502.8756
1505.2171	1506.7950	1511.8780
1513.1431	1513.7700	1517.6786
1520.4622	1525.0183	1528.5231
1530.6963	1533.7921	1536.4779
1548.3948	1551.6389	1563.8292
1575.4497	1608.5451	1625.7456
1627.5397	1631.1103	1636.5894
1644.0824	1645.0080	1648.1384
1653.6750	1664.8706	1672.4958
1723.6492	1745.9549	2990.3329
3024.1135	3034.6816	3036.7953
3043.7433	3050.8436	3053.0251
3056.5503	3065.9721	3091.0902
3092.3350	3101.1514	3102.9262
3106.4736	3108.4049	3112.9272
3114.9743	3119.2616	3124.8377
3126.3715	3129.5945	3133.4011
3135.2025	3144.2714	3160.3248
3174.1060	3174.4188	3174.4986
3174.5193	3175.7688	3181.1615
3183.5540	3184.1710	3187.9282
3189.1715	3190.5530	3193.7814
3194.2060	3196.1088	3196.9098
3198.6713	3200.9394	3202.6770
3204.3629	3206.8924	3208.2799
3209.2354	3210.3895	3222.8190
3225.0137	3235.2997	3252.8502

3265.3844

3379.9993

3619.5847

## TS5RR2

Zero-point correction= 0.961467

Thermal correction to Energy= 1.019109

Thermal correction to Enthalpy= 1.020054

Thermal correction to Gibbs Free Energy= 0.868829

Sum of electronic and zero-point Energies= -2949.507768

Sum of electronic and thermal Energies= -2949.450125

Sum of electronic and thermal Enthalpies= -2949.449181

Sum of electronic and thermal Free Energies= -2949.600406

## Cartesian coordinates

C	-3.075664	-1.232278	-3.697849
C	-2.096644	-1.689030	-2.774108
C	-2.358401	-1.353126	-1.389426
C	-3.507675	-0.609387	-1.044449
C	-4.422645	-0.207266	-2.015420
N	-4.160695	-0.534057	-3.321772
H	-2.951614	-1.439204	-4.751676
C	-3.759506	-0.247854	0.388377
C	-4.494533	-1.172755	1.198177
C	-3.278151	0.935438	0.941809
C	-4.976745	-2.411554	0.688489
C	-4.755444	-0.851496	2.570818
C	-3.569966	1.247332	2.299547
C	-5.674764	-3.281839	1.495569
H	-4.787001	-2.670403	-0.346967
C	-5.480833	-1.770080	3.375001
C	-4.287852	0.383676	3.088432
H	-3.249974	2.199144	2.709896

C	-5.930440	-2.960863	2.850950
H	-6.033153	-4.222897	1.090290
H	-5.672819	-1.514799	4.413103
H	-4.509878	0.641991	4.119559
H	-6.482201	-3.657688	3.473988
C	-1.417933	-1.739836	-0.384129
H	-1.628771	-1.558211	0.663331
O	-1.067361	-2.324779	-3.167641
C	-5.626192	0.634984	-1.710201
H	-5.784747	0.678892	-0.634470
H	-5.478108	1.660878	-2.065001
H	-6.537213	0.241415	-2.167765
C	-2.432954	1.875641	0.116628
O	-2.577073	1.994673	-1.103908
N	-1.487889	2.554858	0.817089
H	-1.360743	2.373131	1.802383
C	-0.460710	3.396173	0.209899
C	0.888336	2.936293	0.793240
H	1.124527	1.957739	0.368260
H	1.690192	3.613252	0.490601
O	0.865185	2.868656	2.224696
H	0.900877	1.936922	2.484104
C	-0.781089	4.919284	0.331259
C	-0.793096	5.388099	1.797271
H	-1.532587	4.832142	2.383254
H	0.180716	5.252801	2.273824
H	-1.058211	6.449926	1.848004
C	-2.164591	5.184402	-0.294461
H	-2.386222	6.256795	-0.278617
H	-2.203397	4.839551	-1.332261
H	-2.955251	4.670020	0.259216

C	0.273047	5.719323	-0.458977
H	0.324985	5.384562	-1.501083
H	0.011353	6.782561	-0.462406
H	1.273031	5.631342	-0.024128
N	-0.274320	-2.303348	-0.690548
C	0.790301	-2.546654	0.193259
C	1.838265	-3.387738	-0.433462
O	1.957470	-3.515941	-1.645869
O	2.628297	-3.906220	0.503847
C	3.789144	-4.768788	0.177980
C	4.744741	-4.067793	-0.788002
H	4.335518	-4.034936	-1.796752
H	4.931449	-3.039471	-0.472874
H	5.690756	-4.618580	-0.806646
C	4.441074	-4.960535	1.546744
H	3.729191	-5.392174	2.256005
H	5.298538	-5.633294	1.458949
H	4.788927	-4.001013	1.940050
C	3.260061	-6.090751	-0.380138
H	4.095770	-6.775139	-0.553684
H	2.571093	-6.558538	0.329407
H	2.740727	-5.927627	-1.326199
P	3.669746	-0.022390	-0.903726
O	4.683167	-0.811872	-1.707662
C	4.499481	1.417360	-0.122548
C	4.048233	1.948672	1.093286
C	5.574799	2.035080	-0.778258
C	4.642319	3.090035	1.633893
H	3.231227	1.465759	1.617817
C	6.176392	3.172185	-0.235538
H	5.937913	1.616927	-1.712338

C	5.706139	3.704829	0.968467
H	4.273332	3.497097	2.570862
H	7.008736	3.643568	-0.750274
H	6.170095	4.593036	1.387589
C	2.401294	0.729885	-2.008226
C	2.250915	2.115863	-2.172878
C	1.542225	-0.128853	-2.715747
C	1.263025	2.630546	-3.016080
H	2.904065	2.798895	-1.640260
C	0.553519	0.385364	-3.556076
H	1.648185	-1.205243	-2.611717
C	0.408087	1.766862	-3.703827
H	1.162945	3.705603	-3.133397
H	-0.099674	-0.300687	-4.082363
H	-0.365407	2.167378	-4.352493
N	2.943373	-0.797351	0.336573
C	1.617626	-0.855217	0.608603
C	1.255314	-0.738020	2.068640
C	2.147893	-1.150888	3.067044
C	0.012442	-0.210886	2.452947
C	1.799375	-1.048098	4.413046
H	3.114051	-1.540191	2.766170
C	-0.338676	-0.105678	3.802680
H	-0.681331	0.132304	1.693711
C	0.556232	-0.525944	4.787616
H	2.501590	-1.371446	5.176010
H	-1.306473	0.305861	4.073385
H	0.291215	-0.444214	5.837168
H	0.467705	-2.886362	1.171828
C	-5.096253	-0.093015	-4.380399
H	-6.064696	-0.572568	-4.235554

H	-5.211706	0.989918	-4.338955
H	-4.690913	-0.378218	-5.347787
H	0.928817	-0.268191	-0.018484
H	-0.150141	-2.465930	-1.716358
H	-0.449375	3.150023	-0.856314

Vibrational frequencies

-340.9198	14.6612	21.5828
24.4646	26.9374	32.4314
36.7466	39.8623	41.3429
42.5740	44.8038	46.9632
53.2386	58.6598	59.8949
60.1734	72.2499	75.1367
78.4142	81.3535	86.5611
92.6783	99.1576	107.2547
114.1588	116.8787	129.3945
130.5968	140.8327	144.7370
151.2844	153.5233	156.6844
160.5392	180.1368	185.8872
189.0893	190.7359	196.7587
212.7705	217.5521	226.7327
232.9387	237.8547	238.6702
247.7340	253.2756	255.2886
261.6864	271.4297	278.7976
280.2429	283.1869	285.2076
287.7713	297.9040	304.4497
309.7800	326.0462	328.2451
334.7257	340.9083	348.0995
357.5391	360.9473	362.7853
364.0279	381.0857	382.7889
393.5665	394.9124	397.4423

407.9645	414.3430	419.0781
421.4617	423.7197	430.9281
438.1331	442.6114	443.4333
446.1375	462.3289	469.4227
480.9008	482.6198	483.2939
517.8935	520.8896	528.6435
530.7586	535.0360	553.8384
554.0874	561.2158	562.6470
575.5245	591.3092	615.9251
626.8483	630.6521	631.8546
634.0911	638.3503	649.4824
665.6965	672.4841	682.2058
694.9471	700.8014	714.5522
718.3745	722.3734	727.6765
734.5574	742.0240	753.2617
756.0171	756.2873	763.0505
769.0012	775.0085	779.8426
784.4461	794.8425	800.3940
813.9607	818.8927	849.7335
851.3614	851.6213	857.3633
868.9367	876.0416	879.1540
884.5367	889.3464	891.4164
893.9534	912.2681	926.2279
934.2313	939.9749	941.0418
943.6666	946.2022	947.9973
949.7147	952.2125	964.1985
972.8685	975.8910	976.1868
983.1577	987.8381	991.8399
993.5803	997.1693	999.5189
1009.0771	1009.3075	1011.1921
1012.4912	1014.6807	1015.6694

1029.8813	1031.3459	1037.0176
1048.2620	1049.7957	1052.0361
1054.3920	1054.5410	1058.1884
1062.9027	1068.1196	1070.3629
1082.4566	1087.9065	1091.4113
1102.9136	1106.0190	1108.4186
1117.2158	1128.1093	1129.4112
1134.6157	1145.7805	1154.2701
1166.1530	1173.8396	1183.7133
1188.9663	1189.1561	1190.1458
1192.2057	1197.4791	1200.5381
1203.7331	1205.0236	1206.3973
1214.8129	1219.5207	1221.7664
1222.7572	1242.0866	1248.0936
1254.7949	1257.9163	1258.8916
1266.5335	1269.1316	1274.8957
1289.7450	1295.0536	1300.5712
1319.2965	1323.6642	1324.4817
1327.9342	1338.6701	1347.7025
1353.0688	1354.3116	1360.1681
1363.0017	1363.5837	1377.4106
1396.9354	1402.7521	1410.1516
1410.4560	1411.3472	1415.2640
1415.8863	1417.0616	1420.0763
1425.8346	1427.2621	1436.6441
1439.9924	1443.9553	1448.6369
1454.8382	1467.0308	1470.6078
1473.5232	1479.7221	1481.5949
1485.1631	1488.7725	1489.0589
1493.5475	1495.1181	1495.7442
1498.0602	1498.1855	1501.4449



1502.2094	1506.1041	1508.9965
1510.4062	1510.9980	1516.2592
1520.4689	1524.7722	1525.1521
1527.7829	1530.7181	1532.0661
1541.1547	1549.9591	1554.5275
1581.5122	1609.8610	1623.0827
1626.0683	1633.1102	1637.5777
1643.6713	1643.9166	1644.7059
1650.6801	1670.9999	1671.6407
1719.6277	1746.3929	2977.0402
3036.6526	3039.0659	3045.5502
3047.1622	3049.8553	3054.0957
3057.0744	3061.2944	3082.2577
3091.6233	3091.6964	3104.7439
3106.5016	3114.3071	3116.0577
3122.1957	3124.5727	3125.7985
3129.3788	3131.8655	3134.5943
3135.3285	3145.2873	3151.6644
3175.4851	3176.6194	3178.9867
3179.2380	3182.2481	3185.0726
3187.4720	3187.5019	3187.6273
3191.2450	3191.5925	3193.5763
3196.5610	3197.0862	3197.3535
3203.4497	3205.2517	3207.1876
3208.8303	3209.2556	3209.9043
3216.7128	3217.2707	3219.6512
3222.5037	3228.7372	3231.1080
3255.9374	3630.9300	3770.9063

### **TS5RR3**

Zero-point correction= 0.960683

Thermal correction to Energy= 1.018546

Thermal correction to Enthalpy= 1.019490

Thermal correction to Gibbs Free Energy= 0.865162

Sum of electronic and zero-point Energies= -2949.491853

Sum of electronic and thermal Energies= -2949.433991

Sum of electronic and thermal Enthalpies= -2949.433047

Sum of electronic and thermal Free Energies= -2949.587374

#### Cartesian coordinates

C	2.560346	-2.714967	3.197528
C	1.471007	-2.263553	2.409561
C	1.811436	-1.859411	1.056513
C	3.156572	-1.933917	0.619261
C	4.150987	-2.474163	1.437076
N	3.812606	-2.828382	2.716541
H	2.386156	-3.020057	4.220007
C	3.514738	-1.482399	-0.765858
C	3.164200	-2.327240	-1.870728
C	4.136572	-0.256566	-1.004619
C	2.553232	-3.601524	-1.688484
C	3.428485	-1.887393	-3.209548
C	4.419606	0.144960	-2.340145
C	2.206206	-4.380621	-2.768831
H	2.363182	-3.960638	-0.683884
C	3.056645	-2.715381	-4.302742
C	4.067919	-0.638567	-3.409554
H	4.950533	1.074385	-2.514507
C	2.453771	-3.933615	-4.089808
H	1.741476	-5.348204	-2.607611
H	3.258755	-2.366687	-5.311322
H	4.290808	-0.314568	-4.421673

H	2.170989	-4.557923	-4.931481
C	0.751099	-1.522636	0.147595
H	0.959745	-1.228014	-0.873629
O	0.287472	-2.243458	2.880605
C	5.563643	-2.703861	0.985640
H	5.652711	-2.481895	-0.075774
H	6.260702	-2.050688	1.516551
H	5.868280	-3.743316	1.139233
C	4.567051	0.648429	0.118777
O	5.021768	0.203208	1.186602
N	4.468013	1.976090	-0.114525
H	3.993201	2.271003	-0.952760
C	5.034253	3.015045	0.766940
C	4.247108	3.104112	2.098302
H	4.376703	4.091971	2.547597
H	3.172887	2.989129	1.882482
O	4.691689	2.163123	3.061066
H	4.811321	1.321976	2.575745
C	5.161311	4.362660	-0.008779
C	3.780085	4.997352	-0.268478
H	3.124699	4.347363	-0.858047
H	3.260741	5.236168	0.664421
H	3.897562	5.928655	-0.831086
C	5.886784	4.132230	-1.352593
H	6.103703	5.094901	-1.825652
H	6.834819	3.604880	-1.203149
H	5.290439	3.556438	-2.066790
C	6.022940	5.336593	0.821922
H	7.012529	4.912624	1.023147
H	6.162878	6.269877	0.267793
H	5.562156	5.592708	1.779344

N	-0.505545	-1.690581	0.495583
C	-1.635100	-1.543280	-0.304887
C	-2.765594	-2.342211	0.223839
O	-2.908057	-2.596812	1.414087
O	-3.575962	-2.716494	-0.770564
C	-4.665276	-3.704138	-0.576424
C	-5.688207	-3.218471	0.449799
H	-5.257032	-3.188454	1.450176
H	-6.034869	-2.220937	0.171067
H	-6.537618	-3.909786	0.451712
C	-5.291116	-3.768654	-1.968993
H	-4.547210	-4.065343	-2.714083
H	-6.104808	-4.499323	-1.978140
H	-5.693999	-2.789771	-2.241712
C	-4.029632	-5.039273	-0.184134
H	-4.802335	-5.812471	-0.139592
H	-3.282040	-5.339262	-0.924663
H	-3.552055	-4.966771	0.794631
P	-4.857492	0.814537	-0.310132
O	-5.996279	-0.123307	-0.657659
C	-5.263123	2.510129	-0.879619
C	-6.604829	2.917822	-0.909441
C	-4.263046	3.420518	-1.250311
C	-6.941203	4.215815	-1.296751
H	-7.381543	2.208711	-0.639090
C	-4.598631	4.720412	-1.634873
H	-3.225477	3.099923	-1.248368
C	-5.937491	5.119706	-1.657138
H	-7.983147	4.522030	-1.320470
H	-3.817702	5.418975	-1.921617
H	-6.198673	6.130085	-1.958423

C	-4.697261	0.988808	1.512663
C	-5.272315	0.021849	2.347682
C	-3.956898	2.033510	2.090276
C	-5.111793	0.095085	3.732925
H	-5.846448	-0.783823	1.905550
C	-3.794103	2.106511	3.474124
H	-3.510290	2.795460	1.457290
C	-4.371279	1.135740	4.298012
H	-5.564376	-0.659285	4.370148
H	-3.219480	2.919018	3.909239
H	-4.245311	1.192482	5.375286
N	-3.383059	0.522969	-0.970822
C	-2.240764	0.367727	-0.275321
C	-1.000898	0.959518	-0.862281
C	-0.805573	1.009605	-2.252155
C	-0.013943	1.480137	-0.017537
C	0.354707	1.565797	-2.781725
H	-1.579467	0.613184	-2.901341
C	1.138376	2.063891	-0.549843
H	-0.155220	1.444415	1.058867
C	1.328309	2.103774	-1.930118
H	0.501176	1.592848	-3.857298
H	1.879845	2.477154	0.122756
H	2.218754	2.555045	-2.358810
H	-1.448773	-1.647008	-1.368638
C	4.852588	-3.361885	3.623166
H	5.216749	-4.317482	3.243975
H	5.678800	-2.654425	3.690414
H	4.417960	-3.505724	4.609074
H	-2.258199	0.446479	0.818848
H	-0.619245	-1.952755	1.507721

H	6.046886	2.683840	1.028664
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Vibrational frequencies

-376.9881	7.5839	17.5322
19.1034	25.3399	27.5794
29.7617	35.8554	37.2684
41.4138	42.8806	43.6880
48.9685	53.0477	57.5160
60.7616	64.0414	70.3561
71.9599	75.9940	79.7741
82.2650	91.2480	95.3461
102.5670	110.7626	122.1475
128.6808	135.1665	140.9870
145.8104	149.2056	153.4548
157.6681	169.4950	174.5436
185.0185	195.8975	202.6937
210.1777	218.0062	222.8234
237.9896	239.5857	242.2497
243.5224	246.6794	251.1373
260.1174	270.2885	271.5385
287.9733	289.8046	297.8540
299.3416	305.1855	309.3086
311.3968	329.9436	334.6788
341.3939	347.8910	353.4417
359.9817	369.3489	376.9492
381.6716	382.6882	388.1592
397.4594	406.5945	409.6478
412.9918	413.2240	417.4805
420.1037	427.1171	434.2177
441.0260	444.8866	452.2923
462.7791	475.1240	479.9484

484.2884	484.6406	485.5401
510.6687	522.0862	532.2895
535.2978	538.7486	541.3149
548.5365	558.2975	561.1806
578.1149	581.3035	596.8446
613.6925	626.9468	628.4709
630.6641	632.0934	636.0141
643.0810	664.6587	674.9848
690.6829	700.7297	712.1092
712.8600	716.6096	725.4042
743.8750	747.2444	751.7951
755.3606	761.4870	764.9785
768.0477	770.4250	779.5007
780.0667	794.3616	799.3346
812.3219	817.5543	844.2590
852.0996	856.6421	861.8016
862.5861	871.2198	873.8126
874.9775	889.7849	890.0826
905.2986	911.6478	916.2308
924.3517	938.7707	939.3801
941.4744	942.5917	945.7700
947.5388	947.7758	974.1627
976.0566	978.2906	980.6987
987.4229	991.4655	991.7522
992.3357	999.8782	1003.5340
1008.4560	1009.5961	1011.0425
1012.5571	1014.1660	1014.9151
1028.5423	1031.9958	1036.3974
1049.3723	1050.2624	1054.2617
1055.7447	1059.0051	1060.9365
1067.4667	1077.7362	1082.8036

1085.7493	1098.0501	1099.6452
1101.1822	1103.1642	1109.9630
1113.5853	1119.8545	1122.1345
1127.9458	1132.4716	1144.6632
1153.2293	1169.4815	1183.6382
1184.6039	1189.4740	1190.1904
1191.1168	1200.2461	1202.9198
1206.2440	1207.8730	1211.3828
1215.9795	1219.3838	1221.0088
1235.5417	1248.8791	1251.7306
1254.3399	1261.9455	1262.9726
1265.0361	1280.6829	1281.3719
1284.9553	1293.8445	1306.8787
1320.0912	1325.4600	1325.5130
1328.0673	1334.9132	1344.4287
1353.3257	1356.6308	1357.2232
1360.4396	1367.8812	1386.0412
1399.6745	1408.9460	1409.0798
1409.6507	1411.7532	1415.2368
1417.3023	1421.7684	1427.4033
1429.4831	1436.1855	1438.2552
1451.3798	1455.2978	1461.6120
1465.5763	1473.1712	1475.1140
1480.1550	1481.6342	1481.9091
1487.7171	1490.9888	1493.4827
1495.6452	1498.5329	1499.3082
1499.8783	1501.5126	1504.9979
1506.9937	1512.6907	1513.6407
1516.0517	1516.7008	1519.5874
1521.1437	1523.4317	1523.6877
1531.5596	1535.1391	1548.1780



1549.0061	1552.8336	1552.8895
1578.4259	1607.4684	1622.4456
1625.1274	1626.2720	1637.3619
1643.1870	1643.9397	1645.4585
1655.3528	1669.0628	1670.9591
1691.7549	1741.0615	2946.5620
2985.4341	3033.1062	3042.4810
3044.2383	3048.5110	3048.9927
3050.4682	3052.4360	3056.6175
3063.6024	3090.6545	3100.0068
3112.5056	3113.2082	3117.8043
3118.7650	3122.2605	3124.3671
3128.3065	3129.4098	3130.7297
3132.5614	3141.2576	3150.5274
3170.3984	3174.7534	3177.0860
3178.0982	3179.7272	3180.5767
3183.9231	3185.5757	3187.7943
3187.8011	3193.0270	3193.4620
3193.6574	3194.6874	3196.2637
3197.3497	3200.2878	3202.1633
3205.3977	3207.1754	3210.5057
3210.9475	3213.1558	3223.2468
3229.5611	3229.6668	3233.7752
3255.6717	3564.1701	3666.1941

### **TS5RS**

Zero-point correction= 0.961281

Thermal correction to Energy= 1.018979

Thermal correction to Enthalpy= 1.019924

Thermal correction to Gibbs Free Energy= 0.868020

Sum of electronic and zero-point Energies= -2949.520532

Sum of electronic and thermal Energies= -2949.462834

Sum of electronic and thermal Enthalpies= -2949.461890

Sum of electronic and thermal Free Energies= -2949.613794

Cartesian coordinates

C	2.417517	-0.809717	4.082289
C	1.344061	-0.269765	3.314238
C	1.602960	-0.189802	1.890251
C	2.818490	-0.669245	1.355864
C	3.817288	-1.182185	2.185617
N	3.568396	-1.233398	3.535461
H	2.310549	-0.896541	5.154749
C	3.035715	-0.688510	-0.128720
C	2.897134	-1.927499	-0.834019
C	3.323667	0.472012	-0.835437
C	2.535141	-3.139817	-0.183468
C	3.120667	-1.952828	-2.251491
C	3.525720	0.439228	-2.240001
C	2.425687	-4.314344	-0.891256
H	2.318093	-3.127740	0.878241
C	3.004749	-3.184570	-2.949911
C	3.444268	-0.746909	-2.926710
H	3.763161	1.361539	-2.759855
C	2.668416	-4.341098	-2.285019
H	2.120891	-5.222779	-0.384326
H	3.177863	-3.192602	-4.022270
H	3.617605	-0.773047	-3.998432
H	2.566952	-5.274522	-2.828463
C	0.631122	0.420673	1.034207
H	0.871089	0.614463	0.002857
O	0.272135	0.110794	3.870807

C	5.147207	-1.665956	1.681520
H	5.251240	-1.424329	0.625626
H	5.977380	-1.190995	2.211842
H	5.255371	-2.750873	1.789843
C	3.374982	1.786025	-0.111767
O	4.097565	1.957565	0.883457
N	2.545366	2.728027	-0.610818
H	1.924663	2.446324	-1.358965
C	2.420691	4.100718	-0.083512
C	1.799840	4.082180	1.335241
H	1.342370	5.049442	1.558143
H	0.994593	3.331427	1.357310
O	2.761342	3.850123	2.352767
H	3.334463	3.127673	2.027035
C	1.668216	4.999030	-1.112986
C	0.177752	4.616268	-1.202572
H	0.034766	3.580758	-1.524219
H	-0.336303	4.753109	-0.245952
H	-0.327059	5.244788	-1.942393
C	2.319035	4.862248	-2.506436
H	1.874197	5.588418	-3.194045
H	3.396137	5.054718	-2.458092
H	2.168594	3.873464	-2.948271
C	1.796285	6.473341	-0.678564
H	2.847389	6.771659	-0.601412
H	1.316860	7.119101	-1.420880
H	1.316028	6.670458	0.283376
N	-0.496405	0.921216	1.488650
C	-1.444041	1.482226	0.632152
C	-2.747113	1.698906	1.283717
O	-3.059817	1.212517	2.363682

O	-3.542454	2.430802	0.482775
C	-4.967432	2.669399	0.794017
C	-5.083318	3.477789	2.087989
H	-4.734556	2.898570	2.942888
H	-4.492145	4.395625	2.014509
H	-6.129346	3.754689	2.250175
C	-5.435784	3.490446	-0.407160
H	-5.333300	2.914475	-1.331510
H	-6.487725	3.762440	-0.284073
H	-4.846130	4.406897	-0.499312
C	-5.703806	1.332056	0.865425
H	-6.778064	1.512338	0.970109
H	-5.539761	0.756752	-0.050178
H	-5.362021	0.734723	1.709237
P	-1.444609	-2.229468	0.383619
O	-0.844775	-2.382227	1.764699
C	-1.073724	-3.690961	-0.650234
C	-0.947010	-4.941747	-0.028756
C	-0.957261	-3.602500	-2.043705
C	-0.712500	-6.087727	-0.789252
H	-1.017622	-5.007066	1.052871
C	-0.725185	-4.749239	-2.805097
H	-1.028659	-2.630097	-2.520809
C	-0.603937	-5.992473	-2.179799
H	-0.610436	-7.052244	-0.300158
H	-0.627709	-4.671735	-3.884036
H	-0.419357	-6.883626	-2.772718
C	-3.278906	-2.224534	0.498140
C	-3.878497	-2.116096	1.759266
C	-4.093003	-2.317466	-0.641940
C	-5.269323	-2.115603	1.882667

H	-3.243739	-2.037991	2.635682
C	-5.482919	-2.310282	-0.519820
H	-3.639652	-2.407833	-1.625454
C	-6.072511	-2.213700	0.744359
H	-5.725857	-2.036253	2.865028
H	-6.105211	-2.384488	-1.406863
H	-7.154315	-2.211523	0.840011
N	-0.946722	-0.963128	-0.554084
C	-1.691264	0.134070	-0.815701
C	-1.264408	0.934515	-2.014400
C	-0.007488	0.729621	-2.603393
C	-2.106930	1.922025	-2.544876
C	0.402953	1.507274	-3.688866
H	0.629798	-0.057566	-2.216343
C	-1.702850	2.688772	-3.638466
H	-3.071702	2.099149	-2.079253
C	-0.443487	2.489674	-4.211221
H	1.379611	1.333975	-4.131085
H	-2.367594	3.449048	-4.038046
H	-0.124867	3.092897	-5.055794
H	-1.081946	2.307812	0.031307
C	4.605032	-1.774670	4.442390
H	4.883606	-2.778696	4.123100
H	5.481923	-1.126674	4.424570
H	4.203352	-1.813597	5.451726
H	-2.780088	0.078983	-0.712817
H	-0.721988	0.676353	2.468407
H	3.439957	4.491630	0.024396

Vibrational frequencies

-357.8197                      14.5870                      16.2592

22.9753	25.8304	32.6734
34.2250	37.6172	42.5142
47.5791	49.1085	52.9526
54.6664	58.7599	61.9372
65.4759	68.6937	71.4347
75.3006	79.1158	82.9617
89.6275	95.1919	98.6513
103.3569	105.0223	110.6434
123.2691	130.0602	132.8531
140.9775	149.4246	156.7042
164.1234	169.7730	177.0413
186.5848	194.9768	197.9914
208.3435	220.2210	224.1312
232.2506	235.9996	243.0138
244.0196	245.0311	257.8130
263.4605	263.7415	271.1206
280.8141	283.5035	293.0593
298.7442	301.0659	304.0148
316.8079	325.5490	331.9970
342.9038	343.2419	355.7667
364.8668	372.7618	375.7633
378.0820	385.8079	398.0950
399.5809	407.5354	408.0428
410.0459	416.4437	422.4714
423.6140	437.8722	440.4023
445.5101	449.0750	457.6931
462.2771	471.1160	475.7105
480.6117	486.1460	497.4691
520.2044	524.0673	533.3881
536.4144	541.3766	552.3311
555.2496	573.2683	577.6168

584.3965	589.9212	601.1252
608.4931	614.3496	625.7125
630.1353	631.5884	633.9367
647.6775	665.1793	671.7192
696.0438	702.8140	709.2294
710.9682	717.8103	727.0390
740.2080	750.9862	754.2279
756.9196	761.6376	763.0913
763.9606	767.8602	776.8222
783.5808	795.6410	798.0459
812.1405	822.6071	843.8366
850.3066	851.7820	857.4832
864.1190	869.5676	870.3488
875.9833	886.8935	887.4081
890.9878	904.1510	910.7801
930.2397	935.6530	936.7524
939.4792	940.7447	943.7102
946.5748	951.4047	953.4324
970.1458	979.6063	979.9794
985.0851	986.3178	986.9032
987.7232	987.9774	991.6492
1002.2627	1006.9377	1007.1991
1010.5492	1012.6105	1013.5112
1017.6376	1027.9479	1032.0515
1036.6726	1049.5603	1050.2546
1052.6914	1055.9798	1056.2606
1062.9716	1063.3520	1070.4085
1080.1691	1086.6361	1100.1429
1101.1010	1102.6349	1104.8618
1112.5461	1116.9483	1120.5468
1129.9803	1133.0909	1145.5205

1154.0297	1175.6980	1182.1729
1184.3995	1186.9687	1190.2527
1191.2167	1192.1192	1201.6594
1203.0240	1204.1901	1209.6321
1211.9281	1219.8848	1221.0192
1233.4151	1247.6500	1249.2170
1256.1326	1261.3281	1262.9204
1264.7301	1277.1078	1282.3709
1290.4059	1292.6921	1313.1252
1314.1123	1325.4070	1325.6583
1327.7043	1329.8035	1343.4437
1353.2825	1357.8182	1359.0932
1360.9984	1363.5561	1388.3060
1404.6396	1409.1560	1409.6057
1413.3816	1414.6805	1415.3160
1423.2446	1427.3877	1429.9648
1430.9077	1436.9460	1439.2884
1441.8179	1454.0044	1456.4244
1467.2097	1473.9735	1476.0117
1478.5113	1480.3998	1483.5220
1489.2414	1492.2348	1495.0866
1496.0447	1496.9957	1498.5699
1499.5138	1501.2593	1502.3905
1502.7841	1507.3153	1511.0517
1513.7608	1518.2898	1520.7182
1521.1458	1522.1176	1525.3725
1530.7922	1532.5902	1533.2331
1548.9273	1555.5282	1558.2212
1583.9416	1613.5974	1625.0037
1626.3448	1632.2680	1643.1142
1643.5765	1644.4172	1646.5510



1651.4969	1663.3282	1672.7406
1701.2606	1741.2765	2997.2973
3041.9276	3045.0171	3050.3223
3050.4267	3051.0381	3053.6962
3054.5981	3055.0985	3061.6305
3093.1391	3101.6212	3111.7580
3112.1354	3115.3604	3118.4542
3123.1258	3123.6132	3126.2937
3127.9668	3130.1876	3131.0875
3136.4713	3167.0389	3176.6663
3177.5265	3177.6095	3178.3176
3178.7184	3181.8651	3183.1329
3185.3271	3186.4645	3190.0158
3190.7762	3192.6366	3194.1306
3199.8838	3201.2209	3203.8292
3204.7244	3206.3209	3206.8703
3208.0118	3208.7971	3210.7290
3211.1400	3215.0432	3217.4843
3227.8831	3234.7281	3254.1440
3304.9355	3569.0795	3595.0333

### **TS5RS1**

Zero-point correction= 0.961633

Thermal correction to Energy= 1.019194

Thermal correction to Enthalpy= 1.020138

Thermal correction to Gibbs Free Energy= 0.867559

Sum of electronic and zero-point Energies= -2949.522846

Sum of electronic and thermal Energies= -2949.465285

Sum of electronic and thermal Enthalpies= -2949.464340

Sum of electronic and thermal Free Energies= -2949.616920

Cartesian coordinates

C	3.503889	-3.923723	-1.368902
C	2.246275	-3.259398	-1.363525
C	2.253038	-1.940729	-0.757982
C	3.445015	-1.419087	-0.197933
C	4.624486	-2.169238	-0.200614
N	4.609144	-3.398258	-0.814322
H	3.586577	-4.901834	-1.822253
C	3.458226	-0.053426	0.421395
C	4.173066	1.011182	-0.222994
C	2.770264	0.202468	1.601315
C	4.844940	0.843403	-1.466704
C	4.224493	2.299236	0.407227
C	2.777252	1.497237	2.179739
C	5.565717	1.874157	-2.028467
H	4.786356	-0.111176	-1.977228
C	4.979395	3.340108	-0.197533
C	3.504613	2.512670	1.611400
H	2.214191	1.664624	3.091451
C	5.646262	3.132396	-1.383359
H	6.073787	1.722448	-2.975667
H	5.013481	4.308588	0.293083
H	3.530472	3.495383	2.072839
H	6.220395	3.934695	-1.835921
C	1.019697	-1.229469	-0.631978
H	0.976659	-0.237089	-0.199179
O	1.216825	-3.805055	-1.868198
C	5.898903	-1.716352	0.455157
H	5.704312	-0.844915	1.076755
H	6.318884	-2.493778	1.098630
H	6.661870	-1.438403	-0.280435

C	2.038514	-0.901762	2.318249
O	2.639314	-1.927720	2.687508
N	0.726357	-0.680414	2.527848
H	0.293049	0.113008	2.043958
C	-0.094196	-1.595884	3.332363
C	-0.564563	-2.808273	2.501233
H	-0.999808	-3.545727	3.190342
H	-1.352718	-2.509965	1.804476
O	0.472543	-3.399100	1.728534
H	1.320723	-3.197996	2.164647
C	-1.241311	-0.829690	4.062731
C	-2.250799	-0.197514	3.081781
H	-1.780256	0.549499	2.439327
H	-2.731874	-0.940986	2.439848
H	-3.041171	0.307794	3.647241
C	-0.617854	0.288024	4.923329
H	-1.397090	0.802100	5.495633
H	0.112105	-0.117820	5.632630
H	-0.111209	1.035098	4.305754
C	-1.988491	-1.808768	4.991621
H	-1.296908	-2.339424	5.655737
H	-2.697792	-1.256909	5.617044
H	-2.560321	-2.552375	4.428740
N	-0.132033	-1.791821	-0.915933
C	-1.369711	-1.229933	-0.605980
C	-2.466557	-2.202124	-0.695870
O	-2.400242	-3.257090	-1.316549
O	-3.537463	-1.743382	-0.023872
C	-4.763380	-2.549326	0.145218
C	-4.421229	-3.812576	0.938675
H	-3.760374	-4.464651	0.366388

H	-3.929816	-3.546931	1.879867
H	-5.340260	-4.358139	1.172257
C	-5.659767	-1.614648	0.957196
H	-5.839964	-0.687291	0.405986
H	-6.621005	-2.097346	1.154394
H	-5.191180	-1.365136	1.913393
C	-5.393081	-2.863264	-1.213167
H	-6.356427	-3.357984	-1.055582
H	-5.561594	-1.941273	-1.774054
H	-4.750387	-3.516507	-1.802586
P	-1.149554	2.173387	-0.087025
O	-0.215584	1.362962	0.815106
C	-2.184170	3.273211	0.919277
C	-1.717025	3.636660	2.191007
C	-3.419125	3.761647	0.468712
C	-2.473601	4.483914	3.001074
H	-0.771123	3.236220	2.542480
C	-4.171696	4.612965	1.279305
H	-3.791494	3.459130	-0.504536
C	-3.699557	4.975346	2.543993
H	-2.111041	4.756526	3.987751
H	-5.128638	4.987526	0.928148
H	-4.288995	5.634530	3.174492
C	-0.111531	3.225860	-1.162990
C	1.227747	2.865056	-1.362561
C	-0.643777	4.316644	-1.868329
C	2.023286	3.573912	-2.265509
H	1.644004	2.039514	-0.798033
C	0.155259	5.033990	-2.757781
H	-1.678620	4.610152	-1.715310
C	1.487974	4.659076	-2.961799

H	3.057505	3.282174	-2.412978
H	-0.259222	5.882974	-3.293566
H	2.106790	5.216001	-3.659410
N	-2.212529	1.359444	-1.043287
C	-1.731889	0.351576	-1.808145
C	-2.620559	-0.193888	-2.875071
C	-3.972076	0.167303	-2.946302
C	-2.104663	-1.093019	-3.820844
C	-4.789852	-0.352782	-3.949963
H	-4.361683	0.860929	-2.209645
C	-2.921842	-1.616627	-4.820920
H	-1.059743	-1.387837	-3.762795
C	-4.268877	-1.247039	-4.889164
H	-5.835293	-0.061578	-3.998747
H	-2.510082	-2.311374	-5.547047
H	-4.906370	-1.652477	-5.669319
H	-1.346832	-0.619382	0.284170
C	5.851194	-4.201357	-0.866923
H	6.657457	-3.604004	-1.291462
H	6.122615	-4.525590	0.138389
H	5.678127	-5.072530	-1.493629
H	-0.673695	0.361043	-2.116148
H	-0.062040	-2.733204	-1.355050
H	0.579285	-1.985572	4.105609

Vibrational frequencies

-383.6295	8.2794	18.7619
22.7209	27.2657	29.0132
29.5785	34.1907	38.8416
40.4705	43.5463	48.0275
50.5040	50.5732	55.7613

60.1178	63.8069	72.6944
77.9585	81.4828	86.1618
92.4530	97.6374	104.0430
112.1742	126.8052	131.6933
136.4299	139.4092	144.9019
149.2099	152.2261	157.5712
162.5649	174.5519	184.7289
188.8394	191.7840	199.2286
209.2243	218.1191	219.2063
221.1608	236.9175	242.3323
246.6741	249.3051	253.7986
256.1438	265.2164	273.8441
278.5606	280.4483	286.2766
289.5048	298.0076	308.0655
312.7759	317.5093	332.6861
343.9376	353.9702	357.4190
358.8027	364.4403	374.6370
383.7546	390.1863	403.3360
408.1536	409.3952	411.5562
412.6934	413.7733	416.7623
423.9263	429.2834	438.6627
440.3198	446.1344	451.9895
458.1853	466.1482	473.3072
479.1941	483.9186	510.7651
525.3689	530.5830	533.2731
537.6812	541.5673	547.1160
551.1686	553.7701	561.1365
576.3041	582.1602	601.7634
609.4924	630.2027	631.8555
632.3067	635.3864	649.4188
662.1245	673.5206	700.0883

704.9208	709.2138	711.0149
715.0713	736.1876	742.9629
744.8558	750.8828	759.3471
760.8848	764.4681	769.4309
770.5975	774.4144	777.2428
793.4024	797.1782	805.3639
817.6157	827.8733	847.9520
849.0638	849.8870	864.8347
866.2901	872.8185	873.8532
886.1389	890.9369	894.3664
906.2028	917.3766	933.4401
933.6758	937.4637	939.2550
943.8410	947.1814	949.4673
950.2701	958.2427	963.8997
971.4495	976.7483	981.1098
982.9776	983.2915	987.7685
990.0273	992.5970	1003.4539
1004.2159	1011.0334	1012.3708
1013.5506	1014.3712	1015.4243
1020.1364	1029.2920	1046.2341
1049.7346	1050.5622	1052.0486
1052.2706	1057.1726	1061.1089
1062.9650	1070.7145	1079.2972
1083.7503	1089.4769	1096.3328
1105.5974	1107.4029	1111.1434
1116.7282	1128.9821	1133.0179
1136.1088	1141.4284	1143.5353
1147.5668	1154.7243	1182.5038
1188.0999	1189.6516	1191.3849
1193.2159	1194.5413	1199.6500
1201.4574	1205.7361	1208.5017

1216.6319	1218.6584	1221.4656
1228.5543	1246.1831	1253.8713
1258.4693	1262.0538	1265.6145
1274.8977	1276.0551	1287.6834
1290.0029	1295.6641	1306.2382
1325.7080	1327.6734	1330.4558
1331.1652	1339.6993	1346.2148
1354.4371	1355.1862	1361.0763
1361.8533	1365.8509	1395.5566
1402.8481	1406.9882	1410.4555
1414.3627	1417.4966	1418.3406
1420.6676	1425.7155	1430.3041
1433.1922	1436.4305	1437.6179
1450.2011	1452.9396	1459.9709
1466.0159	1474.2334	1476.5732
1478.9044	1479.9522	1480.5675
1487.5585	1490.1230	1492.8803
1493.7718	1496.0712	1497.6989
1500.8553	1503.0651	1504.4448
1505.3557	1508.5208	1511.2413
1512.2378	1520.2657	1521.6546
1524.6480	1524.8280	1531.1385
1532.9551	1534.7038	1537.0106
1548.2235	1553.4117	1576.9216
1598.7838	1612.4025	1624.8491
1626.5841	1633.4513	1635.4562
1644.0078	1645.4716	1646.2000
1654.3058	1666.3867	1670.9789
1687.4901	1739.0203	2961.4830
3013.1045	3035.3613	3039.1935
3045.7365	3050.1919	3050.8476



3053.9974	3054.6883	3063.9856
3092.6633	3105.0396	3105.3085
3109.4121	3114.9581	3116.2810
3117.2720	3121.2627	3123.8153
3125.6755	3130.0572	3134.1467
3140.2618	3146.7630	3159.3546
3172.5324	3172.5466	3177.8320
3179.8989	3180.2524	3180.9239
3182.4524	3185.9486	3189.3544
3191.0002	3191.3037	3191.4686
3195.0527	3199.6498	3202.5737
3204.6448	3204.7813	3206.6918
3208.4016	3211.9436	3212.1822
3216.5802	3217.3516	3218.4986
3218.9879	3236.2974	3250.1288
3255.6266	3356.8077	3635.2274

## TS5RS2

Zero-point correction= 0.961849

Thermal correction to Energy= 1.019397

Thermal correction to Enthalpy= 1.020341

Thermal correction to Gibbs Free Energy= 0.869552

Sum of electronic and zero-point Energies= -2949.519537

Sum of electronic and thermal Energies= -2949.461990

Sum of electronic and thermal Enthalpies= -2949.461046

Sum of electronic and thermal Free Energies= -2949.611834

## Cartesian coordinates

C	-3.512274	-1.003126	2.861895
C	-2.284582	-1.242261	2.178728
C	-1.913947	-0.219882	1.220176

C	-2.710890	0.945296	1.075060
C	-3.862944	1.125380	1.837964
N	-4.239041	0.110385	2.688011
H	-3.888734	-1.747140	3.550246
C	-2.357486	1.969919	0.036823
C	-1.241014	2.845837	0.237616
C	-3.120255	2.084273	-1.121562
C	-0.404204	2.765443	1.385793
C	-0.926661	3.817965	-0.768852
C	-2.848097	3.104029	-2.069055
C	0.725010	3.546378	1.494074
H	-0.662028	2.073718	2.179129
C	0.236217	4.619969	-0.617567
C	-1.773602	3.941974	-1.902829
H	-3.494934	3.190893	-2.935044
C	1.056392	4.475288	0.478373
H	1.371569	3.446401	2.359686
H	0.476361	5.339445	-1.394926
H	-1.546732	4.698598	-2.647897
H	1.961929	5.064021	0.566491
C	-0.750816	-0.410080	0.415781
H	-0.478607	0.310733	-0.347630
O	-1.612288	-2.297488	2.385956
C	-4.732198	2.347955	1.764197
H	-4.243612	3.119218	1.172842
H	-5.689689	2.111575	1.292299
H	-4.928583	2.762888	2.756300
C	-4.296044	1.187431	-1.408066
O	-5.395692	1.660907	-1.733353
N	-4.059715	-0.137091	-1.308807
H	-3.134011	-0.433189	-1.044434

C	-5.075164	-1.173792	-1.496152
C	-5.920503	-1.330021	-0.216740
H	-6.747943	-2.021501	-0.420175
H	-5.316512	-1.756446	0.590859
O	-6.425004	-0.086233	0.266004
H	-6.516399	0.521431	-0.487192
C	-4.409291	-2.488063	-2.011051
C	-3.366534	-3.043425	-1.016249
H	-2.518877	-2.366270	-0.864460
H	-3.799546	-3.260718	-0.035929
H	-2.950467	-3.976698	-1.407822
C	-3.717224	-2.194025	-3.358424
H	-3.261193	-3.107354	-3.753252
H	-4.439077	-1.829089	-4.097049
H	-2.927739	-1.442884	-3.259828
C	-5.499230	-3.554008	-2.240982
H	-6.308546	-3.164304	-2.867850
H	-5.067760	-4.421366	-2.750019
H	-5.933320	-3.908321	-1.301849
N	0.045008	-1.447155	0.566779
C	1.299456	-1.550351	-0.038058
C	1.887227	-2.906281	0.020916
O	1.600517	-3.739034	0.870818
O	2.807541	-3.023362	-0.942290
C	3.761387	-4.148120	-1.009272
C	3.001148	-5.453527	-1.249866
H	2.379134	-5.706467	-0.390955
H	2.364432	-5.361466	-2.134963
H	3.715770	-6.263848	-1.423051
C	4.622613	-3.774840	-2.216495
H	5.112568	-2.810620	-2.053017

H	5.387166	-4.540040	-2.378545
H	4.005630	-3.703977	-3.117271
C	4.599328	-4.179758	0.269435
H	5.376282	-4.944367	0.175833
H	5.077045	-3.208281	0.419801
H	3.981548	-4.409940	1.138155
P	4.149890	0.497815	-0.899649
O	5.419213	0.007384	-1.564125
C	4.303091	2.235451	-0.319966
C	4.422657	3.284700	-1.245370
C	4.359629	2.528077	1.050193
C	4.607793	4.596896	-0.810149
H	4.362707	3.075114	-2.310017
C	4.548282	3.841221	1.487547
H	4.255456	1.721867	1.769571
C	4.677669	4.876212	0.558570
H	4.696963	5.400941	-1.534771
H	4.592477	4.055949	2.551339
H	4.824645	5.897408	0.897948
C	2.773368	0.552768	-2.113502
C	2.767515	-0.414670	-3.130755
C	1.648842	1.380345	-1.953976
C	1.651168	-0.576179	-3.952192
H	3.635377	-1.053204	-3.254763
C	0.530892	1.217375	-2.777329
H	1.639328	2.149472	-1.187341
C	0.525704	0.231608	-3.767959
H	1.655653	-1.335494	-4.728761
H	-0.335040	1.856697	-2.646787
H	-0.349584	0.100626	-4.397571
N	3.708278	-0.400733	0.401900

C	2.456841	-0.397627	0.928123
C	2.347167	-0.855560	2.356359
C	3.265258	-1.770757	2.890041
C	1.317679	-0.378584	3.179623
C	3.144863	-2.211154	4.206558
H	4.071991	-2.123272	2.259252
C	1.193942	-0.818482	4.498747
H	0.614528	0.349359	2.790029
C	2.105602	-1.740300	5.015856
H	3.862898	-2.922825	4.604322
H	0.388869	-0.436372	5.119643
H	2.012796	-2.084380	6.041783
H	1.337909	-1.085516	-1.014990
C	-5.530960	0.212943	3.404316
H	-5.521787	1.080349	4.064047
H	-6.324069	0.301160	2.661433
H	-5.674375	-0.688085	3.995561
H	1.803843	0.476415	0.749791
H	-0.244164	-2.105293	1.320746
H	-5.742818	-0.807186	-2.285572

Vibrational frequencies

-337.7849	8.5805	20.6199
27.6606	29.5118	34.5853
37.3795	42.5821	42.8801
46.4987	48.2702	54.7247
58.2331	62.2695	64.6278
67.4419	68.8131	76.6819
84.4445	87.3135	92.1503
96.0593	98.0306	100.3666
103.4919	113.7636	124.1251

124.7518	133.4562	140.4086
144.7601	154.1380	155.5516
161.5075	164.6632	179.4780
194.2252	199.3358	201.4869
204.0676	221.8008	223.2453
235.0252	243.0094	245.4069
249.9404	254.7901	256.9950
265.4909	273.5220	280.4136
284.8302	286.3109	289.9446
292.5908	301.8019	312.1672
315.3841	320.3538	338.0494
341.1708	351.7521	354.9406
358.5156	363.0292	367.2240
369.8254	384.3189	385.7693
397.2217	408.0070	411.1350
412.0564	413.3510	414.4650
422.2812	424.2596	433.6252
437.5721	444.1418	446.2396
448.9140	469.6238	474.9918
480.9075	483.0903	501.2841
511.1610	513.3240	523.3176
530.7842	532.4210	535.0715
550.6664	552.8042	557.1397
561.8403	573.4451	576.7379
595.4325	614.7423	628.2337
631.7473	632.7753	634.9511
646.5984	664.0159	669.3964
697.9849	699.5871	712.0101
712.6642	715.6839	726.0733
748.7528	750.4661	753.4004
759.1198	765.5343	766.8995

769.6490	770.8809	779.3360
786.1504	793.0972	798.1982
815.5215	830.6783	840.5396
851.8299	860.4774	864.0477
866.6196	871.8529	879.4526
883.0570	886.3457	891.2374
913.2099	914.8859	923.1863
933.1265	938.4857	939.6816
943.3379	944.4238	944.8318
945.5736	952.4061	970.8708
975.7863	978.3261	981.5751
982.3881	987.3198	990.0435
991.0218	994.2988	1003.1789
1007.5084	1010.8736	1012.4463
1013.4570	1014.1841	1017.1611
1017.5462	1030.8180	1046.8919
1049.3054	1049.6105	1053.7992
1055.2979	1059.0606	1060.7390
1068.0597	1070.3164	1076.2946
1080.0591	1080.7527	1100.8748
1105.3066	1110.1929	1110.2413
1116.4260	1127.2865	1129.1381
1136.5051	1152.0311	1152.7120
1170.4235	1178.8370	1183.0570
1189.0500	1191.0542	1191.2725
1192.8346	1197.2060	1206.6597
1208.0830	1209.4938	1211.6759
1213.3026	1214.6462	1222.4829
1227.3163	1246.3219	1253.5587
1254.7778	1257.7876	1265.2303
1269.9648	1279.9184	1280.1697

1291.1439	1292.3747	1305.4466
1311.6393	1321.2375	1325.6344
1327.9855	1339.9553	1342.7522
1356.7419	1357.5130	1359.4571
1360.6890	1364.5693	1391.1049
1399.4226	1406.7161	1408.5031
1411.7044	1412.6042	1417.9511
1422.2158	1423.3749	1425.2560
1426.5707	1436.6690	1441.7447
1441.9588	1454.1822	1460.3254
1467.5453	1470.4034	1471.8490
1474.4296	1479.1818	1481.8011
1485.5444	1492.3824	1493.8768
1495.4267	1499.2745	1499.5128
1500.8587	1501.0446	1502.6583
1506.2521	1506.4194	1513.9204
1517.0157	1518.2442	1520.7871
1522.2135	1523.1065	1527.3649
1529.9762	1534.0056	1540.1328
1543.5052	1551.3836	1563.3060
1586.2531	1606.8446	1621.8158
1624.0639	1634.3331	1636.9920
1640.7653	1643.2849	1643.6756
1656.2006	1665.7733	1670.2308
1698.6097	1751.8172	2920.4378
3032.8668	3039.0343	3042.6602
3047.9894	3048.1049	3052.1852
3054.5871	3061.7966	3069.0838
3090.1790	3091.3762	3109.3422
3111.6914	3114.7507	3117.9968
3118.2967	3121.3677	3123.3869



3127.9261	3128.6796	3132.8365
3133.3952	3138.7420	3160.8236
3163.4730	3177.0060	3178.7353
3183.2590	3183.2982	3183.7238
3184.0895	3187.7300	3192.1361
3192.3819	3195.0676	3196.5249
3199.4959	3200.6682	3201.0936
3201.7429	3202.0094	3207.8234
3212.9581	3214.9777	3215.6096
3218.4706	3220.5897	3226.5642
3230.5841	3230.7720	3237.1370
3254.3965	3667.7358	3700.5227

### TS5RS3

Zero-point correction= 0.961406

Thermal correction to Energy= 1.019167

Thermal correction to Enthalpy= 1.020111

Thermal correction to Gibbs Free Energy= 0.866925

Sum of electronic and zero-point Energies= -2949.513510

Sum of electronic and thermal Energies= -2949.455750

Sum of electronic and thermal Enthalpies= -2949.454806

Sum of electronic and thermal Free Energies= -2949.607992

### Cartesian coordinates

C	-3.481850	-1.828300	3.321634
C	-2.221039	-1.732215	2.667940
C	-2.105225	-0.631404	1.731918
C	-3.217826	0.197380	1.466863
C	-4.429222	0.010388	2.128538
N	-4.507682	-1.002760	3.052799
H	-3.641246	-2.603838	4.058092

C	-3.109457	1.252565	0.409115
C	-2.822069	2.603565	0.773060
C	-3.230249	0.905976	-0.930600
C	-2.631919	3.001284	2.125106
C	-2.707713	3.594186	-0.256842
C	-3.126663	1.897354	-1.940707
C	-2.340257	4.309234	2.439381
H	-2.709745	2.258243	2.911458
C	-2.410368	4.936258	0.102200
C	-2.885287	3.209395	-1.610268
H	-3.257369	1.610247	-2.979298
C	-2.226727	5.287250	1.420424
H	-2.192775	4.595761	3.476046
H	-2.324665	5.679695	-0.685279
H	-2.815247	3.964933	-2.387295
H	-1.994214	6.314247	1.684359
C	-0.867729	-0.412779	1.046982
H	-0.704956	0.481257	0.449128
O	-1.289871	-2.563685	2.907285
C	-5.663376	0.811332	1.831981
H	-5.425644	1.607753	1.129998
H	-6.435446	0.184737	1.372894
H	-6.087217	1.269360	2.730143
C	-3.503629	-0.524274	-1.321930
O	-4.444087	-1.159245	-0.818685
N	-2.654425	-1.016304	-2.251468
H	-1.915713	-0.392264	-2.549231
C	-2.601775	-2.364920	-2.851084
C	-3.970209	-3.076772	-2.858193
H	-3.898271	-3.917277	-3.553091
H	-4.195940	-3.476736	-1.865648

O	-5.025734	-2.246698	-3.320330
H	-5.270230	-1.716706	-2.543588
C	-1.450197	-3.220757	-2.219952
C	-1.712643	-3.497761	-0.726945
H	-1.988264	-2.584924	-0.196858
H	-2.519713	-4.221818	-0.582343
H	-0.812401	-3.899736	-0.251227
C	-0.123659	-2.454056	-2.375414
H	0.705838	-3.042543	-1.974201
H	0.095028	-2.240117	-3.425995
H	-0.134726	-1.501209	-1.842306
C	-1.319641	-4.555330	-2.980590
H	-1.192046	-4.389580	-4.056467
H	-0.441492	-5.101415	-2.620330
H	-2.189361	-5.202192	-2.834313
N	0.112311	-1.281803	1.127998
C	1.366451	-1.128231	0.522647
C	2.105221	-2.407046	0.468682
O	1.818181	-3.392448	1.138453
O	3.128021	-2.300716	-0.389280
C	4.051893	-3.422102	-0.660430
C	3.276759	-4.564130	-1.320832
H	2.527040	-4.970463	-0.640563
H	2.781396	-4.212692	-2.230759
H	3.971649	-5.363118	-1.595947
C	5.044751	-2.792091	-1.636694
H	5.559991	-1.950755	-1.164571
H	5.789195	-3.531806	-1.943558
H	4.524843	-2.427130	-2.527273
C	4.751487	-3.857692	0.628112
H	5.536180	-4.579920	0.382791

H	5.209582	-2.995413	1.117611
H	4.048725	-4.319240	1.321325
P	1.813346	2.111655	-0.214209
O	0.435259	2.388949	0.366614
C	1.588278	1.354453	-1.877892
C	0.378355	1.573149	-2.553736
C	2.572494	0.550888	-2.471905
C	0.159564	1.007094	-3.811230
H	-0.386459	2.177432	-2.079368
C	2.350968	-0.019150	-3.727334
H	3.491194	0.348213	-1.931106
C	1.148005	0.211916	-4.400266
H	-0.777293	1.186950	-4.332356
H	3.113290	-0.648218	-4.177767
H	0.977222	-0.232847	-5.376145
C	2.711841	3.667746	-0.520512
C	1.974086	4.858978	-0.569790
C	4.098866	3.703514	-0.726591
C	2.615748	6.072861	-0.823218
H	0.902736	4.825100	-0.394648
C	4.737854	4.917636	-0.980574
H	4.672632	2.783697	-0.674790
C	3.997078	6.102761	-1.031079
H	2.040252	6.993522	-0.855924
H	5.812586	4.941454	-1.136127
H	4.496603	7.046819	-1.228483
N	2.866114	1.151732	0.603212
C	2.327406	0.250343	1.471541
C	3.281386	-0.473482	2.374621
C	4.665780	-0.381714	2.189260
C	2.785847	-1.256251	3.428567

C	5.540647	-1.051339	3.046364
H	5.037140	0.228745	1.373669
C	3.658044	-1.931402	4.281250
H	1.711429	-1.343437	3.572439
C	5.040048	-1.829940	4.093272
H	6.613403	-0.967218	2.896650
H	3.261610	-2.534625	5.092768
H	5.720426	-2.352459	4.759315
H	1.310567	-0.631734	-0.436634
C	-5.777391	-1.217711	3.781353
H	-6.013602	-0.331673	4.371170
H	-6.580453	-1.411031	3.070106
H	-5.664440	-2.073896	4.441354
H	1.417098	0.557952	2.008071
H	-0.069395	-2.082919	1.770062
H	-2.334326	-2.185237	-3.900276

Vibrational frequencies

-352.4171	10.6208	14.2876
24.0456	26.6122	28.5837
30.5937	34.2546	36.2388
37.8430	43.9328	48.4190
51.9306	58.4533	59.1145
61.8398	66.7064	73.4323
76.5736	78.7620	82.8415
86.7101	90.9692	97.6660
102.6475	111.0915	120.4761
126.6299	134.5658	137.5240
147.5670	159.9053	161.1681
165.8694	171.9982	176.0926
183.1647	191.8743	195.2306

204.5560	214.6832	223.7021
226.2287	231.8596	237.8887
244.7390	247.8217	257.6029
260.8359	267.9172	268.9577
278.3156	287.4871	293.1637
294.9505	303.8941	312.7900
313.6218	327.5785	330.8695
341.4302	342.1454	344.7487
362.2540	363.7005	368.9651
375.3182	384.0889	398.6897
400.2977	405.0029	410.0859
412.1677	414.5791	417.4840
427.1950	434.3665	438.4307
440.6512	449.0039	450.4692
460.3599	467.2153	470.3877
472.3345	484.6438	501.2654
522.7010	523.5841	535.3767
537.3573	540.2506	546.8501
557.8577	563.2677	574.6446
592.8391	599.5819	614.8642
625.5010	629.6388	630.6026
632.2638	637.6088	645.9500
648.2768	664.7216	682.3010
696.5191	705.7351	710.1602
712.7453	713.7769	726.9435
740.3407	747.3766	754.9958
759.1833	764.9495	767.0077
771.1801	772.0314	777.4916
781.0563	794.4824	797.8334
813.0502	823.6906	845.8965
850.4829	854.0832	864.1444

868.1793	868.6414	872.9061
877.5799	885.9711	889.3150
892.9763	908.7888	923.4620
930.8148	934.1944	938.2796
942.5464	945.2795	946.0222
947.0673	949.7582	955.0495
967.0811	973.3109	980.0632
982.9445	983.3780	986.3006
990.3587	993.8074	1003.2832
1003.8963	1010.6071	1011.3719
1012.7074	1013.9261	1014.4926
1024.0090	1034.5207	1043.3209
1049.6215	1050.0412	1051.9733
1054.9898	1056.2393	1058.3146
1064.2934	1070.1587	1072.7492
1082.9664	1088.0036	1092.7503
1098.6981	1100.9675	1105.8873
1115.1177	1117.7772	1129.0105
1133.2986	1145.6801	1155.3299
1159.4055	1171.5151	1182.7380
1187.7379	1190.4129	1190.8345
1191.5935	1201.7694	1203.4044
1206.0080	1207.1397	1210.2666
1212.9142	1214.6746	1220.9598
1222.2765	1247.4401	1253.4880
1258.4140	1261.8377	1262.8741
1265.9675	1269.1246	1277.8933
1290.9650	1293.4256	1317.9100
1319.8674	1322.7944	1331.1583
1337.3017	1343.4001	1344.3971
1353.0882	1356.0425	1360.5494

1361.8213	1368.1237	1393.6064
1402.1363	1410.0291	1411.7219
1412.2385	1412.3820	1419.2146
1420.3733	1424.4363	1429.9473
1431.3622	1433.3100	1435.0306
1435.4039	1440.4646	1448.6868
1460.4411	1469.2803	1472.6261
1475.7306	1479.9839	1481.0358
1486.1872	1488.5612	1494.3004
1494.9865	1495.8820	1496.8456
1497.7828	1501.6596	1502.1222
1502.6841	1507.2868	1508.0308
1510.1990	1510.6827	1518.4138
1520.7645	1521.7572	1525.1933
1531.9080	1534.2583	1535.4777
1547.5071	1553.9920	1577.3403
1583.7173	1612.3014	1622.2221
1625.9462	1634.9902	1639.3602
1639.9161	1643.6211	1644.0491
1654.9890	1672.2553	1675.1789
1702.3235	1740.6902	2979.5756
3034.1807	3036.3487	3050.1526
3053.5376	3055.6564	3055.6820
3060.2708	3063.7207	3067.2396
3091.3919	3099.5091	3104.5273
3112.3441	3115.1265	3119.7163
3123.3785	3124.9150	3129.1903
3130.4082	3134.5821	3141.0918
3141.6324	3157.3010	3159.6821
3169.3737	3170.9567	3173.5694
3175.7807	3176.1094	3179.5167



3179.6056	3182.1066	3183.7194
3186.0276	3187.4314	3188.0684
3190.5593	3193.3169	3196.3599
3200.8781	3203.2425	3203.5505
3203.7299	3204.9635	3205.5860
3209.2369	3210.1849	3214.6014
3214.8638	3218.5532	3220.9178
3253.5286	3602.0060	3718.4774

### TS5SR

Zero-point correction= 0.961821

Thermal correction to Energy= 1.019108

Thermal correction to Enthalpy= 1.020052

Thermal correction to Gibbs Free Energy= 0.869789

Sum of electronic and zero-point Energies= -2949.524785

Sum of electronic and thermal Energies= -2949.467498

Sum of electronic and thermal Enthalpies= -2949.466554

Sum of electronic and thermal Free Energies= -2949.616817

### Cartesian coordinates

C	-0.984797	1.958914	4.189023
C	0.019284	1.546121	3.272172
C	-0.281399	1.820996	1.882968
C	-1.536314	2.356772	1.518897
C	-2.447068	2.777884	2.489251
N	-2.128669	2.556960	3.803093
H	-0.834684	1.806793	5.248934
C	-1.886015	2.447673	0.062556
C	-1.321113	3.501282	-0.726580
C	-2.658887	1.460833	-0.548781
C	-0.545678	4.547604	-0.148369

C	-1.521395	3.509775	-2.146205
C	-2.846838	1.490222	-1.958709
C	0.007020	5.534719	-0.932316
H	-0.393175	4.560162	0.925282
C	-0.936121	4.543189	-2.926982
C	-2.290935	2.476473	-2.735891
H	-3.460045	0.726524	-2.423868
C	-0.184229	5.532220	-2.336385
H	0.594047	6.323448	-0.472185
H	-1.093471	4.534938	-4.001795
H	-2.444487	2.479075	-3.811046
H	0.262288	6.314605	-2.941971
C	0.738339	1.619227	0.888209
H	0.574550	1.956650	-0.122197
O	1.095309	0.997604	3.674474
C	-3.725593	3.494620	2.169173
H	-3.820336	3.601691	1.090599
H	-4.598609	2.939985	2.519114
H	-3.740938	4.494899	2.615209
C	-3.430699	0.425264	0.239956
O	-4.027186	0.727872	1.278219
N	-3.531678	-0.803074	-0.328861
H	-2.885085	-1.051291	-1.064944
C	-4.475671	-1.826316	0.127984
C	-3.703935	-3.082873	0.561287
H	-4.416959	-3.870774	0.820123
H	-3.105415	-3.455420	-0.280789
O	-2.911988	-2.861487	1.710665
H	-2.195558	-2.217477	1.495309
C	-5.601795	-2.062190	-0.931252
C	-6.629851	-3.070683	-0.379620

H	-6.219623	-4.081484	-0.302457
H	-6.985476	-2.770433	0.612635
H	-7.498191	-3.121770	-1.045030
C	-5.030360	-2.592448	-2.260521
H	-5.837471	-2.733598	-2.987332
H	-4.312810	-1.892441	-2.701627
H	-4.522003	-3.552810	-2.134310
C	-6.328350	-0.726579	-1.187078
H	-5.653834	0.027365	-1.601906
H	-7.147763	-0.870170	-1.899493
H	-6.751454	-0.325049	-0.259782
N	1.967407	1.264405	1.205965
C	2.932690	1.041166	0.230070
C	4.180597	0.475360	0.786465
O	4.289854	0.073925	1.936883
O	5.131851	0.422106	-0.161928
C	6.446325	-0.208146	0.086265
C	6.248127	-1.685677	0.427340
H	5.737148	-1.807175	1.381616
H	5.652592	-2.175562	-0.348656
H	7.222810	-2.180444	0.477703
C	7.154211	-0.045626	-1.258935
H	7.212847	1.010319	-1.537260
H	8.169390	-0.446743	-1.194278
H	6.620270	-0.584624	-2.046560
C	7.187687	0.555295	1.186309
H	8.206533	0.165928	1.272716
H	7.246411	1.618445	0.934398
H	6.684996	0.445250	2.146964
P	0.264541	-1.643509	0.339051
O	-0.811159	-1.210468	1.324407

C	1.640214	-2.459636	1.220429
C	2.500913	-3.371422	0.587143
C	1.871683	-2.110243	2.559046
C	3.563787	-3.941031	1.289220
H	2.327976	-3.653362	-0.447351
C	2.937193	-2.679670	3.256213
H	1.230829	-1.379263	3.041682
C	3.779985	-3.598254	2.626466
H	4.220865	-4.649860	0.794417
H	3.111960	-2.403703	4.291955
H	4.606442	-4.042801	3.173202
C	-0.398873	-2.901344	-0.813876
C	-0.851715	-2.505337	-2.082479
C	-0.566142	-4.235345	-0.413243
C	-1.478171	-3.423675	-2.927196
H	-0.696250	-1.479222	-2.402581
C	-1.178042	-5.155936	-1.264947
H	-0.220817	-4.554836	0.565029
C	-1.641826	-4.750026	-2.519655
H	-1.833038	-3.105921	-3.902922
H	-1.300701	-6.187062	-0.947406
H	-2.125257	-5.465576	-3.177931
N	0.794305	-0.423568	-0.627980
C	2.079756	-0.256711	-1.018882
C	2.270899	0.432865	-2.337358
C	1.227543	1.172678	-2.912296
C	3.503539	0.369548	-3.001238
C	1.417251	1.845391	-4.119059
H	0.267170	1.202690	-2.410142
C	3.690990	1.034522	-4.213778
H	4.316862	-0.192840	-2.555053

C	2.649752	1.779388	-4.775452
H	0.600849	2.421366	-4.545202
H	4.650523	0.972561	-4.719449
H	2.797042	2.300564	-5.716904
H	3.066121	1.853774	-0.475954
C	-3.083441	2.963963	4.856409
H	-3.244794	4.041271	4.812163
H	-4.031201	2.444992	4.710710
H	-2.670197	2.699991	5.826666
H	2.802928	-1.061678	-0.849423
H	2.091730	0.927441	2.177907
H	-4.941842	-1.412954	1.025815

Vibrational frequencies

-330.7772	11.6585	23.4802
27.3512	34.7740	35.5759
37.0422	39.8206	40.7998
45.8360	48.5997	50.2661
54.0602	62.6190	64.2999
66.5286	67.9529	73.3739
74.1819	74.5427	85.3738
86.7311	92.8678	99.9796
104.4247	110.9327	121.7102
131.0001	134.8592	139.0841
144.5905	157.4921	168.7661
179.8991	182.9978	186.3950
193.9230	200.8934	202.7483
214.3733	222.0073	225.6007
230.3587	230.7000	241.9827
252.2497	255.7261	259.5843
265.2610	270.7170	275.3055

286.1561	290.0574	291.6883
294.1816	300.3944	312.5254
316.3448	319.4472	332.6860
345.6155	353.0227	358.6755
361.6454	365.2916	372.3423
381.5113	384.4847	390.8258
397.7582	404.1134	408.5497
410.4929	415.2144	419.0062
421.6153	438.7533	441.8937
445.8897	454.1040	461.6795
469.0213	476.9095	486.8066
489.4569	494.0877	514.2164
519.7787	524.8031	533.1944
537.2639	543.2191	546.6137
557.5691	564.5015	570.6729
579.1558	585.7379	598.2199
614.9142	626.6909	629.8068
631.2974	633.9471	643.5010
662.9196	677.2031	693.7513
701.1014	712.8976	713.6566
715.1083	730.5975	742.7327
746.0125	750.6074	757.9567
762.0414	763.5709	766.2257
775.5082	778.0644	781.2462
782.2883	795.5839	800.5283
812.1141	816.9706	845.2571
851.1081	856.9355	859.3883
865.0265	867.0351	872.8624
873.7248	889.2269	891.1307
904.5122	910.7004	916.1611
921.7769	935.2034	936.8523

938.9301	944.2876	945.7259
946.1051	947.6745	956.0640
965.3960	974.2068	977.0670
981.9583	985.7668	987.9662
992.4528	993.2116	1003.4020
1007.4524	1008.7857	1012.7956
1013.9830	1014.7531	1015.6065
1024.1901	1027.4053	1032.3396
1035.3118	1049.7085	1051.4809
1052.0058	1053.7192	1056.8504
1058.1759	1066.2934	1070.6490
1081.6819	1097.3581	1104.5176
1104.9719	1108.6936	1113.8105
1114.5320	1116.5012	1127.3235
1132.1568	1132.5473	1144.1782
1148.8473	1154.4069	1183.0120
1184.1062	1187.4098	1188.0083
1191.9045	1192.5417	1200.7758
1204.6826	1208.6211	1210.5037
1214.7403	1223.3451	1224.3577
1234.9366	1247.5257	1249.3568
1251.4473	1262.2233	1264.5700
1267.0915	1271.4260	1276.4634
1290.7720	1292.8867	1308.3096
1311.5076	1323.2076	1325.8850
1330.9985	1341.4791	1344.6616
1352.4005	1357.0645	1359.6298
1360.8418	1363.6175	1381.5829
1398.9315	1410.1343	1411.5437
1414.5646	1415.4243	1415.9763
1420.7017	1423.2249	1426.5840

1438.2923	1438.7273	1439.0422
1442.6133	1448.2864	1453.9867
1465.3331	1466.4026	1471.7610
1475.7128	1477.3947	1478.8031
1480.3091	1485.2859	1491.7562
1493.5880	1494.4682	1497.0522
1499.0072	1501.5406	1502.0104
1502.7566	1505.0971	1506.3015
1512.8850	1517.0903	1519.2809
1521.0127	1523.3169	1525.6861
1529.9162	1532.1346	1534.0018
1550.0189	1552.1166	1560.8218
1577.3557	1607.5277	1622.4024
1625.5369	1634.9175	1639.2159
1642.5906	1644.7651	1645.6590
1653.6815	1656.7395	1672.4871
1716.1072	1749.4532	3035.1374
3038.0721	3041.2413	3045.6586
3052.4079	3053.8631	3054.3985
3055.6391	3060.5279	3090.7175
3096.2554	3102.7406	3104.2537
3107.8426	3109.7009	3119.9675
3123.8840	3123.9056	3124.9671
3125.2809	3128.6149	3132.2199
3137.0579	3166.9044	3174.2566
3175.7159	3178.3830	3179.3515
3180.3351	3182.7993	3185.1635
3185.8777	3186.6307	3188.1295
3189.0104	3190.1573	3194.5743
3194.9842	3195.8994	3201.2799
3201.8870	3202.5287	3205.6833



3207.3222	3210.5278	3210.9469
3211.2718	3213.7776	3214.3000
3216.2356	3224.2915	3253.4613
3290.5239	3389.5568	3623.8816

### TS5SR1

Zero-point correction= 0.961895

Thermal correction to Energy= 1.019180

Thermal correction to Enthalpy= 1.020124

Thermal correction to Gibbs Free Energy= 0.870390

Sum of electronic and zero-point Energies= -2949.521455

Sum of electronic and thermal Energies= -2949.464170

Sum of electronic and thermal Enthalpies= -2949.463226

Sum of electronic and thermal Free Energies= -2949.612960

### Cartesian coordinates

C	-1.364660	0.388601	4.171266
C	-0.361388	0.747602	3.231169
C	-0.863300	1.261919	1.971855
C	-2.252470	1.381250	1.750263
C	-3.168387	1.024246	2.740051
N	-2.679877	0.524771	3.919426
H	-1.076497	-0.017313	5.130789
C	-2.756768	1.963171	0.461192
C	-2.800265	3.392753	0.351512
C	-3.151967	1.171728	-0.614477
C	-2.389818	4.251294	1.411093
C	-3.270760	3.991712	-0.863348
C	-3.647252	1.787179	-1.798053
C	-2.433926	5.620323	1.269252
H	-2.037459	3.819190	2.340334

C	-3.304422	5.407081	-0.976734
C	-3.703899	3.152301	-1.920999
H	-4.015332	1.166738	-2.608483
C	-2.892655	6.206772	0.064931
H	-2.115049	6.256858	2.088720
H	-3.662103	5.846332	-1.903538
H	-4.089101	3.604036	-2.830279
H	-2.919958	7.287567	-0.031801
C	0.060985	1.597655	0.933371
H	-0.303737	1.943406	-0.026320
O	0.874238	0.590065	3.489690
C	-4.653704	1.087087	2.543732
H	-4.882135	1.652679	1.642612
H	-5.063293	0.080102	2.411854
H	-5.166773	1.565289	3.381523
C	-3.053444	-0.332635	-0.533339
O	-3.184541	-0.933594	0.535396
N	-2.802490	-0.963448	-1.712108
H	-2.639910	-0.389419	-2.526377
C	-2.425798	-2.381661	-1.830614
C	-1.247767	-2.409049	-2.838350
H	-1.628062	-2.163426	-3.841571
H	-0.563889	-1.604320	-2.545699
O	-0.559804	-3.642449	-2.894308
H	0.303406	-3.506351	-2.435324
C	-3.650921	-3.290702	-2.167257
C	-4.232553	-2.951405	-3.551931
H	-4.492486	-1.889110	-3.623538
H	-3.533509	-3.187811	-4.360127
H	-5.146204	-3.529028	-3.729492
C	-4.747612	-3.080527	-1.103607

H	-5.583027	-3.765142	-1.289239
H	-4.360319	-3.267207	-0.098253
H	-5.138588	-2.059543	-1.123261
C	-3.228014	-4.772319	-2.129648
H	-2.806943	-5.030995	-1.151613
H	-4.102038	-5.411151	-2.302398
H	-2.471941	-4.996070	-2.882616
N	1.361689	1.556629	1.102633
C	2.275369	1.718117	0.065240
C	3.681534	1.646602	0.512974
O	4.028712	1.353415	1.648454
O	4.495016	1.901157	-0.526800
C	5.965578	1.788908	-0.424011
C	6.343652	0.355550	-0.051597
H	6.022244	0.108966	0.959185
H	5.876377	-0.351873	-0.742320
H	7.429465	0.237348	-0.118739
C	6.420233	2.125464	-1.843998
H	6.082676	3.125977	-2.129042
H	7.511716	2.095094	-1.902676
H	6.014065	1.402960	-2.558032
C	6.491389	2.816378	0.580111
H	7.585434	2.812096	0.563491
H	6.147091	3.819533	0.311271
H	6.153063	2.583414	1.589876
P	1.526716	-2.192396	-0.408222
O	1.785338	-3.063418	-1.640164
C	0.234904	-2.970334	0.606498
C	0.025820	-4.351778	0.471464
C	-0.535886	-2.245091	1.518380
C	-0.938729	-4.993632	1.247398

H	0.605810	-4.908416	-0.257040
C	-1.496541	-2.887061	2.299316
H	-0.403470	-1.176227	1.586773
C	-1.698851	-4.261428	2.166439
H	-1.102367	-6.061287	1.134119
H	-2.100368	-2.307869	2.990190
H	-2.451629	-4.761740	2.768756
C	3.031011	-2.222560	0.636056
C	3.027666	-1.650794	1.917058
C	4.189828	-2.857416	0.166702
C	4.167258	-1.720722	2.717246
H	2.140618	-1.152167	2.296608
C	5.330489	-2.923173	0.968826
H	4.180053	-3.306096	-0.821383
C	5.318603	-2.357628	2.246344
H	4.158556	-1.270890	3.705428
H	6.225481	-3.415217	0.599173
H	6.204827	-2.410804	2.872116
N	1.015840	-0.657237	-0.709407
C	1.909532	0.223784	-1.232748
C	1.435328	1.057840	-2.385895
C	0.065872	1.228872	-2.632647
C	2.360658	1.711244	-3.213645
C	-0.372155	2.045495	-3.675530
H	-0.641381	0.708508	-1.998613
C	1.923545	2.513316	-4.267794
H	3.422608	1.600143	-3.013918
C	0.555370	2.687744	-4.500005
H	-1.436996	2.181080	-3.840730
H	2.650389	3.006666	-4.906768
H	0.216653	3.318469	-5.316555

H	2.054387	2.543665	-0.600311
C	-3.628069	0.102545	4.974921
H	-4.180748	0.969366	5.338471
H	-4.322057	-0.633543	4.569756
H	-3.067234	-0.340138	5.794046
H	2.960963	-0.069750	-1.338326
H	1.665477	1.181818	2.023447
H	-2.041162	-2.682588	-0.853413

Vibrational frequencies

-358.1404	20.8010	22.5982
26.6164	30.6370	32.7743
34.9715	40.8397	42.7442
43.7763	46.9327	52.9935
56.4169	57.5146	66.5806
67.8700	69.5061	72.4304
76.5499	83.6248	88.3951
93.0184	99.4964	101.2188
111.8474	117.8876	124.3423
129.2079	131.8529	139.6738
144.9810	154.3858	168.6428
170.8720	175.1004	183.9661
187.0566	194.7159	203.2435
211.2349	217.6416	229.0833
233.3927	236.3996	239.0428
246.2564	251.2444	257.5236
262.6996	270.3987	276.4463
286.2041	290.0020	295.3559
297.5544	306.4777	309.0947
324.1090	332.1737	337.0426
340.3386	346.2117	361.7722

372.3075	375.4785	379.7296
382.1099	392.3235	395.9318
396.3347	403.5840	409.4554
411.3770	414.1907	420.3262
425.4213	431.7309	438.5205
440.4076	442.9445	451.3328
464.2055	469.9655	470.8975
484.4389	486.6177	491.9920
520.4259	522.8084	529.4147
535.9438	541.4767	552.5922
560.8827	562.7134	573.7273
579.8312	592.8460	597.8956
629.0979	629.3882	629.9461
633.6215	633.9895	640.3646
666.5338	680.1555	687.9290
700.9843	707.1043	713.9952
716.0065	718.0912	730.4216
737.5725	739.1357	746.2154
749.9637	759.5276	762.3971
764.3585	766.2619	777.9482
783.6506	795.0192	797.8790
811.3781	816.4802	848.0181
848.2873	856.3336	862.5236
863.8132	870.3824	872.6994
876.9640	888.9267	889.1338
894.9602	911.6516	925.3411
933.4017	936.3798	937.6921
940.4123	942.3412	944.5993
945.9234	949.8873	955.3475
972.3494	977.6913	980.5083
980.5929	986.3186	991.2677

995.9036	1002.4152	1006.3515
1008.4732	1009.6402	1012.9826
1013.6844	1015.3330	1018.3603
1023.5656	1033.2859	1039.6496
1050.1550	1052.6746	1053.7103
1057.0897	1059.0444	1063.9134
1069.6004	1070.6976	1076.9606
1084.1734	1087.2018	1090.7892
1102.5809	1104.8311	1111.6784
1112.4404	1115.1078	1121.4667
1131.2878	1132.5601	1146.4009
1147.0179	1154.7306	1182.6187
1183.7501	1190.6789	1191.0992
1191.6444	1192.8386	1204.4731
1206.6046	1209.4742	1210.1402
1212.7296	1219.4440	1226.9022
1231.5356	1247.5754	1248.7085
1250.9204	1262.5503	1264.4310
1267.5365	1276.8327	1277.7869
1290.5717	1292.5011	1298.2688
1313.1344	1324.9059	1328.2016
1333.3700	1337.2406	1349.6411
1353.8463	1356.9181	1359.7914
1361.2525	1362.6700	1399.8132
1408.0945	1409.3682	1411.2997
1411.5077	1413.0946	1414.3734
1418.4750	1424.0101	1425.0052
1434.6570	1435.4471	1438.3214
1439.2222	1450.5153	1457.3420
1467.1082	1473.7652	1478.2163
1478.9802	1480.3219	1483.3232

1487.9650	1491.2051	1491.8703
1494.4985	1496.6774	1496.9126
1499.5452	1500.7170	1502.3583
1503.5181	1506.2659	1510.3380
1512.0107	1514.8441	1517.4214
1522.9305	1524.7986	1527.1879
1531.6667	1533.0395	1533.9993
1550.1486	1552.3573	1554.6546
1576.9094	1609.5945	1625.8799
1628.7527	1633.6195	1639.4750
1644.6261	1646.1233	1649.0773
1653.1657	1669.9723	1671.0725
1726.6635	1751.0933	2994.9154
3032.5388	3034.8858	3036.2775
3042.7361	3050.0432	3055.3591
3059.3260	3061.1507	3073.4238
3092.5574	3097.6859	3101.2700
3112.1836	3112.7132	3124.1309
3124.7582	3124.8504	3126.8397
3129.6249	3131.5547	3136.3783
3154.8080	3155.4264	3164.9690
3176.8647	3177.8496	3178.2678
3179.0448	3179.9994	3181.6775
3186.7122	3188.9226	3188.9902
3189.1685	3194.6759	3196.2277
3196.7316	3197.6214	3204.4470
3204.6269	3205.4353	3206.4463
3206.6534	3206.9452	3209.2979
3209.9406	3211.7837	3222.7831
3232.1234	3234.5055	3256.5897
3279.7138	3376.3495	3633.7228



## TS5SR2

Zero-point correction= 0.961843

Thermal correction to Energy= 1.019395

Thermal correction to Enthalpy= 1.020339

Thermal correction to Gibbs Free Energy= 0.871158

Sum of electronic and zero-point Energies= -2949.512901

Sum of electronic and thermal Energies= -2949.455349

Sum of electronic and thermal Enthalpies= -2949.454405

Sum of electronic and thermal Free Energies= -2949.603585

### Cartesian coordinates

C	-2.059432	1.659734	4.383178
C	-0.837990	1.430959	3.684772
C	-0.916855	1.653435	2.256068
C	-2.161137	1.901174	1.637362
C	-3.313831	2.085889	2.393433
N	-3.208287	1.972437	3.757827
H	-2.085306	1.565454	5.459867
C	-2.227537	1.901186	0.137932
C	-2.023321	3.140766	-0.547771
C	-2.401613	0.718070	-0.586439
C	-1.791468	4.360706	0.149744
C	-2.032619	3.166569	-1.981273
C	-2.403295	0.771385	-2.009169
C	-1.587763	5.537155	-0.536012
H	-1.772382	4.355748	1.233519
C	-1.827183	4.397843	-2.658403
C	-2.227357	1.952185	-2.684677
H	-2.560074	-0.125782	-2.594840
C	-1.608746	5.559331	-1.952526

H	-1.408834	6.456636	0.012087
H	-1.835149	4.402393	-3.744249
H	-2.228121	1.960601	-3.770027
H	-1.445571	6.494796	-2.478016
C	0.247356	1.500007	1.450741
H	0.219716	1.763843	0.400903
O	0.217392	1.062283	4.282429
C	-4.669750	2.287999	1.784336
H	-4.570758	2.453099	0.712747
H	-5.295307	1.399706	1.926561
H	-5.195450	3.147457	2.208509
C	-2.659107	-0.589702	0.128420
O	-3.013916	-0.622807	1.311081
N	-2.499091	-1.734499	-0.598807
H	-2.174415	-1.670370	-1.553329
C	-3.040984	-3.030365	-0.162997
C	-2.054697	-4.131144	-0.579096
H	-2.451716	-5.106626	-0.290435
H	-1.949160	-4.140021	-1.671328
O	-0.782524	-4.011739	0.039212
H	-0.568171	-3.072882	0.135968
C	-4.505816	-3.267086	-0.670967
C	-5.079124	-4.524259	0.014580
H	-4.554306	-5.437357	-0.279416
H	-5.026720	-4.436796	1.105444
H	-6.130984	-4.651994	-0.260737
C	-4.554384	-3.443678	-2.201231
H	-5.594226	-3.520956	-2.534800
H	-4.108962	-2.587886	-2.719557
H	-4.037816	-4.350053	-2.531591
C	-5.390092	-2.064278	-0.284384

H	-5.092925	-1.156611	-0.817748
H	-6.432284	-2.272368	-0.547095
H	-5.336265	-1.858266	0.788023
N	1.374481	0.997841	1.903285
C	2.386599	0.545465	1.049981
C	3.609081	0.105396	1.744157
O	3.650594	-0.203951	2.928607
O	4.616337	0.037710	0.861654
C	5.948375	-0.491941	1.211101
C	5.825245	-1.962535	1.612370
H	5.215302	-2.074167	2.509155
H	5.369766	-2.534876	0.799905
H	6.821265	-2.371582	1.806370
C	6.713035	-0.343742	-0.104440
H	6.756354	0.707025	-0.405076
H	7.734451	-0.716518	0.012304
H	6.220482	-0.911688	-0.898599
C	6.574599	0.367179	2.311692
H	7.612996	0.058958	2.465915
H	6.568667	1.420499	2.015621
H	6.030240	0.259974	3.249867
P	2.468734	-0.761411	-2.352209
O	3.658383	-1.269504	-3.137454
C	2.555644	1.065925	-2.194441
C	1.425502	1.879345	-2.003910
C	3.831110	1.643912	-2.104951
C	1.570279	3.236937	-1.707823
H	0.429348	1.456299	-2.087148
C	3.976303	2.999471	-1.807371
H	4.705018	1.019098	-2.255987
C	2.846639	3.795687	-1.600109

H	0.691614	3.855755	-1.560589
H	4.969065	3.433602	-1.733313
H	2.958934	4.849148	-1.361889
C	0.890845	-1.055125	-3.255384
C	0.090381	-2.169489	-2.958820
C	0.519592	-0.220310	-4.322231
C	-1.048294	-2.440754	-3.725352
H	0.357267	-2.821840	-2.131910
C	-0.633723	-0.473963	-5.065248
H	1.127895	0.645699	-4.564801
C	-1.420141	-1.589556	-4.769582
H	-1.646805	-3.322012	-3.520351
H	-0.913055	0.192404	-5.875721
H	-2.312210	-1.800929	-5.351099
N	2.346813	-1.457514	-0.868728
C	1.592166	-0.987485	0.149488
C	1.334186	-1.942688	1.280718
C	2.245957	-2.970917	1.560167
C	0.191925	-1.818392	2.088499
C	2.039332	-3.832640	2.634429
H	3.110491	-3.082413	0.917096
C	-0.017935	-2.686143	3.162132
H	-0.557321	-1.065506	1.873223
C	0.908537	-3.689550	3.445776
H	2.759017	-4.620193	2.839058
H	-0.912290	-2.576599	3.768508
H	0.747045	-4.363291	4.282074
H	2.549964	1.184431	0.193719
C	-4.415922	2.164492	4.591090
H	-4.791889	3.179628	4.460828
H	-5.182355	1.447784	4.295787

H	-4.153370	2.006148	5.633966
H	0.689178	-0.394232	-0.085712
H	1.368621	0.741203	2.907455
H	-3.062487	-2.990981	0.929398

Vibrational frequencies

-365.8154	23.5600	25.9512
31.8220	34.9882	41.2379
41.4360	42.0730	44.9040
47.4252	50.4123	52.8856
53.7984	57.6830	62.5656
63.7697	71.0299	80.3191
85.7107	87.7790	88.6117
95.3419	99.7221	101.3824
111.2544	113.7110	121.5422
129.4869	134.9906	141.0501
143.0251	144.9935	154.4828
158.8618	179.1476	185.1903
188.4104	195.4430	198.3985
198.7270	223.8065	228.3812
230.6396	231.3555	245.2357
254.9811	260.4535	263.2324
268.9293	274.9113	280.1327
283.0338	290.4886	292.6040
297.0382	303.5696	306.4317
312.4310	330.8615	335.4115
344.3663	346.5136	353.1209
355.6231	361.0499	364.2073
369.3139	378.7974	381.5488
390.5540	394.5135	397.2635
402.9570	411.8160	414.5722

418.3881	424.3125	428.5208
429.6577	437.3582	441.5742
443.4302	462.4556	476.5551
484.6573	493.5943	500.1293
503.1205	517.2500	521.9892
534.2403	535.2248	543.6878
548.6646	556.8013	560.8317
563.0563	577.6499	584.8605
595.2622	615.4410	627.4534
631.8753	632.1655	633.4310
635.2451	662.5986	674.5446
687.9353	698.4755	716.5957
717.4965	718.3669	725.8539
737.8903	744.1879	746.6301
759.5092	761.4361	766.9324
770.7171	779.9981	780.9417
782.2563	794.6651	799.1561
805.8402	815.0218	836.2173
838.6111	849.5022	866.6030
872.8410	878.4783	880.2957
886.0686	888.8061	889.9025
894.5534	903.1591	913.7708
921.3256	936.9195	938.9045
944.4443	946.2445	947.8256
948.5804	950.8544	956.9890
959.2956	965.3086	976.9255
979.9378	984.8660	990.8711
998.2084	1003.0934	1004.8478
1009.6675	1012.1948	1012.9764
1014.0798	1015.0545	1023.0955
1026.9865	1034.8885	1041.6314

1047.8583	1051.5915	1053.0388
1054.0870	1055.0463	1055.6175
1057.6913	1067.0268	1071.9342
1080.5490	1084.2974	1103.5037
1106.4983	1110.2533	1110.9464
1118.6158	1126.9474	1130.7705
1133.6556	1146.1987	1155.5269
1167.5478	1175.6509	1181.9926
1188.2256	1192.0032	1194.8754
1194.9792	1200.4605	1203.1325
1207.1005	1209.6283	1214.6354
1222.0355	1222.3583	1224.5286
1229.3154	1235.5127	1247.3647
1253.6860	1257.7730	1261.1129
1264.5322	1268.7727	1277.9610
1278.5195	1290.7236	1304.2118
1319.2853	1321.9041	1323.1386
1323.5436	1330.6615	1343.1321
1359.3517	1359.8382	1360.8003
1362.7384	1363.2044	1367.2799
1388.9934	1400.5059	1408.9939
1411.0895	1411.4789	1414.6816
1418.3654	1421.0505	1422.9939
1429.5866	1436.9413	1440.1430
1441.3591	1443.9734	1451.9165
1462.8218	1468.0758	1470.7745
1476.1593	1480.5783	1483.3822
1485.9870	1491.2190	1491.5055
1494.1386	1495.6721	1499.3535
1499.7656	1500.1997	1502.9570
1503.2315	1506.5955	1513.1288

1513.8524	1517.9793	1522.8274
1524.4257	1525.2369	1527.2448
1532.3461	1533.5413	1534.7931
1548.5072	1552.3013	1559.6029
1586.1337	1602.5640	1622.2880
1624.4624	1633.1435	1640.0968
1641.3834	1642.6888	1643.6212
1654.4663	1665.8579	1669.7766
1711.9651	1746.4078	2917.7340
3038.5315	3039.5666	3044.4993
3050.2839	3051.2791	3053.9016
3055.0913	3061.7971	3092.6481
3099.5864	3109.0184	3109.9805
3112.6412	3117.0122	3118.0161
3118.3083	3124.1368	3125.7220
3129.5712	3131.9476	3132.8677
3137.8025	3164.5122	3167.1588
3173.6952	3176.8538	3179.9398
3184.5062	3185.2990	3187.9445
3189.1243	3190.3195	3195.7407
3197.0204	3198.9893	3200.4864
3200.6856	3203.3949	3203.9325
3205.1788	3211.7363	3212.4932
3212.8721	3215.1542	3221.3024
3224.3234	3225.0119	3228.9343
3231.7327	3241.4985	3252.3654
3256.4144	3616.4912	3788.6768

### **TS5SR3**

Zero-point correction= 0.961497

Thermal correction to Energy= 1.019080



Thermal correction to Enthalpy= 1.020024

Thermal correction to Gibbs Free Energy= 0.870430

Sum of electronic and zero-point Energies= -2949.512755

Sum of electronic and thermal Energies= -2949.455172

Sum of electronic and thermal Enthalpies= -2949.454228

Sum of electronic and thermal Free Energies= -2949.603823

Cartesian coordinates

C	2.119778	-0.872780	4.017665
C	1.253964	-1.198361	2.938101
C	1.849664	-1.101125	1.618678
C	3.189461	-0.672925	1.486937
C	3.978393	-0.397820	2.603508
N	3.399725	-0.502457	3.842676
H	1.744436	-0.921041	5.030488
C	3.769821	-0.431171	0.127932
C	4.329180	-1.507510	-0.627363
C	3.736031	0.847976	-0.411494
C	4.354323	-2.843978	-0.139525
C	4.874604	-1.238032	-1.926640
C	4.289337	1.105345	-1.691595
C	4.881860	-3.861366	-0.902618
H	3.948516	-3.055397	0.844021
C	5.412788	-2.311897	-2.685845
C	4.854659	0.090212	-2.424318
H	4.259970	2.116674	-2.083837
C	5.414597	-3.595214	-2.188255
H	4.890500	-4.876415	-0.517890
H	5.820005	-2.100565	-3.670499
H	5.278208	0.291826	-3.403689
H	5.824478	-4.408569	-2.778833

C	1.087828	-1.499927	0.471897
H	1.536262	-1.507630	-0.515412
O	0.052533	-1.548222	3.152465
C	5.406190	0.056212	2.512660
H	5.773161	-0.084873	1.497931
H	5.486189	1.122604	2.745110
H	6.060033	-0.502331	3.187014
C	3.073323	1.966307	0.349538
O	3.423450	2.301579	1.489455
N	2.060401	2.562528	-0.323094
H	1.730791	2.091929	-1.153123
C	1.178535	3.550360	0.305098
C	0.046465	2.817587	1.053165
H	-0.547120	3.550283	1.615731
H	-0.623504	2.308967	0.353426
O	0.547680	1.801324	1.920053
H	1.391227	2.100751	2.291875
C	0.723672	4.640675	-0.710164
C	-0.149309	4.058976	-1.839386
H	0.401996	3.341509	-2.456600
H	-1.050192	3.570240	-1.461021
H	-0.472295	4.863933	-2.507152
C	1.978248	5.293561	-1.323807
H	1.686996	6.091869	-2.014197
H	2.613843	5.732610	-0.546556
H	2.578431	4.567594	-1.879825
C	-0.075280	5.724756	0.041006
H	0.490336	6.111097	0.896238
H	-0.284239	6.563611	-0.630929
H	-1.035769	5.350969	0.401221
N	-0.140722	-1.945313	0.591472

C	-0.956349	-2.435637	-0.432530
C	-2.179748	-3.075967	0.098755
O	-2.560534	-2.974686	1.257402
O	-2.815862	-3.727385	-0.887990
C	-4.103401	-4.423037	-0.665070
C	-5.155329	-3.450119	-0.127918
H	-4.959273	-3.191509	0.912551
H	-5.152952	-2.527394	-0.714169
H	-6.141517	-3.920608	-0.195859
C	-4.465293	-4.890181	-2.074826
H	-3.675161	-5.526000	-2.484521
H	-5.396686	-5.462476	-2.050760
H	-4.601020	-4.030730	-2.737641
C	-3.868153	-5.611013	0.269233
H	-4.792971	-6.187917	0.365699
H	-3.092389	-6.268225	-0.135241
H	-3.564302	-5.268743	1.259439
P	-3.429762	0.463594	-0.489280
O	-4.539618	-0.283599	-1.209523
C	-3.592613	2.273553	-0.764497
C	-3.812933	2.719221	-2.077848
C	-3.498880	3.220014	0.264492
C	-3.930042	4.080430	-2.357163
H	-3.898045	1.994083	-2.882368
C	-3.623203	4.584078	-0.013599
H	-3.329328	2.894359	1.285618
C	-3.835089	5.017102	-1.323591
H	-4.097065	4.411484	-3.378092
H	-3.555237	5.307003	0.794157
H	-3.926855	6.077587	-1.538708
C	-3.584809	0.264103	1.321104

C	-2.464259	0.281209	2.160473
C	-4.861869	0.094847	1.877621
C	-2.618038	0.128717	3.539793
H	-1.471408	0.394537	1.742643
C	-5.015106	-0.052968	3.256285
H	-5.728993	0.062901	1.224643
C	-3.891266	-0.034587	4.089132
H	-1.734434	0.104800	4.168480
H	-6.005808	-0.188595	3.681123
H	-4.010172	-0.156430	5.162264
N	-1.870322	0.163433	-0.911284
C	-1.549078	-0.957635	-1.595656
C	-0.361340	-0.843139	-2.514620
C	0.372643	0.347475	-2.558639
C	-0.001430	-1.886936	-3.380975
C	1.455259	0.488764	-3.427408
H	0.032034	1.154903	-1.921367
C	1.088778	-1.755073	-4.240091
H	-0.581613	-2.806799	-3.384372
C	1.828247	-0.568260	-4.259640
H	2.010676	1.421286	-3.463542
H	1.358224	-2.574578	-4.899724
H	2.679806	-0.464965	-4.924835
H	-0.427224	-3.034798	-1.163265
C	4.196977	-0.182162	5.046950
H	5.006330	-0.905170	5.154298
H	4.610538	0.822020	4.955460
H	3.549872	-0.229940	5.919082
H	-2.356716	-1.552325	-2.040277
H	-0.519519	-1.885523	1.564836
H	1.799774	4.048833	1.057201

Vibrational frequencies

-386.0406	22.0756	25.2148
26.5473	33.1573	37.0725
40.4028	40.8916	44.4516
50.3447	52.4628	54.8750
58.0934	61.3308	64.6445
66.0983	71.7658	80.1368
83.6113	86.2687	92.1261
94.9552	98.3387	104.0392
107.9898	110.8063	121.2424
128.6572	138.7902	141.8447
145.8667	150.5740	156.2292
160.1436	165.5259	176.5884
182.3721	190.3960	195.3693
199.6876	211.7394	218.0907
228.1066	233.1917	237.0716
246.3924	248.5609	256.3250
257.2905	262.4535	268.0409
281.9992	290.3096	294.0744
296.8109	310.5047	314.7130
316.0710	332.5307	334.8106
339.6159	353.1517	357.2905
360.2258	362.2843	368.2461
370.0321	377.8890	383.9490
390.9086	404.7214	406.3777
411.0210	413.3326	420.3701
422.1968	425.3055	428.2738
440.7872	443.7135	445.6529
450.7236	467.1214	473.5426
478.1086	483.4303	486.7443

518.9486	520.8901	530.4039
533.0774	533.8973	541.0838
550.7434	555.3621	565.8359
571.0253	577.0705	581.4600
600.0657	612.3340	630.2836
631.0304	635.0550	637.6400
648.1385	663.1420	675.2434
698.4940	706.6968	710.5121
714.7713	718.3800	730.0573
744.0674	747.4470	754.1788
758.4416	764.4846	764.7377
766.2177	768.4018	778.7710
779.4871	793.6498	798.2730
811.8672	826.0651	850.4603
852.4733	859.3477	864.6744
867.8221	868.9243	878.3263
886.6500	889.1221	894.8768
910.1209	912.0057	923.5174
929.8331	935.4377	937.2428
938.8441	939.5858	941.6521
948.0722	951.7548	954.4039
971.0720	982.0916	984.8805
985.4263	986.6780	987.4916
991.1674	998.2356	1004.2989
1006.6491	1007.7843	1012.7813
1013.0788	1013.8847	1017.1548
1020.4164	1029.8773	1035.0576
1048.0244	1051.2044	1052.0573
1056.7647	1058.7232	1060.4241
1065.0082	1072.8219	1074.6783
1077.9266	1083.5034	1100.7555

1102.6370	1104.5964	1105.6196
1117.8277	1128.7195	1132.3494
1134.3046	1136.6340	1146.2767
1154.7025	1159.9674	1182.6870
1184.9937	1188.9773	1189.4836
1191.3091	1192.5999	1198.2147
1200.8610	1204.5191	1209.3359
1211.3343	1213.2668	1218.9485
1230.4024	1247.5075	1251.8680
1254.2681	1261.2640	1266.6728
1270.4753	1277.1574	1277.7172
1289.9820	1290.6170	1304.8970
1307.8499	1326.2999	1327.3556
1327.7521	1342.7718	1347.4082
1354.1338	1355.4346	1359.4201
1363.8654	1367.3831	1391.8199
1398.0013	1405.8091	1411.1005
1411.2904	1412.0513	1417.4411
1418.4673	1420.5437	1424.4672
1426.1830	1437.1428	1439.6274
1440.8913	1452.3130	1453.6538
1465.2105	1468.7861	1473.0100
1474.3373	1480.7133	1481.4230
1483.7647	1489.2733	1494.4503
1495.0577	1495.9426	1497.6635
1499.5769	1499.9120	1500.7818
1503.9705	1507.0803	1513.8290
1515.8961	1519.5166	1519.9291
1524.2402	1525.3459	1526.5857
1532.0181	1534.6906	1539.4124
1550.4226	1554.9614	1558.9116

1583.8102	1612.7899	1625.0486
1626.8156	1634.5093	1634.7929
1644.1717	1645.0114	1645.5580
1653.7771	1668.6869	1672.7861
1705.1876	1749.6574	3022.6511
3037.3480	3037.4052	3042.4865
3044.0417	3049.7215	3050.4072
3051.7883	3057.3614	3062.5366
3068.6995	3091.8868	3101.6688
3105.6509	3106.3514	3110.2176
3121.9512	3123.3590	3127.6946
3129.3858	3131.5968	3136.7509
3145.8403	3150.8621	3157.5230
3165.7876	3169.6595	3176.0358
3176.0924	3177.6143	3178.5314
3183.5825	3183.8108	3185.0280
3189.2213	3190.0949	3192.8306
3193.4821	3194.1583	3200.5408
3201.8597	3204.7736	3205.8730
3208.4238	3208.5549	3208.7958
3210.2399	3212.2561	3214.9645
3223.6385	3223.8773	3239.2866
3255.0348	3649.7522	3758.7341

### **TS5SS**

Zero-point correction= 0.960928

Thermal correction to Energy= 1.017877

Thermal correction to Enthalpy= 1.018821

Thermal correction to Gibbs Free Energy= 0.869271

Sum of electronic and zero-point Energies= -2949.534510

Sum of electronic and thermal Energies= -2949.477561



Sum of electronic and thermal Enthalpies= -2949.476616

Sum of electronic and thermal Free Energies= -2949.626166

Cartesian coordinates

C	3.590652	-3.740022	0.806905
C	2.253112	-3.283073	0.641321
C	2.121384	-1.853872	0.439638
C	3.272274	-1.049255	0.297577
C	4.550748	-1.584335	0.450034
N	4.658280	-2.925996	0.717604
H	3.775787	-4.787482	1.001003
C	3.112073	0.382370	-0.111765
C	3.243299	0.718887	-1.497105
C	2.729803	1.354842	0.800458
C	3.566591	-0.246233	-2.493332
C	3.018511	2.074376	-1.906113
C	2.489598	2.687241	0.380298
C	3.664946	0.112755	-3.819141
H	3.721835	-1.279161	-2.202598
C	3.136712	2.411633	-3.281471
C	2.648349	3.041340	-0.936154
H	2.169605	3.420085	1.112932
C	3.451676	1.454813	-4.218991
H	3.904653	-0.639223	-4.564603
H	2.953927	3.439233	-3.579366
H	2.449465	4.058486	-1.257653
H	3.531298	1.723260	-5.267854
C	0.816670	-1.263346	0.408057
H	0.678893	-0.192573	0.388738
O	1.272210	-4.089444	0.676098
C	5.803864	-0.763016	0.355362

H	5.543576	0.285669	0.225372
H	6.407361	-0.844594	1.264381
H	6.429780	-1.064550	-0.491506
C	2.495375	0.953930	2.227871
O	3.360047	0.337081	2.879988
N	1.276221	1.269690	2.706154
H	0.554080	1.555853	2.032412
C	0.859836	0.873972	4.057407
C	0.328961	-0.568721	4.016263
O	1.322261	-1.510091	3.612293
H	2.169264	-1.039507	3.517017
C	-0.108640	1.915974	4.697344
C	-0.183674	1.658765	6.216399
H	-0.602381	0.675170	6.448489
H	0.806958	1.724045	6.680267
H	-0.826140	2.408353	6.690031
C	-1.525103	1.836993	4.094258
H	-2.152557	2.628167	4.518970
H	-1.502845	1.963422	3.009155
H	-2.008185	0.880389	4.318768
C	0.458402	3.331894	4.471698
H	0.445681	3.608140	3.413925
H	-0.142044	4.066626	5.018282
H	1.492316	3.405627	4.827388
N	-0.268079	-1.999617	0.419876
C	-1.560111	-1.497847	0.280101
C	-2.604566	-2.526025	0.366936
O	-2.395547	-3.731103	0.281173
O	-3.810807	-1.934405	0.457917
C	-5.069684	-2.704842	0.482732
C	-5.237724	-3.462460	-0.835998

H	-5.205704	-2.764779	-1.678419
H	-4.454854	-4.211028	-0.960484
H	-6.210286	-3.963597	-0.846564
C	-5.082735	-3.635642	1.697347
H	-4.882612	-3.065553	2.609482
H	-6.070399	-4.097099	1.789746
H	-4.333069	-4.420668	1.598158
C	-6.124047	-1.607356	0.619416
H	-7.123448	-2.051018	0.637959
H	-5.973179	-1.042871	1.543733
H	-6.062745	-0.907967	-0.218500
P	-1.297478	1.729515	-0.604564
O	-0.786848	1.723457	0.836493
C	-3.122027	1.889746	-0.567346
C	-3.800138	1.913005	0.658431
C	-3.858680	1.930185	-1.761985
C	-5.194172	1.984992	0.690927
H	-3.229648	1.869097	1.579858
C	-5.251415	1.998900	-1.728900
H	-3.342436	1.907174	-2.718134
C	-5.920467	2.027931	-0.501129
H	-5.712906	2.002577	1.644833
H	-5.814631	2.028934	-2.656853
H	-7.004833	2.080355	-0.475367
C	-0.680546	3.189578	-1.491540
C	-0.546798	4.393343	-0.783670
C	-0.342466	3.143114	-2.849210
C	-0.082522	5.538936	-1.428305
H	-0.786119	4.420005	0.275258
C	0.123109	4.291144	-3.493672
H	-0.420374	2.202477	-3.384204

C	0.253350	5.488159	-2.785620
H	0.024778	6.467188	-0.875144
H	0.393590	4.248178	-4.544447
H	0.618799	6.379026	-3.287797
N	-0.866225	0.445433	-1.529578
C	-1.609024	-0.689578	-1.559601
C	-1.081293	-1.788496	-2.416758
C	0.267073	-1.794163	-2.806075
C	-1.906382	-2.852495	-2.809012
C	0.782143	-2.849503	-3.557320
H	0.894866	-0.958668	-2.520825
C	-1.393380	-3.904647	-3.566871
H	-2.952283	-2.854580	-2.519519
C	-0.045081	-3.909922	-3.938045
H	1.828646	-2.839510	-3.849422
H	-2.044222	-4.720637	-3.867244
H	0.354614	-4.731749	-4.525066
H	-1.748443	-0.572744	0.812355
C	5.998718	-3.520063	0.910294
H	6.614056	-3.332991	0.030286
H	6.471558	-3.079582	1.788738
H	5.891021	-4.591916	1.055971
H	-2.703983	-0.620704	-1.546256
H	-0.094880	-3.026103	0.419768
H	1.774942	0.870667	4.660354
H	-0.058177	-0.848581	5.004712
H	-0.507011	-0.625454	3.306199

Vibrational frequencies

-407.5081	-9.1332	18.8807
21.9253	28.0908	29.4977

32.3708	37.2159	40.0705
43.2684	43.9056	47.8571
50.8693	54.0287	55.2747
60.6542	64.5246	65.9774
70.9447	75.7733	78.2325
85.7912	88.2777	94.8308
102.7025	111.3015	116.7616
124.7142	131.1128	133.9947
139.6810	149.0292	155.0169
160.0713	162.5484	180.8095
184.5565	195.2674	198.8091
203.8792	220.2698	225.5876
230.0791	236.6495	241.0790
246.2390	246.5153	253.5301
259.4892	269.8359	271.7955
277.0793	282.7436	288.3083
298.8299	304.2002	307.7404
313.5361	323.6362	332.1899
335.9574	342.9637	351.4903
362.4628	363.5322	373.7413
375.4667	387.3986	394.8875
404.1936	405.8967	407.5488
410.0661	412.4384	416.7550
426.7369	432.6307	438.0349
441.5285	443.1571	458.6979
460.6136	464.9320	473.2570
479.8719	483.4085	486.0507
498.4708	520.6191	528.5888
534.1802	536.5551	549.8023
550.6989	554.4368	573.5068
579.1386	580.8599	593.4646

609.0823	630.0607	630.3174
633.4951	641.0186	649.4696
664.9673	670.3055	695.0697
703.8719	707.8895	710.4209
717.1628	733.4897	744.9489
750.4136	753.3900	762.1784
763.1120	764.9103	768.7090
770.0677	776.2332	782.0236
796.1903	797.7895	811.6146
818.3079	836.0471	845.6428
847.2353	852.8563	866.9697
867.9711	871.2268	871.9457
884.4070	888.3737	891.7829
896.9336	913.1463	920.7221
935.2358	936.1009	939.3981
939.8986	944.0116	946.2545
950.5275	951.7955	956.4110
970.4348	982.0234	983.6209
985.6755	986.8482	988.7277
989.4273	990.8489	1003.0407
1007.0719	1009.7124	1010.2934
1013.1659	1014.0669	1015.7713
1022.1382	1024.1511	1032.9582
1042.9592	1048.9988	1050.3628
1051.8533	1053.1624	1056.3842
1060.4783	1064.6362	1072.4904
1080.6996	1085.6213	1092.0810
1103.0943	1108.2436	1110.7943
1112.7125	1125.4491	1130.6431
1131.2503	1134.5660	1146.5353
1147.3017	1156.2151	1183.3452

1185.0192	1188.0208	1190.9184
1191.1897	1192.0469	1203.4470
1204.1431	1206.0187	1207.5878
1213.1777	1224.8292	1231.0452
1235.7009	1247.1251	1251.3762
1256.5897	1265.6955	1268.2037
1275.0061	1276.7541	1289.9739
1293.4371	1296.6317	1312.9195
1325.3506	1325.9497	1329.6454
1330.6897	1339.9318	1343.6167
1355.6251	1356.8777	1357.2589
1362.8271	1366.9482	1395.8351
1402.8128	1408.3256	1409.3197
1413.4910	1416.5028	1418.0700
1422.3989	1423.9691	1429.5398
1433.4406	1438.5030	1441.5764
1441.6899	1449.7331	1462.0536
1468.0437	1473.9741	1474.6633
1476.3689	1480.1898	1481.0320
1488.3993	1490.5586	1495.1575
1495.7303	1497.0852	1497.5839
1500.7895	1501.8005	1502.1567
1503.5620	1508.7038	1510.0358
1512.6409	1519.3329	1522.0436
1522.5247	1522.6408	1528.3202
1531.3942	1532.8285	1533.4326
1550.4992	1555.4013	1582.8503
1605.5416	1618.4076	1625.3699
1626.7989	1634.3615	1638.1638
1643.7781	1645.6637	1648.0993
1655.6883	1671.9525	1673.2480

1684.6998	1737.4556	3016.6840
3036.0469	3036.8632	3036.9788
3043.2959	3049.9043	3051.8921
3052.0013	3053.3570	3059.9948
3067.7190	3091.7566	3103.9132
3104.8146	3109.2097	3109.8400
3119.1111	3122.3556	3123.0218
3125.0097	3127.8408	3134.6391
3137.5549	3139.2738	3161.9673
3166.9764	3175.2346	3177.6168
3177.8640	3178.1587	3182.1443
3185.6368	3187.2093	3187.7922
3189.4955	3195.6801	3196.7569
3197.8771	3199.7085	3199.9888
3203.3412	3204.1589	3206.2479
3206.9951	3208.6471	3210.8840
3212.2101	3215.0395	3217.0327
3217.0579	3229.2788	3254.4983
3269.9633	3309.0864	3649.9096

### **TS5SS1**

Zero-point correction= 0.960940

Thermal correction to Energy= 1.018838

Thermal correction to Enthalpy= 1.019782

Thermal correction to Gibbs Free Energy= 0.867691

Sum of electronic and zero-point Energies= -2949.517125

Sum of electronic and thermal Energies= -2949.459226

Sum of electronic and thermal Enthalpies= -2949.458282

Sum of electronic and thermal Free Energies= -2949.610374

Cartesian coordinates



C	-3.338598	-1.317162	-3.510875
C	-2.164374	-0.747828	-2.937018
C	-2.139933	-0.752171	-1.489245
C	-3.224646	-1.281202	-0.750408
C	-4.341659	-1.805595	-1.396796
N	-4.347482	-1.807838	-2.772869
H	-3.437638	-1.360116	-4.586775
C	-3.156948	-1.282225	0.748590
C	-2.837105	-2.494028	1.441072
C	-3.294199	-0.099263	1.466298
C	-2.640108	-3.730107	0.764599
C	-2.698593	-2.467067	2.869596
C	-3.147079	-0.082277	2.877048
C	-2.337935	-4.877171	1.463603
H	-2.720817	-3.762406	-0.315618
C	-2.383772	-3.669165	3.559114
C	-2.867112	-1.239618	3.562097
H	-3.271512	0.855337	3.408829
C	-2.208960	-4.849447	2.873791
H	-2.192413	-5.810700	0.929032
H	-2.281838	-3.637206	4.639972
H	-2.764543	-1.225394	4.643000
H	-1.968446	-5.761906	3.410060
C	-1.065576	-0.111096	-0.809803
H	-1.078948	-0.045069	0.267401
O	-1.229773	-0.294139	-3.660568
C	-5.543831	-2.339418	-0.671932
H	-5.423504	-2.190928	0.399381
H	-6.459528	-1.824289	-0.977334
H	-5.686544	-3.410797	-0.847869
C	-3.550394	1.187813	0.733495

O	-4.520186	1.327975	-0.025466
N	-2.619152	2.150760	0.936105
H	-1.838536	1.942740	1.545679
C	-2.720233	3.493177	0.343509
C	-2.237827	3.485938	-1.123896
O	-2.756458	2.404043	-1.884783
H	-3.619390	2.156418	-1.509194
C	-2.021843	4.553413	1.249449
C	-2.257938	5.956873	0.655053
H	-1.739049	6.093916	-0.297658
H	-3.324945	6.146538	0.495172
H	-1.880794	6.718250	1.345004
C	-0.503713	4.308024	1.372092
H	-0.062811	5.059925	2.033844
H	-0.266306	3.336486	1.815131
H	0.013011	4.378107	0.410409
C	-2.656357	4.505771	2.655062
H	-2.470440	3.553859	3.161165
H	-2.235426	5.297725	3.282465
H	-3.740295	4.654067	2.602219
N	-0.084445	0.507382	-1.413813
C	0.849630	1.298096	-0.720285
C	1.808375	1.951431	-1.627928
O	2.066180	1.533542	-2.747963
O	2.359479	3.009605	-1.019122
C	3.488629	3.756952	-1.611123
C	4.693369	2.825390	-1.741738
H	4.955412	2.415732	-0.763665
H	4.479755	1.986244	-2.403138
H	5.546764	3.390436	-2.130051
C	3.063578	4.371094	-2.947053

H	2.140219	4.944827	-2.820342
H	3.845623	5.051952	-3.296607
H	2.900596	3.601034	-3.700422
C	3.741877	4.845846	-0.568831
H	4.583733	5.471032	-0.879186
H	2.858969	5.481332	-0.453173
H	3.977806	4.399090	0.401007
P	3.732954	-1.128891	-0.748752
O	4.562467	-0.702985	-1.941422
C	2.328032	-2.189891	-1.275334
C	1.773219	-1.982745	-2.545861
C	1.708022	-3.097750	-0.401150
C	0.623617	-2.670694	-2.938084
H	2.234681	-1.261579	-3.212402
C	0.555545	-3.781665	-0.790085
H	2.124915	-3.269119	0.587248
C	0.009841	-3.565259	-2.058498
H	0.187114	-2.477565	-3.911392
H	0.075510	-4.469054	-0.101141
H	-0.893862	-4.088413	-2.358066
C	4.735083	-2.203672	0.349023
C	5.747774	-2.997076	-0.210012
C	4.494139	-2.276797	1.728614
C	6.499824	-3.855477	0.593520
H	5.948790	-2.928213	-1.274893
C	5.243440	-3.138052	2.533203
H	3.726949	-1.645322	2.166659
C	6.245772	-3.929409	1.966206
H	7.284016	-4.463932	0.152075
H	5.049889	-3.187583	3.600998
H	6.830321	-4.597657	2.592011

N	3.161440	0.050030	0.247586
C	1.848638	0.211190	0.537571
C	1.545740	0.937734	1.821468
C	2.345861	1.997526	2.266300
C	0.425980	0.569344	2.583208
C	2.027115	2.680486	3.440120
H	3.212378	2.276211	1.678024
C	0.105540	1.252626	3.759993
H	-0.183557	-0.278062	2.278152
C	0.904396	2.314893	4.189673
H	2.652689	3.505095	3.769429
H	-0.758737	0.944420	4.340016
H	0.656351	2.850756	5.100666
H	0.371222	1.974959	-0.023455
C	-5.515626	-2.368793	-3.487582
H	-5.667742	-3.404437	-3.183809
H	-6.404520	-1.782246	-3.253702
H	-5.325911	-2.328382	-4.557102
H	1.176631	-0.652174	0.411564
H	-0.051856	0.394230	-2.442595
H	-3.792129	3.724791	0.328979
H	-2.516920	4.447711	-1.575920
H	-1.146939	3.407053	-1.172243

Vibrational frequencies

-352.3520	15.8436	19.8400
26.6570	28.5740	32.4750
34.3615	36.0726	38.3399
42.5261	44.7000	47.6934
51.0474	58.0909	61.3199
63.7700	66.2063	74.5463

77.0663	82.6299	86.0821
90.6020	92.5709	97.8081
112.7028	113.5087	115.7808
127.3239	132.2310	141.1949
144.9688	150.7792	153.5282
159.3741	171.0563	175.8132
185.5485	191.6770	198.7507
204.5019	215.7584	221.0593
224.8280	231.1450	238.5589
248.5986	253.1114	264.0695
266.0777	269.5614	277.5962
281.9418	284.5729	288.1990
292.4277	298.1838	307.1293
310.9321	319.1030	328.9390
337.8198	341.9984	346.8464
362.7529	369.7969	371.7727
382.2930	385.1296	385.7816
390.6523	392.6679	402.3009
403.3531	410.5923	412.3526
418.9427	420.0767	422.2815
438.0329	444.0796	449.9410
453.0785	461.6078	472.2838
484.4007	486.8704	496.5470
515.0130	518.9396	520.7371
535.7375	537.7707	543.4405
548.7387	552.5863	561.3971
569.3840	576.0486	582.2722
594.5259	612.8239	629.3503
631.6410	632.0007	638.1905
648.0127	663.9561	675.2525
694.0807	699.9669	712.3350

714.7708	716.2184	725.2621
734.3671	742.4835	754.2367
761.0077	766.2354	768.5356
770.4298	775.5363	778.3271
781.7893	795.4576	796.9206
809.6242	817.4122	840.2235
843.9418	853.2289	864.7560
869.6462	874.9053	877.5646
884.2357	888.2522	890.6597
891.3396	901.7539	908.4037
928.1223	931.9881	937.1981
937.8940	938.6366	947.6281
949.6585	950.1513	952.7206
968.2424	972.6136	974.9939
981.5239	982.2357	992.9127
994.9673	996.8419	1001.2055
1006.4118	1012.0803	1013.4243
1014.2414	1014.5852	1016.3699
1022.8675	1031.7767	1042.5313
1050.7704	1051.4708	1052.3867
1052.8425	1056.5590	1060.0559
1065.1276	1067.3877	1070.8774
1076.0666	1081.5635	1096.0376
1104.1449	1107.2054	1108.6045
1110.5195	1119.6577	1129.8418
1130.9266	1134.4007	1146.5572
1154.9910	1180.1243	1183.8295
1186.1925	1188.6235	1190.3818
1192.8239	1192.9465	1195.7445
1202.8560	1204.5031	1213.4023
1215.5357	1217.2930	1232.3590

1242.7340	1246.9390	1248.4421
1251.7818	1259.0112	1264.4597
1271.4269	1277.0972	1278.7832
1288.7581	1290.8904	1309.9724
1318.0310	1323.4401	1329.3193
1331.1010	1344.9064	1354.3178
1358.1523	1359.9297	1361.5106
1362.1873	1365.8759	1384.2948
1399.9806	1405.4131	1409.2446
1410.3208	1411.9612	1414.5347
1417.4002	1419.4903	1431.8384
1433.2958	1434.6247	1435.5485
1439.8282	1448.1507	1457.7092
1466.1800	1467.5009	1471.0794
1474.5552	1479.8515	1480.1427
1487.6372	1489.2668	1492.0039
1494.9674	1495.6637	1496.6022
1501.7194	1501.9046	1503.4401
1507.3776	1511.5089	1512.1677
1513.1180	1514.1451	1518.7880
1520.7900	1522.4758	1525.0456
1529.6592	1532.7860	1533.9755
1550.2471	1554.7598	1563.6727
1577.2267	1612.9738	1621.9555
1624.9277	1626.6237	1635.3029
1641.2202	1644.7204	1645.4817
1655.3400	1672.3990	1675.4539
1729.6902	1742.3120	3013.2313
3035.5573	3035.6606	3040.1897
3045.9659	3049.5608	3050.6787
3053.1329	3053.9450	3059.6233

3062.8826	3091.1137	3105.1514
3106.6027	3110.9522	3115.4716
3115.6849	3116.5006	3117.5966
3122.3340	3126.9652	3129.0898
3129.2256	3136.4900	3163.4348
3166.6736	3175.5935	3178.1446
3179.0310	3181.1883	3183.4662
3185.8758	3185.9139	3187.6859
3190.2022	3191.3665	3194.8516
3195.5063	3195.7747	3199.0024
3202.6169	3203.2579	3205.0894
3208.3761	3208.6588	3210.3258
3210.5851	3216.4550	3217.6829
3218.0790	3249.2093	3254.0932
3256.2011	3600.2446	3810.3810

## TS5SS2

Zero-point correction= 0.961352

Thermal correction to Energy= 1.019168

Thermal correction to Enthalpy= 1.020112

Thermal correction to Gibbs Free Energy= 0.865689

Sum of electronic and zero-point Energies= -2949.503794

Sum of electronic and thermal Energies= -2949.445978

Sum of electronic and thermal Enthalpies= -2949.445034

Sum of electronic and thermal Free Energies= -2949.599457

## Cartesian coordinates

C	-1.779886	-2.828493	-3.287496
C	-1.047583	-1.879418	-2.518217
C	-1.578824	-1.631649	-1.193335
C	-2.787383	-2.244520	-0.782046



C	-3.463285	-3.129613	-1.619786
N	-2.911387	-3.403376	-2.849895
H	-1.429703	-3.095749	-4.274981
C	-3.360356	-1.907599	0.560641
C	-3.259381	-2.849113	1.634271
C	-3.919494	-0.654981	0.790299
C	-2.640848	-4.121635	1.478984
C	-3.791180	-2.500513	2.920591
C	-4.425352	-0.317029	2.072729
C	-2.572293	-5.006359	2.531461
H	-2.214667	-4.390355	0.518919
C	-3.707149	-3.439444	3.984123
C	-4.376723	-1.221595	3.105370
H	-4.871201	0.660931	2.223292
C	-3.113839	-4.666570	3.795564
H	-2.096439	-5.972247	2.393594
H	-4.117010	-3.166529	4.952364
H	-4.781210	-0.963266	4.079626
H	-3.053173	-5.375650	4.615210
C	-0.934829	-0.680034	-0.348754
H	-1.321046	-0.487402	0.644467
O	-0.015320	-1.310143	-2.986713
C	-4.776462	-3.768957	-1.269116
H	-5.127696	-3.391980	-0.310963
H	-5.543694	-3.543284	-2.015987
H	-4.694443	-4.858123	-1.190573
C	-3.986980	0.364907	-0.320647
O	-4.453341	0.097043	-1.430101
N	-3.478766	1.580748	0.012302
H	-3.042301	1.704206	0.915429
C	-3.424553	2.726915	-0.894539

C	-1.973489	3.221367	-0.950464
H	-1.369183	2.422052	-1.400670
H	-1.899581	4.096532	-1.606907
O	-1.509679	3.519616	0.366973
H	-0.547520	3.647421	0.317440
C	-4.522562	3.789095	-0.556345
C	-4.414004	4.299275	0.892899
H	-4.534341	3.482311	1.612353
H	-3.448394	4.773650	1.077353
H	-5.207480	5.028536	1.089767
C	-5.903529	3.132501	-0.755564
H	-6.698635	3.853231	-0.537714
H	-6.033617	2.782049	-1.784819
H	-6.037473	2.275286	-0.089603
C	-4.397869	4.978859	-1.527198
H	-4.379726	4.643195	-2.570594
H	-5.253993	5.650908	-1.407500
H	-3.493350	5.565616	-1.341112
N	0.070970	0.060629	-0.745219
C	0.616275	1.097446	0.025176
C	1.376692	2.050635	-0.799681
O	1.964208	1.748032	-1.824536
O	1.353193	3.278093	-0.230295
C	2.133198	4.417442	-0.774848
C	3.623622	4.074312	-0.763333
H	3.943432	3.818779	0.249442
H	3.842727	3.238003	-1.427291
H	4.192392	4.947701	-1.096033
C	1.618697	4.759440	-2.173952
H	0.538765	4.934675	-2.149947
H	2.105704	5.674334	-2.523952

H	1.831432	3.953905	-2.876610
C	1.817045	5.532051	0.221658
H	2.351666	6.443388	-0.059615
H	0.744461	5.750687	0.229282
H	2.122019	5.239460	1.230166
P	3.203831	-1.435314	0.069207
O	2.037303	-2.406432	0.025851
C	4.678700	-2.189371	0.861244
C	5.388435	-3.203085	0.198209
C	5.065296	-1.825077	2.158134
C	6.461151	-3.841447	0.821010
H	5.107142	-3.485908	-0.812903
C	6.138044	-2.464431	2.783628
H	4.525419	-1.030591	2.664106
C	6.837204	-3.473044	2.116421
H	7.005949	-4.621752	0.297304
H	6.431403	-2.172216	3.787995
H	7.674390	-3.967534	2.600617
C	3.793205	-1.046236	-1.620115
C	3.117225	-1.570401	-2.725619
C	4.896279	-0.202474	-1.822215
C	3.532789	-1.250199	-4.021208
H	2.244412	-2.193595	-2.569809
C	5.315070	0.112340	-3.113746
H	5.422433	0.211456	-0.966637
C	4.631559	-0.412096	-4.217166
H	2.994233	-1.651997	-4.874975
H	6.169734	0.766088	-3.263461
H	4.955397	-0.164001	-5.224064
N	3.020592	0.003859	0.835779
C	1.820348	0.375741	1.335239

C	1.843607	1.488468	2.350827
C	2.978724	2.293158	2.503003
C	0.719896	1.748643	3.148361
C	2.984175	3.350806	3.413035
H	3.850967	2.067952	1.899897
C	0.721786	2.803708	4.060829
H	-0.164120	1.121397	3.055350
C	1.852941	3.614853	4.190719
H	3.871752	3.968573	3.516832
H	-0.156829	2.991705	4.671041
H	1.855215	4.439126	4.897830
H	-0.127812	1.553032	0.667896
C	-3.593160	-4.358777	-3.751217
H	-3.703257	-5.319934	-3.249143
H	-4.575240	-3.970116	-4.022288
H	-2.993069	-4.484813	-4.648749
H	1.099070	-0.415697	1.599134
H	0.446540	-0.177342	-1.684915
H	-3.654388	2.334094	-1.890111

#### Vibrational frequencies

-357.1280	11.2775	15.0664
18.6048	26.4115	30.1181
30.7387	33.6867	34.5822
36.3040	38.4859	45.3959
46.7754	53.8412	54.7537
58.4380	62.5000	64.5629
70.3186	70.5391	76.4510
78.4398	88.0254	97.5269
100.0026	107.6414	112.0930
125.0069	127.3553	137.4347

147.5462	152.7448	158.6277
169.3394	177.3855	186.9801
190.3909	191.4359	196.7163
204.2742	217.1213	223.4110
235.2296	237.8463	249.2253
249.7646	254.7180	261.6415
263.3033	267.4769	273.4125
279.6405	286.9196	293.4997
300.9629	301.5148	303.1110
314.6254	320.8303	330.1007
337.8501	338.9260	344.4706
358.0493	367.5557	369.7151
385.6731	393.9959	396.6361
400.2217	403.5733	407.7945
410.6518	413.4893	416.6271
423.3641	425.9447	436.5401
439.8932	445.9130	455.0443
461.8071	478.0159	478.7120
484.2637	485.7809	510.6708
521.5647	524.2584	536.3261
542.6285	547.0641	548.9969
566.0855	570.3231	575.9043
591.0216	609.5500	618.3581
630.7423	631.5620	632.6842
633.3875	636.9567	645.5517
662.2010	670.5983	676.3950
700.2956	706.2085	713.2719
714.8075	716.2976	727.2626
735.7479	741.8841	755.3181
758.0153	760.8625	762.1873
766.2715	767.0909	777.4333

786.8821	795.2976	797.6919
813.2222	820.6264	853.1665
855.2405	857.0464	860.0583
868.1545	870.2254	873.3911
873.7601	887.2951	889.7114
892.1927	904.1157	911.9077
936.0956	939.7656	941.5745
942.6022	943.0694	945.9207
948.3090	952.2072	962.1307
969.4618	973.8113	977.0736
982.2898	988.5546	989.3495
990.1350	991.9773	1006.7050
1007.2357	1007.6770	1008.3873
1011.0181	1012.8610	1014.7037
1014.8718	1030.1078	1042.9270
1048.4273	1050.0291	1050.9010
1051.5809	1055.9447	1059.6049
1063.7574	1064.1403	1077.2778
1079.7176	1080.1703	1104.2437
1105.0899	1106.6495	1113.1198
1119.1847	1130.3430	1133.1202
1136.6254	1146.7726	1153.1978
1156.5374	1165.4498	1183.1274
1186.7641	1189.2594	1189.5577
1190.6348	1194.6893	1200.5947
1202.8393	1208.2242	1209.2211
1212.1694	1215.7528	1220.5589
1224.3586	1245.6020	1249.3154
1253.7301	1258.6432	1261.1690
1266.5510	1270.5224	1280.2585
1290.1498	1294.8074	1305.5479

1313.2320	1316.3515	1326.0617
1327.0359	1332.9465	1343.9791
1356.2196	1358.1244	1360.2018
1361.6039	1365.0549	1374.2116
1387.4613	1402.4135	1407.8299
1410.3998	1411.3504	1415.7326
1416.5603	1417.3696	1427.0807
1431.6163	1438.8202	1439.6680
1440.6149	1446.9093	1464.9779
1467.6205	1470.5274	1473.8039
1475.2743	1480.8558	1482.9270
1487.3893	1490.1661	1491.7553
1495.8248	1496.6947	1497.1433
1498.0838	1499.1654	1499.6734
1504.9544	1505.6379	1511.6761
1513.6517	1516.5651	1519.7506
1523.3643	1525.6096	1528.6516
1533.4352	1533.7506	1539.2106
1542.4304	1544.8884	1553.8768
1583.5939	1610.5856	1625.4306
1628.5837	1635.4912	1636.9454
1644.5124	1644.7926	1646.0008
1653.9362	1670.4820	1672.5496
1728.2695	1767.2729	2955.0150
3025.8363	3033.8793	3039.0277
3045.3153	3048.3829	3054.0016
3056.4719	3065.5089	3067.8468
3086.1020	3092.6619	3102.4449
3103.2788	3111.2319	3111.6955
3115.3473	3122.2593	3122.7670
3127.5444	3137.1287	3141.7640

3146.4832	3164.4384	3166.2080
3166.2897	3169.0803	3174.5088
3174.9653	3177.3256	3180.3662
3181.1559	3182.1248	3182.7547
3185.9286	3190.0401	3190.5325
3190.7473	3191.9906	3195.2038
3199.7931	3202.5415	3203.4152
3204.4399	3204.7938	3206.5393
3207.1772	3208.4622	3217.5399
3217.8917	3230.3522	3230.7513
3254.3297	3629.1841	3710.0284

### TS5SS3

Zero-point correction= 0.962001

Thermal correction to Energy= 1.019435

Thermal correction to Enthalpy= 1.020379

Thermal correction to Gibbs Free Energy= 0.869135

Sum of electronic and zero-point Energies= -2949.499615

Sum of electronic and thermal Energies= -2949.442181

Sum of electronic and thermal Enthalpies= -2949.441237

Sum of electronic and thermal Free Energies= -2949.592481

### Cartesian coordinates

C	4.446793	0.255041	3.489597
C	3.109693	0.115670	3.023408
C	2.989715	-0.218032	1.618614
C	4.140358	-0.313222	0.801037
C	5.412286	-0.097429	1.332239
N	5.514843	0.158618	2.678604
H	4.628572	0.472734	4.533002
C	3.987603	-0.644373	-0.652865



C	4.389407	-1.939573	-1.116337
C	3.387737	0.249886	-1.537213
C	4.952379	-2.922117	-0.253224
C	4.203450	-2.277531	-2.497549
C	3.210947	-0.101925	-2.901389
C	5.328912	-4.156047	-0.732874
H	5.071989	-2.698667	0.800217
C	4.598055	-3.562161	-2.960076
C	3.615878	-1.327225	-3.370554
H	2.768824	0.621257	-3.578628
C	5.153011	-4.482172	-2.100135
H	5.754781	-4.889992	-0.056019
H	4.450044	-3.804942	-4.008409
H	3.486860	-1.582542	-4.418199
H	5.450733	-5.460550	-2.463846
C	1.692026	-0.314956	1.033733
H	1.574222	-0.612598	0.000745
O	2.116943	0.278897	3.798823
C	6.667404	-0.096558	0.505761
H	6.411669	-0.133274	-0.551338
H	7.257765	0.808567	0.672548
H	7.304935	-0.959910	0.725717
C	2.929834	1.610829	-1.056072
O	3.639761	2.287870	-0.309673
N	1.710913	1.982036	-1.529191
H	1.170876	1.251766	-1.976501
C	0.917158	3.193027	-1.235423
C	-0.402289	2.999607	-2.017942
H	-1.085796	3.818908	-1.790736
H	-0.192259	3.023789	-3.092872
O	-1.033143	1.747334	-1.758808

H	-1.542750	1.830519	-0.934053
C	1.622336	4.565505	-1.576094
C	2.590853	4.403975	-2.761635
H	3.446364	3.778550	-2.497594
H	2.093376	3.957827	-3.629336
H	2.973589	5.384954	-3.062346
C	2.378277	5.088756	-0.337160
H	2.896682	6.022883	-0.581586
H	1.675078	5.302804	0.476662
H	3.105070	4.359430	0.015835
C	0.578363	5.647446	-1.943678
H	-0.175667	5.771104	-1.158435
H	1.090537	6.608335	-2.055266
H	0.065580	5.443706	-2.888228
N	0.606865	0.058594	1.669649
C	-0.655034	0.159664	1.075070
C	-1.476893	1.139350	1.823864
O	-1.430983	1.256162	3.039235
O	-2.224417	1.888816	0.987879
C	-2.971352	3.085158	1.483187
C	-3.648706	3.614070	0.222224
H	-2.911762	3.846577	-0.551442
H	-4.355787	2.886706	-0.174197
H	-4.187502	4.535008	0.461501
C	-4.011839	2.670066	2.522692
H	-3.538090	2.392507	3.463862
H	-4.688346	3.512422	2.699567
H	-4.580569	1.812441	2.158865
C	-1.955999	4.093809	2.022792
H	-2.479501	5.010922	2.308488
H	-1.437860	3.701028	2.897983

H	-1.218713	4.345784	1.254033
P	-4.192421	-1.021838	0.630876
O	-4.458591	-0.585121	2.059499
C	-5.167176	-2.539211	0.269451
C	-6.276065	-2.846767	1.069673
C	-4.838186	-3.386360	-0.799319
C	-7.047196	-3.980942	0.805029
H	-6.519564	-2.197005	1.904758
C	-5.608096	-4.519585	-1.064473
H	-3.969638	-3.159150	-1.409855
C	-6.715261	-4.817343	-0.263786
H	-7.902875	-4.213602	1.432710
H	-5.344521	-5.172507	-1.891833
H	-7.313736	-5.700113	-0.469918
C	-4.851115	0.183744	-0.581753
C	-6.120568	0.740991	-0.364455
C	-4.122287	0.566128	-1.715549
C	-6.653355	1.662255	-1.267152
H	-6.686824	0.460844	0.519443
C	-4.653212	1.491012	-2.616793
H	-3.131734	0.155535	-1.870893
C	-5.919826	2.037623	-2.397298
H	-7.634868	2.091602	-1.087959
H	-4.071771	1.792092	-3.483548
H	-6.331992	2.757920	-3.098028
N	-2.676549	-1.338780	0.111545
C	-1.632404	-1.533727	0.945863
C	-0.516021	-2.382044	0.421518
C	-0.286550	-2.472164	-0.961331
C	0.359034	-3.039549	1.296165
C	0.790660	-3.204404	-1.454064

H	-0.964024	-1.955466	-1.632627
C	1.432968	-3.785798	0.800475
H	0.204274	-2.957965	2.368854
C	1.652406	-3.868695	-0.574165
H	0.969723	-3.252451	-2.524064
H	2.106728	-4.285998	1.489669
H	2.497890	-4.427465	-0.959830
H	-0.585635	0.333791	0.008765
C	6.852432	0.362061	3.277482
H	7.496995	-0.481445	3.032301
H	7.290396	1.284040	2.892904
H	6.745873	0.434370	4.356882
H	-1.810998	-1.667064	2.020936
H	0.752651	0.284932	2.674746
H	0.674689	3.195110	-0.163523

#### Vibrational frequencies

-379.5759	13.6330	16.8918
19.8919	23.2498	26.9677
32.5028	39.3033	43.6250
47.2955	51.8485	53.1927
56.2105	61.0697	63.5861
66.1760	68.8781	79.6272
82.5829	86.8099	90.6686
92.8829	94.8717	101.3400
108.6007	115.5593	124.6296
132.7130	142.2812	150.0034
152.2384	158.0700	159.6504
164.6813	175.1709	185.4582
188.0054	188.9098	196.0880
204.0526	219.3736	227.4050

232.4116	237.0952	242.0292
245.2963	250.2866	254.1626
262.3401	266.2862	269.1584
279.6233	282.4024	291.5897
296.5705	298.7038	302.1843
317.7215	338.1228	340.5925
345.7825	347.2918	355.1433
360.3862	368.4179	375.8372
379.6125	388.2502	394.8525
399.8085	409.8616	410.9437
411.5145	412.6511	416.1543
416.8737	428.2542	440.7081
442.5173	446.7289	453.5637
456.4531	471.3054	477.2695
479.4019	487.9125	500.4221
515.1926	527.6564	537.8554
539.4598	541.3001	545.7846
548.8672	558.3564	576.0850
584.3406	590.8154	603.5484
618.4529	628.4564	630.4852
631.7545	633.1719	636.0539
643.7990	663.7889	678.6059
690.4763	706.1470	710.6877
714.4200	716.7338	722.6104
740.2744	745.4044	752.5553
758.6245	762.8015	769.4105
770.7955	771.6386	779.8967
787.3188	796.4389	800.3101
813.0725	820.8455	847.5933
847.8869	849.4776	857.7217
865.4923	868.0951	871.7511

873.0238	887.9789	892.2685
895.2258	910.7922	919.8803
937.3273	941.0216	942.4370
944.5451	945.6056	946.3353
946.6842	959.0956	960.9006
973.7528	979.6800	981.1259
987.4844	988.8649	989.4938
990.8870	1005.9116	1006.7346
1009.0698	1010.0727	1011.6625
1012.0665	1013.6864	1015.0851
1017.8408	1031.8656	1039.9307
1048.7709	1049.8098	1052.4104
1053.5020	1057.8098	1062.8002
1064.3879	1073.0988	1074.8227
1079.8878	1080.2110	1091.9949
1099.6173	1099.7341	1104.0155
1118.0442	1120.3427	1124.3090
1126.9226	1133.4377	1147.0493
1156.3555	1166.5732	1173.7216
1183.3678	1188.8784	1189.1504
1189.6686	1191.4668	1198.2951
1199.5571	1203.6968	1205.0813
1208.3017	1210.8294	1217.9794
1227.7211	1243.2517	1247.2535
1252.6058	1260.5199	1261.2932
1263.4814	1266.8169	1279.7436
1294.4960	1294.6152	1310.2103
1316.8725	1322.2139	1323.5297
1327.5788	1341.6223	1344.9942
1351.2737	1353.7412	1357.8853
1361.6577	1364.8760	1373.1639

1401.0044	1407.8531	1408.4139
1411.2129	1415.9657	1417.3481
1421.0533	1422.6207	1428.8592
1435.6436	1437.5925	1439.0266
1445.6736	1446.6011	1448.0195
1466.6438	1470.7636	1472.4821
1475.2623	1481.6725	1482.2735
1488.1381	1488.8074	1491.2668
1495.7946	1497.8042	1500.3494
1501.5320	1502.1144	1503.1492
1504.9133	1506.3603	1512.7521
1515.0618	1515.6684	1519.3943
1519.8208	1521.2776	1529.2530
1531.7157	1533.3234	1539.5124
1548.3435	1553.4877	1559.1235
1578.4423	1608.8527	1623.4524
1625.6714	1632.5942	1635.1763
1642.2625	1643.3953	1643.5194
1651.9608	1666.0712	1671.8368
1735.7581	1753.9279	3018.5280
3023.3483	3031.3611	3036.5746
3045.1563	3054.1213	3054.8509
3058.3581	3062.0931	3069.1255
3091.8953	3092.8381	3104.7205
3108.8743	3115.6257	3115.9386
3123.7634	3131.3153	3133.0956
3137.4349	3141.1465	3143.6640
3161.7934	3171.3288	3176.9490
3177.0988	3177.1211	3177.2600
3177.5390	3178.8815	3184.1460
3185.0851	3186.3627	3189.2392

3190.9667	3193.1651	3194.8077
3196.0719	3196.0858	3196.4202
3202.0039	3204.2466	3205.1846
3207.2470	3209.7386	3210.3909
3210.9104	3213.9197	3222.6010
3223.2487	3224.4747	3246.1206
3255.2343	3592.7682	3691.0508

## MSRR

Zero-point correction= 0.964017

Thermal correction to Energy= 1.021220

Thermal correction to Enthalpy= 1.022164

Thermal correction to Gibbs Free Energy= 0.871540

Sum of electronic and zero-point Energies= -2949.547579

Sum of electronic and thermal Energies= -2949.490375

Sum of electronic and thermal Enthalpies= -2949.489431

Sum of electronic and thermal Free Energies= -2949.640055

## Cartesian coordinates

C	-2.902055	-2.076370	-3.593925
C	-1.675250	-1.979561	-2.872066
C	-1.820448	-1.653199	-1.468165
C	-3.104159	-1.479988	-0.905097
C	-4.254322	-1.648188	-1.674257
N	-4.098558	-1.929204	-3.010635
H	-2.879481	-2.294089	-4.652709
C	-3.245120	-1.089998	0.534244
C	-3.239565	-2.101444	1.546379
C	-3.355166	0.248699	0.883242
C	-3.085733	-3.483637	1.244380
C	-3.395474	-1.712291	2.917925



C	-3.482831	0.619397	2.247427
C	-3.082844	-4.428506	2.246324
H	-2.968170	-3.790632	0.210727
C	-3.394676	-2.713874	3.926049
C	-3.522893	-0.334196	3.234987
H	-3.553230	1.672311	2.496322
C	-3.239740	-4.042887	3.600281
H	-2.961220	-5.478247	1.998048
H	-3.511755	-2.408926	4.962097
H	-3.633566	-0.042896	4.275396
H	-3.236137	-4.798910	4.379189
C	-0.642951	-1.534761	-0.654673
H	-0.716540	-1.259531	0.388807
O	-0.564210	-2.170682	-3.455356
C	-5.642777	-1.494352	-1.128521
H	-5.601301	-1.419401	-0.043883
H	-6.102883	-0.575104	-1.501528
H	-6.282355	-2.342864	-1.385320
C	-3.388898	1.321822	-0.182135
O	-4.207332	1.262657	-1.112211
N	-2.499206	2.314441	0.004177
H	-1.763775	2.167954	0.714491
C	-2.259353	3.335640	-1.010164
C	-0.883011	3.066760	-1.665865
H	-0.794181	3.688347	-2.565321
H	-0.077098	3.363933	-0.981153
O	-0.740157	1.708850	-2.027054
H	-0.195500	1.298871	-1.299167
C	-2.448777	4.773002	-0.437147
C	-2.255778	5.805609	-1.565242
H	-1.224661	5.825433	-1.930770

H	-2.914121	5.591980	-2.415393
H	-2.494456	6.811167	-1.201732
C	-1.454841	5.069278	0.704330
H	-1.671634	6.049034	1.144362
H	-1.513958	4.316681	1.495146
H	-0.419727	5.090923	0.348916
C	-3.886194	4.895725	0.104341
H	-4.058862	4.191557	0.923375
H	-4.070522	5.908262	0.480129
H	-4.621703	4.686504	-0.680855
N	0.539809	-1.813249	-1.134706
C	1.753279	-1.532432	-0.424477
C	2.894263	-2.332172	-1.020875
O	2.823581	-2.931179	-2.078490
O	3.957444	-2.220500	-0.226687
C	5.270128	-2.831531	-0.558099
C	5.788533	-2.258314	-1.877050
H	5.168178	-2.574026	-2.715962
H	5.797298	-1.166213	-1.839489
H	6.810958	-2.611018	-2.041239
C	6.135928	-2.385312	0.618496
H	5.715211	-2.745675	1.561619
H	7.146994	-2.786530	0.509262
H	6.194930	-1.293921	0.657474
C	5.117613	-4.352021	-0.593678
H	6.102720	-4.811053	-0.717930
H	4.685396	-4.711229	0.344810
H	4.478860	-4.661575	-1.421519
P	0.842074	1.312544	1.492931
O	-0.505846	1.915159	1.870643
C	2.191412	2.512889	1.806898

C	2.594012	2.830270	3.113537
C	2.785626	3.182103	0.727284
C	3.575177	3.797052	3.335291
H	2.147369	2.312945	3.958273
C	3.766620	4.150716	0.948911
H	2.482220	2.930898	-0.283825
C	4.162601	4.458746	2.252480
H	3.883745	4.033013	4.349529
H	4.223768	4.659884	0.105433
H	4.928160	5.209363	2.425860
C	1.196912	-0.112206	2.594020
C	0.101707	-0.907174	2.969915
C	2.493870	-0.556932	2.894997
C	0.295512	-2.132624	3.607457
H	-0.901591	-0.554064	2.757826
C	2.689330	-1.783251	3.535521
H	3.353797	0.050350	2.629422
C	1.592801	-2.575968	3.884122
H	-0.563604	-2.737039	3.882579
H	3.697686	-2.119893	3.758179
H	1.748289	-3.532666	4.373873
N	0.924480	0.802699	-0.057098
C	2.080888	0.048689	-0.452080
C	2.647096	0.477225	-1.797824
C	1.914260	0.383659	-2.989886
C	3.952760	0.983200	-1.851064
C	2.483847	0.775631	-4.201838
H	0.897058	0.015263	-2.981656
C	4.521289	1.385186	-3.061942
H	4.527957	1.066542	-0.932841
C	3.787484	1.277480	-4.244271

H	1.904931	0.690174	-5.117100
H	5.534245	1.776804	-3.079222
H	4.225229	1.583528	-5.189941
H	1.635106	-1.790076	0.629141
C	-5.301744	-2.068050	-3.862634
H	-5.880745	-2.932446	-3.536759
H	-5.908400	-1.166469	-3.782874
H	-4.988015	-2.207648	-4.893810
H	2.912943	0.106831	0.262617
H	0.554652	-2.075483	-2.141289
H	-3.023203	3.178412	-1.777697

Vibrational frequencies

16.0167	18.4469	25.5762
28.6668	30.6184	32.1627
36.4759	39.7537	44.2578
45.7606	49.4764	53.8495
55.1975	58.8397	63.4078
65.5776	74.1229	76.7249
84.4510	87.1534	91.0175
94.3695	106.4412	120.0895
122.1326	124.4001	127.2378
134.4943	138.2537	147.6766
156.0358	163.4433	173.8967
180.8976	185.9138	193.6652
195.9836	208.5790	220.3325
222.7425	224.5104	225.1660
233.5015	242.0867	247.2657
251.6903	259.8610	260.9627
268.6555	274.6985	283.7398
287.7006	290.8361	293.8489

297.0716	310.8568	317.6191
321.7979	332.4235	346.5586
350.5285	360.2168	364.7791
370.1438	378.6241	383.8854
388.0609	391.7524	401.5911
406.7185	408.6908	410.2758
412.4226	417.4109	422.8325
428.2750	439.9760	442.7529
446.9352	450.9355	457.2988
472.3276	482.6742	483.9964
508.6110	514.6151	523.5325
528.0808	532.2605	535.3438
554.5151	556.5128	563.7109
569.8277	574.2057	581.5436
589.8405	613.8711	630.1212
631.7874	632.4168	641.4029
648.4263	663.2949	676.8512
695.4100	696.6202	712.5187
714.6895	721.4793	729.0404
732.1795	747.0335	748.2634
755.9498	764.2626	766.0410
769.5464	770.8556	775.5413
785.0205	795.4343	798.3166
810.9479	811.9932	821.4781
825.0262	848.5569	854.0068
858.2631	861.8311	874.8677
879.9642	885.1694	885.9634
888.5555	892.1457	908.9982
920.8167	925.0427	927.9247
936.9136	937.7533	940.2212
942.7015	948.5717	949.3248

949.5255	953.5893	966.7945
973.8906	974.7368	975.7060
980.6188	983.8155	995.2253
998.8206	1001.5927	1003.4034
1009.5861	1012.5596	1013.6402
1013.9459	1015.6969	1020.5912
1023.3598	1033.1143	1036.9535
1049.1859	1050.3354	1051.8517
1056.6825	1057.9946	1058.3277
1065.1659	1069.8019	1080.8609
1094.1178	1098.5506	1101.6681
1104.4434	1107.7503	1112.5680
1120.2295	1130.4652	1131.8471
1138.5364	1143.2786	1145.8340
1150.3800	1162.5541	1180.7220
1186.8365	1189.2284	1190.9680
1191.4938	1192.4778	1198.0153
1210.7841	1211.1105	1213.1591
1215.3195	1223.1951	1226.5209
1242.1822	1247.8531	1253.1030
1253.8325	1262.6371	1279.4284
1279.4648	1284.0968	1292.4061
1294.5085	1297.1855	1320.2191
1322.2487	1329.0279	1330.1620
1340.4205	1348.0257	1354.7736
1357.7655	1358.3139	1359.3572
1367.4123	1369.7588	1386.9301
1403.7534	1409.2970	1411.8770
1412.9501	1413.7465	1415.8652
1418.0347	1420.8876	1424.9277
1425.6020	1426.7061	1438.3784

1439.2529	1445.9073	1452.4452
1466.4923	1471.3529	1475.2380
1480.1195	1480.7289	1482.1726
1487.6105	1494.4095	1494.9121
1495.3441	1495.9067	1497.2490
1499.0273	1500.6814	1503.4781
1507.4892	1508.7744	1510.7406
1512.4226	1518.3559	1519.9320
1520.9506	1523.2288	1528.1960
1532.0169	1540.4649	1548.4408
1553.6176	1570.1473	1588.2853
1610.4107	1621.2469	1624.0849
1625.3503	1637.4382	1641.9304
1644.1015	1646.4096	1654.9070
1657.5674	1671.6905	1682.5260
1709.4527	1783.4254	3012.4429
3019.0680	3030.1520	3033.5924
3042.4395	3051.9646	3057.9132
3060.2339	3065.4731	3065.9457
3086.8588	3094.4276	3097.6166
3101.8285	3105.7995	3112.9389
3119.2907	3122.9720	3128.0514
3130.1462	3130.4970	3130.7947
3133.1532	3136.6878	3141.9267
3161.9645	3166.9896	3167.4513
3174.5046	3177.9394	3180.4816
3180.9043	3181.4910	3181.8524
3184.6086	3184.7883	3190.2807
3191.0203	3191.7148	3194.0347
3194.3146	3199.0536	3201.6671
3204.5272	3204.6024	3206.0921

3206.8885	3207.7619	3210.8619
3215.2070	3216.7429	3221.0434
3245.6430	3257.2056	3257.9107

### M5RS

Zero-point correction= 0.963262

Thermal correction to Energy= 1.020925

Thermal correction to Enthalpy= 1.021869

Thermal correction to Gibbs Free Energy= 0.871648

Sum of electronic and zero-point Energies= -2949.521683

Sum of electronic and thermal Energies= -2949.464020

Sum of electronic and thermal Enthalpies= -2949.463076

Sum of electronic and thermal Free Energies= -2949.613297

### Cartesian coordinates

C	-2.397172	0.885265	4.031496
C	-1.357051	0.277638	3.260864
C	-1.612807	0.240065	1.836178
C	-2.805007	0.775409	1.304360
C	-3.777713	1.332914	2.136225
N	-3.521255	1.369531	3.487030
H	-2.284413	0.962453	5.104203
C	-3.032980	0.785275	-0.178299
C	-2.851535	2.002321	-0.909232
C	-3.378244	-0.376029	-0.855873
C	-2.439798	3.212962	-0.285686
C	-3.091492	2.007085	-2.324073
C	-3.587880	-0.367929	-2.258123
C	-2.304652	4.370187	-1.016170
H	-2.212623	3.214061	0.774290
C	-2.941851	3.221098	-3.047597



C	-3.465962	0.800224	-2.970529
H	-3.859041	-1.292758	-2.756391
C	-2.562874	4.378267	-2.407779
H	-1.963194	5.277005	-0.530750
H	-3.126771	3.214781	-4.118025
H	-3.645715	0.810413	-4.041503
H	-2.439679	5.298418	-2.969513
C	-0.664612	-0.395281	0.969500
H	-0.899549	-0.514429	-0.072583
O	-0.321876	-0.178814	3.821863
C	-5.085065	1.880291	1.638548
H	-5.199867	1.654254	0.580432
H	-5.935395	1.437300	2.164664
H	-5.144774	2.967736	1.757782
C	-3.484371	-1.666624	-0.095478
O	-4.292362	-1.823656	0.832246
N	-2.596000	-2.609791	-0.481625
H	-1.926522	-2.363734	-1.200011
C	-2.514629	-3.940135	0.135577
C	-1.730649	-3.872865	1.462341
H	-1.799675	-4.853420	1.952572
H	-0.670556	-3.673873	1.270802
O	-2.186366	-2.847330	2.334917
H	-3.107878	-2.635415	2.104245
C	-1.978689	-4.986500	-0.888596
C	-0.524716	-4.688238	-1.307826
H	-0.406322	-3.695485	-1.751671
H	0.170291	-4.769440	-0.466810
H	-0.203796	-5.408021	-2.067184
C	-2.879769	-4.965747	-2.141124
H	-2.571193	-5.753242	-2.835974

H	-3.928131	-5.139605	-1.875122
H	-2.819417	-4.013088	-2.674710
C	-2.047279	-6.393353	-0.261285
H	-3.057377	-6.619257	0.097890
H	-1.780883	-7.145633	-1.010488
H	-1.353622	-6.506299	0.576478
N	0.421704	-0.968892	1.416065
C	1.400649	-1.473753	0.505213
C	2.693841	-1.721037	1.241393
O	2.940260	-1.277563	2.349843
O	3.509422	-2.441832	0.467888
C	4.916290	-2.729548	0.843793
C	4.939592	-3.580568	2.113753
H	4.567071	-3.018247	2.970081
H	4.326015	-4.476493	1.980551
H	5.967579	-3.894429	2.317677
C	5.419293	-3.521779	-0.361681
H	5.358586	-2.916514	-1.270772
H	6.461996	-3.811586	-0.206028
H	4.822496	-4.427248	-0.503125
C	5.674051	-1.412456	0.994972
H	6.737447	-1.621758	1.144705
H	5.565731	-0.803636	0.093849
H	5.306280	-0.835707	1.842667
P	1.617413	2.025802	0.390488
O	1.182394	2.125488	1.842940
C	1.197378	3.581520	-0.483606
C	1.067435	4.763620	0.259043
C	1.079790	3.637460	-1.879148
C	0.832507	5.981923	-0.380844
H	1.145002	4.716410	1.341024

C	0.846002	4.854374	-2.520899
H	1.156449	2.718458	-2.451626
C	0.725435	6.029108	-1.773645
H	0.731465	6.892097	0.203817
H	0.748972	4.886559	-3.602366
H	0.542074	6.975883	-2.273701
C	3.461720	2.007548	0.321722
C	4.198302	2.082475	1.510790
C	4.149517	1.938250	-0.900605
C	5.594710	2.101308	1.481805
H	3.663044	2.129537	2.453991
C	5.544645	1.953161	-0.932169
H	3.588986	1.879699	-1.829657
C	6.269601	2.038652	0.260714
H	6.155684	2.163135	2.410115
H	6.066432	1.899844	-1.883503
H	7.355416	2.052242	0.236939
N	1.029303	0.858833	-0.581229
C	1.649645	-0.391187	-0.759676
C	1.155760	-1.095769	-2.021443
C	-0.065323	-0.750760	-2.614256
C	1.904922	-2.140445	-2.580209
C	-0.536909	-1.448726	-3.730454
H	-0.624703	0.085646	-2.208841
C	1.445387	-2.825083	-3.706777
H	2.846508	-2.423327	-2.117279
C	0.217459	-2.487013	-4.282438
H	-1.488948	-1.169062	-4.171079
H	2.041673	-3.628489	-4.129779
H	-0.146154	-3.025356	-5.152497
H	1.061595	-2.403333	0.045926

C	-4.526837	1.965515	4.395744
H	-4.747931	2.984045	4.077879
H	-5.438038	1.367099	4.374637
H	-4.124242	1.978878	5.405251
H	2.747186	-0.348745	-0.808811
H	0.642560	-0.787573	2.408342
H	-3.547747	-4.214457	0.381350

Vibrational frequencies

19.1240	21.7811	26.7812
27.3824	35.2040	36.6684
43.5948	44.5759	46.6848
49.8557	53.7405	58.0667
64.0119	66.7401	70.4376
73.0209	77.6780	79.1188
81.5817	89.4585	95.4124
98.8920	101.5971	106.0502
108.0618	119.1630	125.7215
128.0075	134.3279	142.6830
153.5077	154.8878	159.7122
171.3963	188.3520	193.3619
194.8470	201.9987	211.4568
216.2290	223.8086	233.9400
235.5780	244.3900	244.4688
250.3834	254.9999	262.6980
263.9909	269.9520	281.1527
288.3101	292.4544	296.9706
301.7940	303.3741	306.4038
316.5559	328.0517	343.9355
349.8193	356.5136	357.1842
359.8651	374.1448	376.1035

384.7680	396.4939	402.2253
407.4671	408.9092	411.9185
412.6928	419.1624	425.6069
433.9009	440.7681	442.1295
448.8784	453.6116	457.9774
468.0319	472.1417	478.1215
484.8881	500.3350	504.6460
510.9018	525.2869	531.2804
536.5278	544.4799	549.7795
554.6072	567.9948	578.5915
583.7652	599.4034	609.7478
622.8464	627.3779	629.9422
631.4048	633.4009	646.5678
663.9312	668.8522	671.9725
698.9051	703.0564	708.7688
712.8275	723.2067	723.8084
737.9309	752.9683	756.3163
761.1837	761.3261	762.9147
768.5123	778.7013	780.5680
794.0614	796.1586	804.0804
815.7218	824.1365	827.1820
848.4745	855.8250	858.8910
869.7183	873.1697	877.8862
881.1977	883.7171	888.4531
895.6370	908.1634	915.7578
933.7651	938.9720	939.5762
941.5865	945.8826	948.1281
949.4694	951.5753	966.3253
968.0895	982.1676	982.9861
984.3774	984.8609	986.1679
990.4578	993.9533	1003.0533

1005.9699	1006.7507	1010.0005
1012.3999	1013.3232	1015.2263
1018.9943	1025.6096	1029.8507
1048.6021	1049.0750	1050.3714
1053.7738	1057.5824	1062.2269
1065.1209	1070.0375	1078.9402
1083.6907	1095.2187	1097.4932
1101.4551	1111.0732	1113.8557
1114.2790	1124.2728	1126.8361
1134.3920	1146.5092	1153.0896
1159.9659	1180.1342	1185.4939
1187.9679	1188.2471	1189.0314
1190.1502	1193.6781	1198.8166
1200.1954	1203.9664	1208.3330
1209.6073	1214.6724	1216.3215
1238.1223	1247.6400	1254.6513
1256.1089	1261.0993	1272.1281
1274.3539	1281.1914	1281.6840
1292.7580	1293.4873	1305.7852
1315.6529	1321.1105	1324.3795
1327.8675	1331.5643	1339.1827
1350.9122	1354.3379	1358.9230
1363.9767	1368.2814	1388.7687
1389.4987	1404.4103	1408.5364
1412.1360	1412.7588	1414.2856
1419.5217	1423.3993	1426.6346
1429.8973	1434.1237	1436.6182
1440.1707	1450.5649	1453.1872
1467.8975	1471.1915	1472.2757
1474.7422	1479.2075	1480.4683
1484.1601	1489.6033	1490.0630

1492.8763	1495.5802	1495.6218
1497.1147	1502.0524	1502.5174
1502.9100	1508.1268	1511.6905
1513.2253	1518.6857	1518.8342
1520.0986	1521.5781	1526.1545
1529.7460	1531.0596	1532.8201
1548.2843	1555.8731	1567.0672
1593.0347	1614.5262	1623.5112
1625.6193	1633.0806	1641.9481
1643.5466	1645.2497	1651.0322
1652.2995	1673.5575	1686.2034
1703.5692	1773.9581	2996.5249
3020.0881	3039.7384	3043.1788
3048.7006	3051.5351	3051.9712
3054.0665	3057.8003	3065.1058
3083.4606	3094.5387	3109.5633
3112.4310	3113.6468	3117.6979
3120.1854	3122.0630	3124.0932
3127.0189	3130.1076	3130.2024
3134.7945	3139.2891	3166.5200
3174.9878	3175.2023	3175.3206
3178.7125	3179.7758	3180.2480
3181.3554	3183.7415	3186.0404
3188.8112	3190.5945	3190.7469
3194.9297	3196.4178	3199.8883
3201.2698	3205.6750	3206.0117
3206.2625	3206.3763	3206.8747
3210.0715	3210.8719	3215.1482
3228.3482	3254.0873	3256.9843
3322.6992	3601.4738	3662.9054

## M5SS

Zero-point correction= 0.963551

Thermal correction to Energy= 1.021165

Thermal correction to Enthalpy= 1.022109

Thermal correction to Gibbs Free Energy= 0.870326

Sum of electronic and zero-point Energies= -2949.538186

Sum of electronic and thermal Energies= -2949.480572

Sum of electronic and thermal Enthalpies= -2949.479628

Sum of electronic and thermal Free Energies= -2949.631412

### Cartesian coordinates

C	3.278510	-3.938232	-1.066611
C	2.002344	-3.293206	-1.040915
C	2.009322	-1.970952	-0.452427
C	3.205227	-1.409367	0.050960
C	4.401161	-2.125766	0.012907
N	4.384356	-3.376694	-0.564167
H	3.366147	-4.924218	-1.501773
C	3.199212	-0.017910	0.606706
C	3.739344	1.054653	-0.173715
C	2.614589	0.252498	1.835714
C	4.271924	0.861893	-1.479262
C	3.730378	2.380732	0.372062
C	2.586510	1.570966	2.352240
C	4.785555	1.920428	-2.195364
H	4.264034	-0.130448	-1.916646
C	4.274631	3.447961	-0.391382
C	3.155084	2.603897	1.650183
H	2.107488	1.748683	3.308820
C	4.793675	3.225426	-1.646197
H	5.184090	1.754108	-3.191477



H	4.249349	4.449123	0.026982
H	3.133528	3.614215	2.044933
H	5.198522	4.050575	-2.223851
C	0.780895	-1.248120	-0.338009
H	0.755529	-0.256025	0.088224
O	0.977743	-3.861715	-1.515944
C	5.694127	-1.610156	0.576899
H	5.507810	-0.695886	1.136901
H	6.153740	-2.329356	1.260306
H	6.421427	-1.379730	-0.209240
C	1.962366	-0.863975	2.603302
O	2.618016	-1.849046	2.995307
N	0.636739	-0.718687	2.776815
H	0.171425	0.066457	2.296246
C	-0.162561	-1.705618	3.517806
C	-0.515129	-2.892812	2.603459
O	0.627467	-3.531924	2.045916
H	1.422084	-3.179266	2.488513
C	-1.394879	-1.041627	4.210668
C	-1.939697	-2.003292	5.286512
H	-2.293440	-2.945380	4.857952
H	-1.173969	-2.236067	6.034866
H	-2.785940	-1.540466	5.804699
C	-2.515645	-0.712390	3.203036
H	-3.325659	-0.177814	3.711050
H	-2.148746	-0.067933	2.401199
H	-2.949179	-1.614475	2.760008
C	-0.947089	0.262063	4.903881
H	-0.668589	1.030246	4.177636
H	-1.766385	0.658876	5.512626
H	-0.089176	0.086193	5.562313

N	-0.359870	-1.748995	-0.722961
C	-1.578690	-0.988554	-0.671871
C	-2.768769	-1.902001	-0.828641
O	-2.715025	-3.041445	-1.256878
O	-3.856963	-1.231938	-0.444473
C	-5.221727	-1.806007	-0.489792
C	-5.591048	-2.119007	-1.939773
H	-5.509026	-1.217582	-2.554311
H	-4.943134	-2.893635	-2.351871
H	-6.626917	-2.467843	-1.981944
C	-5.283339	-3.036869	0.415119
H	-4.935097	-2.782668	1.420806
H	-6.319173	-3.381082	0.486119
H	-4.669186	-3.846903	0.020871
C	-6.068281	-0.662351	0.066598
H	-7.122695	-0.951514	0.078647
H	-5.758881	-0.417970	1.086491
H	-5.954363	0.234505	-0.548262
P	-0.860965	2.043252	-0.018034
O	-0.526372	1.365807	1.324009
C	-2.619955	2.575852	0.100753
C	-3.313791	2.476468	1.314547
C	-3.308628	3.008123	-1.043873
C	-4.671507	2.796867	1.383654
H	-2.783778	2.136832	2.197458
C	-4.665468	3.327526	-0.977361
H	-2.779831	3.076533	-1.990783
C	-5.349718	3.219022	0.237480
H	-5.200793	2.712344	2.328587
H	-5.190533	3.654278	-1.870334
H	-6.407216	3.461413	0.288876

C	0.119737	3.570418	-0.180284
C	0.322752	4.368604	0.955188
C	0.659130	3.973634	-1.408491
C	1.047508	5.556632	0.862499
H	-0.074414	4.046375	1.913134
C	1.392063	5.158470	-1.499475
H	0.507362	3.343012	-2.278005
C	1.583650	5.952997	-0.366787
H	1.200616	6.169132	1.746380
H	1.818353	5.458731	-2.452243
H	2.152320	6.875625	-0.439224
N	-0.626983	1.233381	-1.397213
C	-1.547839	0.211215	-1.770082
C	-1.218677	-0.387287	-3.128510
C	0.097865	-0.398480	-3.605800
C	-2.221237	-0.991769	-3.897226
C	0.406710	-1.011883	-4.820927
H	0.865845	0.087262	-3.013521
C	-1.916872	-1.601948	-5.115522
H	-3.248620	-0.980825	-3.542795
C	-0.599097	-1.617199	-5.579456
H	1.433036	-1.015746	-5.177827
H	-2.707469	-2.061326	-5.702013
H	-0.359286	-2.091658	-6.526687
H	-1.655213	-0.488771	0.293088
C	5.644801	-4.151084	-0.640570
H	6.404303	-3.560233	-1.151797
H	5.983153	-4.396365	0.366374
H	5.461162	-5.067015	-1.196053
H	-2.600072	0.539214	-1.779111
H	-0.320171	-2.686410	-1.161267

H	0.494564	-2.085339	4.309775
H	-1.108849	-3.619554	3.174646
H	-1.140816	-2.544868	1.773131

Vibrational frequencies

12.9289	20.5003	24.6600
27.4476	31.7871	34.6214
39.6105	44.0567	44.7490
46.0216	48.6268	51.2704
53.8094	57.0188	62.1729
63.5517	67.8802	75.1548
83.3596	84.3585	90.5446
94.4733	98.7842	103.9494
104.8573	112.6388	122.9618
132.2904	141.9936	146.6273
150.0107	157.6269	159.5837
174.4447	181.8570	188.9811
193.4289	206.2019	211.3225
224.0354	226.4492	227.5994
234.4999	237.9325	242.6219
253.0616	257.5952	261.7069
265.5290	273.9323	281.7525
288.9171	290.3860	295.0229
304.8857	309.2192	320.6170
330.4332	332.4119	337.7136
341.8423	357.4667	359.3628
365.9066	376.4524	378.4207
386.1335	399.7872	404.3009
410.1121	410.9717	412.2822
419.4173	421.6278	425.0273
435.6290	438.6570	441.8479

444.5392	454.8264	461.5121
469.4626	472.7719	477.5416
482.4696	504.8365	518.7001
521.3052	530.1285	535.0586
542.5527	550.7724	552.9845
555.3384	573.6984	581.0490
587.3723	595.3503	609.8126
630.7828	630.8512	633.9823
638.1048	649.3743	664.0213
671.8121	695.6746	698.5141
704.0701	709.6714	717.5492
725.8791	730.6810	744.2803
754.5414	756.9927	762.0673
764.1746	766.5196	769.1393
776.3176	793.9283	795.0398
797.0934	806.2193	822.0239
835.2995	844.2079	857.3417
860.0811	869.5529	871.8543
872.5097	876.7570	883.4169
884.4529	888.8063	904.5951
910.1352	914.1602	917.1079
933.3257	936.2889	940.2985
944.3833	947.1502	948.6866
950.3094	951.0810	965.8390
977.4951	980.1679	982.0705
987.8220	989.5546	991.2485
995.4502	1002.6348	1006.6261
1008.7565	1010.0379	1012.9558
1013.7909	1014.9759	1017.6951
1022.6267	1030.1781	1034.8476
1048.8404	1050.4653	1051.6787

1055.0020	1058.1078	1061.6465
1063.4872	1068.6333	1076.1350
1078.3366	1086.7363	1092.2228
1100.2467	1104.2484	1111.4614
1114.2639	1122.1590	1125.7034
1133.9925	1137.3193	1144.2403
1153.9066	1179.9589	1186.5596
1188.3312	1189.5505	1189.6836
1190.2519	1192.8731	1201.7188
1203.9159	1204.6884	1205.9704
1212.0857	1222.8550	1224.7484
1242.2374	1248.1711	1255.8699
1257.7938	1261.5793	1271.5916
1274.2631	1278.2060	1288.5539
1292.3661	1298.4507	1323.7192
1326.9534	1327.5093	1327.9176
1332.3869	1343.5322	1344.7324
1353.3380	1354.4411	1360.3547
1362.9434	1369.6988	1392.1644
1403.6458	1404.3898	1407.7384
1411.3397	1412.2877	1415.5468
1419.1473	1421.4100	1422.6037
1429.9802	1433.6949	1438.3632
1439.7979	1450.2538	1460.0857
1468.1341	1473.3566	1475.2794
1478.4830	1480.7974	1482.0165
1487.9845	1490.4059	1493.0939
1494.0116	1494.5899	1496.0652
1498.8717	1503.4374	1504.2529
1504.4758	1507.0978	1510.0376
1511.2632	1520.4053	1521.4406

1521.7767	1524.2930	1529.7249
1532.4301	1535.1109	1535.7349
1546.5216	1555.9983	1593.5771
1606.2175	1616.8609	1624.2117
1626.0272	1636.9647	1642.4327
1644.9757	1647.1268	1654.4487
1657.4673	1673.1869	1683.2255
1694.6391	1779.9420	2972.2768
3016.9749	3036.6754	3039.2884
3044.2736	3049.6485	3053.5051
3053.5326	3055.4104	3061.3222
3070.6702	3094.4705	3105.6917
3107.2054	3110.5011	3115.5717
3119.1443	3126.1123	3126.3654
3128.2912	3135.3712	3135.5952
3139.9589	3145.0594	3159.4501
3164.7193	3174.4307	3176.8238
3177.5780	3178.4544	3180.3112
3180.7567	3183.1366	3186.0363
3187.4996	3190.3419	3192.4709
3194.9977	3196.5932	3199.8144
3202.2848	3203.9543	3204.0154
3207.6722	3207.7777	3211.7640
3214.7352	3214.7724	3214.9683
3216.0814	3218.3309	3241.0752
3256.5444	3266.7676	3607.9117

## **TS6RR**

Zero-point correction= 1.030179

Thermal correction to Energy= 1.094469

Thermal correction to Enthalpy= 1.095413

Thermal correction to Gibbs Free Energy= 0.929568

Sum of electronic and zero-point Energies= -3290.969932

Sum of electronic and thermal Energies= -3290.905642

Sum of electronic and thermal Enthalpies= -3290.904698

Sum of electronic and thermal Free Energies= -3291.070543

Cartesian coordinates

C	-2.659574	-1.402132	-3.718715
C	-1.371828	-1.397931	-3.091313
C	-1.397303	-1.644306	-1.667369
C	-2.614698	-1.930333	-1.001512
C	-3.816863	-1.967486	-1.703897
N	-3.784322	-1.673778	-3.054375
H	-2.734752	-1.180782	-4.774480
C	-2.600356	-2.242374	0.463484
C	-2.065113	-3.512324	0.881521
C	-3.106976	-1.358696	1.407106
C	-1.565906	-4.478522	-0.037291
C	-2.035208	-3.832225	2.278251
C	-3.089053	-1.709554	2.784987
C	-1.040177	-5.673649	0.403555
H	-1.599076	-4.273437	-1.100643
C	-1.489796	-5.074075	2.699917
C	-2.556079	-2.897039	3.211232
H	-3.507181	-1.004099	3.493061
C	-0.994768	-5.975976	1.784620
H	-0.661058	-6.391746	-0.316831
H	-1.471086	-5.298064	3.762750
H	-2.529131	-3.139086	4.269690
H	-0.576482	-6.920457	2.117916
C	-0.182245	-1.525146	-0.925266



H	-0.196854	-1.622703	0.153608
O	-0.326111	-1.181612	-3.765794
C	-5.141580	-2.311375	-1.083196
H	-4.993662	-2.635258	-0.055592
H	-5.819838	-1.451601	-1.061249
H	-5.642585	-3.120832	-1.621290
C	-3.796157	-0.038069	1.118491
O	-4.867461	0.187441	1.702850
N	-3.180122	0.823428	0.291667
H	-2.280572	0.578222	-0.112522
C	-3.476413	2.260612	0.132815
C	-3.524390	2.951860	1.504926
H	-3.851620	3.988446	1.374765
H	-4.257492	2.451675	2.148878
O	-2.237730	3.002428	2.108882
H	-1.813661	2.116791	2.055244
C	-4.637832	2.589018	-0.856923
C	-6.027869	2.478698	-0.206245
H	-6.188510	1.481746	0.207480
H	-6.144006	3.199774	0.610110
H	-6.807898	2.690081	-0.946935
C	-4.550982	1.621929	-2.051814
H	-4.789592	0.604230	-1.736210
H	-5.258516	1.913808	-2.835268
H	-3.542511	1.606136	-2.478386
C	-4.425941	4.026668	-1.378249
H	-3.449072	4.130209	-1.864115
H	-5.199743	4.281683	-2.110343
H	-4.479758	4.766491	-0.573365
N	0.963094	-1.279024	-1.496596
C	2.179710	-1.029766	-0.759834

C	3.360889	-1.578886	-1.547337
O	3.288515	-1.953933	-2.701943
O	4.439687	-1.551412	-0.769747
C	5.765845	-2.052528	-1.216863
C	6.239749	-1.265428	-2.438418
H	5.617140	-1.473653	-3.308499
H	6.211848	-0.192206	-2.235059
H	7.271547	-1.549675	-2.665043
C	6.640730	-1.767673	0.002128
H	6.244106	-2.277349	0.884673
H	7.658915	-2.121134	-0.180646
H	6.674891	-0.693743	0.206270
C	5.654364	-3.552669	-1.487941
H	6.647381	-3.955248	-1.707488
H	5.259102	-4.068398	-0.607970
H	5.000928	-3.748925	-2.339042
P	0.777098	0.889215	1.771147
O	-0.722929	0.700079	1.944058
C	1.353012	2.297224	2.775724
C	0.578061	2.727128	3.861889
C	2.574600	2.931074	2.505137
C	1.026818	3.768818	4.675270
H	-0.384987	2.262240	4.043590
C	3.027496	3.964295	3.325541
H	3.156691	2.638122	1.636789
C	2.254814	4.381780	4.413024
H	0.418308	4.104442	5.509845
H	3.974037	4.451102	3.110496
H	2.604818	5.190219	5.048174
C	1.648708	-0.574005	2.443530
C	0.907699	-1.755450	2.602401

C	3.029921	-0.591926	2.692938
C	1.543649	-2.947107	2.954195
H	-0.166276	-1.728648	2.451824
C	3.664512	-1.783611	3.046829
H	3.613269	0.320552	2.614888
C	2.925002	-2.964089	3.164213
H	0.960704	-3.857000	3.055978
H	4.735082	-1.790727	3.227877
H	3.423344	-3.891760	3.428804
N	1.242629	1.133043	0.200094
C	2.409723	0.511606	-0.404347
C	2.878104	1.289977	-1.624441
C	4.195582	1.761151	-1.669191
C	2.029058	1.544324	-2.711389
C	4.664549	2.470862	-2.776993
H	4.858794	1.571659	-0.829519
C	2.497980	2.251543	-3.818881
H	0.997520	1.212581	-2.684062
C	3.815717	2.715644	-3.857588
H	5.688813	2.831520	-2.792629
H	1.829664	2.443299	-4.653400
H	4.175901	3.266918	-4.721144
H	2.123570	-1.563190	0.189386
C	-5.055719	-1.655892	-3.815378
H	-5.493985	-2.653795	-3.815596
H	-5.742881	-0.948669	-3.352208
H	-4.849569	-1.347238	-4.836791
H	3.264294	0.450701	0.279044
O	-0.982734	1.189928	-1.481535
H	-0.231605	1.069836	-0.849354
C	0.442773	4.309400	-0.983438

O	1.253812	3.678405	-0.190421
O	0.717032	5.633492	-0.979383
H	0.080028	6.051029	-1.579873
O	-0.468255	3.853675	-1.679238
H	1.158623	2.604611	-0.110462
H	0.925443	-1.188821	-2.530450
H	-0.956104	2.159508	-1.608618
H	-2.568143	2.638569	-0.339955

Vibrational frequencies

15.3776	21.0778	23.2332
27.5812	31.3761	33.8093
34.6605	38.9649	40.6336
42.1907	46.6131	48.7338
51.4721	54.5645	56.0580
61.2977	68.0454	68.9172
72.3852	74.6661	81.5293
83.2679	89.0671	90.9655
94.0415	106.0073	107.7389
114.1401	117.2927	119.7989
122.4733	127.6578	136.5600
139.6616	140.9807	147.3627
153.7069	162.7843	167.0186
174.8754	187.2076	191.7105
199.7383	205.9898	211.7253
218.9192	224.0816	226.2183
229.4338	231.4402	238.0696
241.0757	250.9284	254.9235
255.8610	262.5037	272.8191
275.3018	281.6641	285.4770
288.6793	292.0737	292.6964

307.6436	311.1654	324.5129
328.2510	333.0948	340.3039
348.2205	352.4279	360.2133
369.4482	382.1758	386.1540
392.3931	397.0015	402.4799
406.8678	409.5259	413.5931
418.8929	422.6795	423.8223
427.0776	433.7048	440.8600
443.2077	445.8117	454.9785
472.4898	478.8192	486.9634
489.2411	509.1778	518.1974
525.1625	534.5603	535.8390
543.8755	552.5854	552.9440
553.9870	569.6704	574.4188
584.4421	598.0191	605.0568
613.7491	624.6165	630.6549
631.7674	632.6801	637.4987
649.2400	665.3738	666.7715
668.0938	681.3125	691.5847
695.5816	701.4443	708.3587
713.0044	717.7996	723.6753
731.9923	734.1006	749.5692
755.3470	756.6095	766.0419
770.8746	771.7377	779.4128
784.8994	788.8721	790.6447
794.9040	795.5906	808.4513
821.1960	832.5305	842.8416
849.3630	852.6955	868.8726
869.4432	874.2908	877.4265
884.9069	887.4878	888.7039
904.7782	912.1966	916.2022

935.9944	939.6087	940.0429
943.3544	943.8736	947.4992
952.3860	952.6391	958.1970
970.2623	973.4050	984.2727
984.9203	985.4748	988.6618
994.6887	1000.8568	1004.9264
1005.6028	1008.4249	1010.4408
1013.3210	1013.7551	1015.2089
1016.2057	1024.2309	1028.1629
1038.1801	1039.8612	1050.5839
1052.4215	1055.2758	1059.9245
1060.6988	1061.8386	1065.8282
1069.8459	1074.9331	1080.3289
1088.1988	1096.8481	1101.4334
1106.4553	1113.8772	1119.8028
1123.6581	1130.2450	1131.9964
1141.4152	1149.0277	1152.6736
1156.6965	1179.5937	1185.2559
1189.4720	1192.1930	1192.6644
1193.7606	1197.0839	1209.8542
1210.7951	1212.0466	1216.3707
1221.2404	1228.2049	1228.5891
1241.4191	1246.7214	1248.4778
1254.7430	1256.2012	1267.4742
1280.0449	1285.2674	1286.6433
1293.9061	1298.7147	1312.7062
1320.9775	1326.5717	1328.0169
1330.5293	1334.6914	1344.1835
1346.4792	1356.1065	1357.5821
1361.1842	1363.1039	1370.9549
1374.3912	1402.4231	1407.4293

1408.1282	1415.0398	1415.0797
1416.0617	1416.7414	1418.3330
1419.2929	1426.1170	1430.9026
1434.7045	1440.0915	1441.1725
1447.6556	1459.9114	1463.8596
1469.1552	1473.5505	1476.4669
1480.5998	1480.8312	1484.7653
1485.4701	1490.2414	1491.9852
1494.8828	1495.5676	1497.5458
1499.0548	1499.3393	1503.6174
1504.5810	1506.9855	1510.8546
1511.4640	1513.2712	1518.1202
1523.5489	1524.7819	1529.8591
1531.3070	1532.0878	1542.2574
1542.9977	1552.5172	1568.9711
1602.0801	1611.6553	1623.3558
1627.2388	1637.8108	1642.8958
1644.7388	1649.5774	1657.1760
1659.3460	1670.8880	1681.0816
1696.7706	1704.6579	1734.7148
1788.7014	1921.9808	3032.6484
3036.0788	3042.8642	3045.1221
3046.0476	3053.0560	3055.1410
3058.5707	3066.2019	3086.8113
3097.6181	3098.2384	3104.9839
3111.2233	3112.6903	3114.3197
3116.1423	3127.8628	3130.0861
3132.2526	3137.3201	3141.8790
3142.2006	3149.0415	3158.6890
3165.8254	3168.5910	3176.8880
3181.8775	3183.8221	3184.7323

3185.4068	3186.0083	3186.4521
3189.0266	3191.0051	3193.6102
3194.1835	3195.3424	3197.5919
3203.1214	3205.8961	3207.3044
3207.8597	3209.6525	3210.6404
3214.3443	3215.2802	3219.3263
3223.7531	3224.3550	3240.3265
3255.3922	3349.5974	3479.1179
3524.8066	3594.6157	3792.3546

### M6RR

Zero-point correction= 1.032761

Thermal correction to Energy= 1.097112

Thermal correction to Enthalpy= 1.098056

Thermal correction to Gibbs Free Energy= 0.933171

Sum of electronic and zero-point Energies= -3290.979819

Sum of electronic and thermal Energies= -3290.915468

Sum of electronic and thermal Enthalpies= -3290.914524

Sum of electronic and thermal Free Energies= -3291.079409

### Cartesian coordinates

C	-2.402273	-1.986212	-3.579218
C	-1.124553	-1.757568	-2.969355
C	-1.110766	-1.910837	-1.532633
C	-2.273494	-2.323032	-0.831791
C	-3.460074	-2.572480	-1.513965
N	-3.473207	-2.366845	-2.883715
H	-2.510567	-1.850799	-4.646598
C	-2.197654	-2.523043	0.650377
C	-1.451686	-3.650699	1.147012
C	-2.819657	-1.656881	1.539835



C	-0.822733	-4.597823	0.289507
C	-1.330412	-3.839349	2.562417
C	-2.711079	-1.884132	2.939690
C	-0.088840	-5.644567	0.804005
H	-0.919879	-4.496309	-0.784785
C	-0.569895	-4.930564	3.060840
C	-1.976248	-2.926887	3.437861
H	-3.223589	-1.199951	3.605204
C	0.047285	-5.812243	2.201961
H	0.386271	-6.349630	0.129152
H	-0.485169	-5.054645	4.136725
H	-1.881035	-3.069838	4.510220
H	0.630290	-6.640069	2.592869
C	0.074208	-1.573340	-0.817074
H	0.073562	-1.597905	0.266376
O	-0.123284	-1.440066	-3.667776
C	-4.724238	-3.046040	-0.854345
H	-4.526799	-3.285784	0.188118
H	-5.506096	-2.278909	-0.873043
H	-5.121813	-3.943543	-1.335950
C	-3.720560	-0.489845	1.179892
O	-4.788787	-0.384039	1.800817
N	-3.285267	0.386919	0.256645
H	-2.378320	0.251498	-0.181237
C	-3.818505	1.743794	0.011406
C	-3.944790	2.513959	1.334335
H	-4.406770	3.486575	1.141070
H	-4.591318	1.969699	2.032132
O	-2.666282	2.779881	1.905432
H	-2.113589	1.973174	1.859320
C	-5.041127	1.805256	-0.954920

C	-6.365007	1.399413	-0.285506
H	-6.312170	0.385128	0.114043
H	-6.612985	2.068530	0.545432
H	-7.184616	1.453974	-1.011728
C	-4.761094	0.868076	-2.144319
H	-4.730383	-0.171340	-1.811714
H	-5.545680	0.963052	-2.902564
H	-3.795679	1.092344	-2.609658
C	-5.155396	3.248542	-1.493830
H	-4.206072	3.580007	-1.928036
H	-5.930139	3.300151	-2.266738
H	-5.434175	3.957797	-0.707945
N	1.174283	-1.204564	-1.413297
C	2.359571	-0.780808	-0.699305
C	3.594933	-1.316267	-1.420976
O	3.556498	-1.833580	-2.519275
O	4.658732	-1.104647	-0.654544
C	6.026906	-1.553394	-1.038125
C	6.453294	-0.867619	-2.335420
H	5.838874	-1.193433	-3.174885
H	6.373523	0.217982	-2.240129
H	7.497181	-1.120437	-2.542852
C	6.861866	-1.076901	0.147939
H	6.499389	-1.527442	1.076111
H	7.906954	-1.362829	0.002875
H	6.807079	0.011129	0.243637
C	6.028538	-3.077675	-1.147198
H	7.053530	-3.425465	-1.304022
H	5.650019	-3.523644	-0.222922
H	5.413765	-3.413162	-1.983365
P	0.723870	1.196100	1.678635

O	-0.721654	0.760479	1.789312
C	1.028283	2.793074	2.475004
C	0.159381	3.215519	3.490521
C	2.129784	3.585817	2.121845
C	0.402700	4.416197	4.158311
H	-0.716228	2.621693	3.728547
C	2.374519	4.779642	2.798613
H	2.778515	3.286703	1.304561
C	1.513030	5.193208	3.818851
H	-0.275666	4.747003	4.938704
H	3.227074	5.392336	2.522617
H	1.701684	6.126281	4.341226
C	1.818584	-0.035094	2.447372
C	1.272463	-1.294455	2.740252
C	3.182132	0.202779	2.678985
C	2.092486	-2.321109	3.210654
H	0.209359	-1.458804	2.600702
C	3.997964	-0.825637	3.150754
H	3.607898	1.185024	2.498282
C	3.456886	-2.089867	3.403725
H	1.665245	-3.297319	3.415899
H	5.054153	-0.640890	3.318814
H	4.097536	-2.890308	3.760584
N	1.249251	1.341942	0.074676
C	2.466217	0.782310	-0.521362
C	2.794088	1.478752	-1.829719
C	4.080622	1.999779	-2.013567
C	1.857419	1.582757	-2.868980
C	4.436921	2.605228	-3.219966
H	4.806657	1.930467	-1.208758
C	2.216094	2.189056	-4.073312

H	0.847130	1.210746	-2.737844
C	3.504716	2.697800	-4.254760
H	5.438356	3.004886	-3.347302
H	1.483999	2.265027	-4.871738
H	3.778200	3.168024	-5.194513
H	2.336375	-1.225488	0.296250
C	-4.736269	-2.582765	-3.628781
H	-5.011903	-3.636083	-3.577749
H	-5.523371	-1.970846	-3.190501
H	-4.586276	-2.292987	-4.665324
H	3.330151	0.897093	0.139263
O	-1.168014	0.978138	-1.611899
H	-0.429622	0.986358	-0.979966
C	-0.795876	4.205111	-1.058881
O	0.291414	3.833781	-0.563504
O	-1.181654	5.486987	-0.707032
H	-2.031636	5.634648	-1.147836
O	-1.577036	3.584730	-1.835890
H	0.972921	2.272910	-0.308216
H	1.128731	-1.194711	-2.450680
H	-1.325329	1.949609	-1.770723
H	-3.002443	2.232121	-0.522173

#### Vibrational frequencies

17.5228	23.7430	27.3669
30.0985	35.7436	36.4819
38.5736	41.5762	43.5621
45.9798	48.2838	51.2602
54.1880	56.7737	60.2891
63.8661	70.6382	70.9837
77.2627	80.6319	84.8756

87.6171	88.8817	91.1650
95.3324	103.4141	110.3303
111.2839	112.9029	118.6143
121.5990	126.2806	128.1963
130.7468	141.8242	145.6026
148.1247	156.7791	162.4777
169.3941	175.0740	188.0173
196.4459	200.5163	207.3178
217.3812	223.2255	228.0987
229.6751	230.3664	236.7928
242.8452	250.0446	253.5889
253.9260	263.0577	269.1018
277.6347	287.6942	291.6123
291.8796	294.9979	298.2005
310.7464	313.2090	322.8899
324.8760	331.4044	335.1319
341.8821	353.8972	358.8585
367.8142	380.0493	384.5143
389.0217	396.2861	402.5089
406.0687	408.3609	413.7632
414.1178	417.6540	424.8753
426.6607	430.6699	438.5664
441.5614	444.9903	454.0137
471.4765	477.2369	482.1970
488.6201	506.7226	517.8116
520.0086	532.0956	534.6440
537.0534	542.9296	552.4074
558.4418	570.3814	583.7350
588.2843	592.1618	597.9985
599.6796	623.2176	626.7729
629.6419	630.8818	633.5429

636.8202	641.2928	656.1293
666.8184	676.1787	686.2607
690.4129	703.5304	709.7957
718.0384	720.7175	723.9498
736.5273	741.2425	752.4760
754.9572	761.2325	766.2864
769.9774	773.5475	780.3446
787.5548	788.9484	794.6996
802.8260	807.1243	809.3736
826.7497	831.0082	848.2759
849.1672	852.0323	869.3218
871.7818	873.8573	882.2030
882.8196	886.1707	887.7658
908.1633	912.1437	916.7650
935.1041	938.7260	941.0602
941.7617	945.6850	948.3670
951.4248	959.1801	959.9077
970.4738	971.2902	982.6865
984.4247	985.8772	990.2691
993.3349	1000.5838	1002.5816
1004.4167	1006.0530	1007.6551
1012.5741	1014.6744	1016.5940
1016.9093	1023.9115	1025.8387
1029.6741	1036.9374	1041.1578
1050.8636	1052.1620	1053.6618
1059.8917	1060.5530	1064.8103
1065.2065	1070.2928	1073.6242
1076.7089	1093.4335	1104.5229
1107.4520	1109.7867	1113.0496
1122.7171	1123.2251	1133.3156
1135.8027	1137.6802	1148.4038

1153.0966	1177.0654	1179.9966
1184.2475	1189.1983	1193.9919
1194.3811	1196.4226	1196.8397
1209.5065	1213.7226	1216.4510
1217.4302	1225.6602	1227.5909
1230.9719	1242.7506	1247.2366
1248.3507	1251.5714	1254.3490
1262.6586	1280.2081	1283.5195
1288.4364	1294.2041	1297.4975
1322.9059	1328.3588	1330.8598
1332.7750	1336.6251	1351.0671
1356.0400	1359.5497	1360.2907
1363.7361	1371.0796	1373.2131
1375.5844	1399.2222	1402.3562
1407.2733	1411.6031	1414.9379
1415.0342	1416.0552	1417.2004
1417.6704	1426.0592	1434.5518
1434.9340	1440.3489	1440.6624
1446.2305	1457.1661	1459.4372
1463.6301	1474.7894	1477.9049
1480.2928	1481.0696	1484.2969
1490.0338	1490.1647	1493.9195
1495.3723	1495.8737	1496.9137
1502.2325	1503.5311	1505.0083
1505.6891	1511.2248	1511.3059
1514.0564	1516.3184	1519.0340
1523.8294	1526.3492	1530.3149
1531.4779	1533.0660	1538.8537
1544.0889	1552.2287	1562.7848
1606.3898	1611.4979	1624.1205
1628.7594	1639.0534	1642.6187

1645.2789	1650.0771	1658.7282
1660.6496	1671.1528	1697.9692
1704.7815	1718.9575	1734.5329
1796.6890	3032.2885	3035.6772
3046.6391	3046.8194	3050.2239
3054.0288	3056.4873	3059.4001
3066.0895	3077.5188	3094.3452
3096.8918	3097.5434	3106.0261
3114.1672	3116.7445	3117.8247
3128.5572	3131.2952	3133.1059
3136.8127	3137.1412	3142.4898
3144.1953	3147.9097	3160.1859
3166.9508	3171.2774	3182.6417
3185.0169	3185.0900	3185.7575
3186.4567	3189.0843	3189.7196
3192.0502	3193.6475	3195.8770
3197.2323	3197.9231	3202.0269
3206.8179	3207.5310	3209.1660
3210.0772	3210.7916	3211.3607
3213.3731	3219.7251	3220.1009
3222.3761	3226.3666	3227.0788
3236.0667	3256.1275	3526.1120
3566.8423	3706.0566	3793.5898

### **TS7RR**

Zero-point correction= 1.030432

Thermal correction to Energy= 1.094390

Thermal correction to Enthalpy= 1.095335

Thermal correction to Gibbs Free Energy= 0.928001

Sum of electronic and zero-point Energies= -3290.969739

Sum of electronic and thermal Energies= -3290.905781



Sum of electronic and thermal Enthalpies= -3290.904836

Sum of electronic and thermal Free Energies= -3291.072170

Cartesian coordinates

C	1.659860	-3.471601	3.445307
C	0.670500	-2.623131	2.866905
C	0.949443	-2.258068	1.500765
C	2.070691	-2.745468	0.825038
C	2.986157	-3.591303	1.463290
N	2.744888	-3.904839	2.771056
H	1.558600	-3.786656	4.474727
C	2.228699	-2.435800	-0.635370
C	1.524207	-3.273889	-1.564133
C	2.941531	-1.336557	-1.099251
C	0.733154	-4.381406	-1.143711
C	1.595371	-2.986630	-2.967391
C	3.009876	-1.075851	-2.497111
C	0.051987	-5.153191	-2.058444
H	0.663022	-4.613472	-0.087708
C	0.889007	-3.809446	-3.885942
C	2.362952	-1.877236	-3.404177
H	3.603096	-0.238552	-2.847364
C	0.128577	-4.867650	-3.443124
H	-0.548627	-5.989867	-1.715560
H	0.957771	-3.582575	-4.946238
H	2.429493	-1.666752	-4.467501
H	-0.412927	-5.486029	-4.152052
C	0.068016	-1.294442	0.813296
H	0.227015	-1.192541	-0.254282
O	-0.351475	-2.241162	3.516892
H	-1.429404	-1.509063	2.131906

C	4.225938	-4.111405	0.799069
H	4.209734	-3.848520	-0.257042
H	5.122915	-3.658119	1.233262
H	4.316147	-5.198649	0.878180
C	3.702172	-0.434477	-0.158080
O	4.317302	-0.881282	0.813884
N	3.711588	0.876972	-0.519966
H	2.999652	1.184736	-1.170568
C	4.483988	1.906578	0.178322
C	3.638585	3.191094	0.251952
H	4.234144	3.983026	0.712515
H	3.382954	3.528664	-0.763024
O	2.468508	3.037814	1.037201
H	1.779873	2.671642	0.456650
C	5.896639	2.118891	-0.468429
C	6.735309	3.056202	0.424276
H	6.330331	4.071336	0.464596
H	6.796648	2.673359	1.449353
H	7.755882	3.129587	0.034003
C	5.776658	2.715868	-1.883682
H	5.375390	3.733892	-1.870979
H	6.761971	2.757774	-2.359966
H	5.127050	2.100456	-2.515656
C	6.632210	0.767589	-0.564444
H	6.126467	0.084355	-1.252179
H	7.649559	0.924194	-0.939164
H	6.690095	0.276731	0.410486
N	-1.213156	-1.190040	1.183657
C	-2.239597	-0.739586	0.274701
C	-3.455426	-1.661645	0.379046
O	-3.593202	-2.511570	1.236157

O	-4.307811	-1.361953	-0.602404
C	-5.585816	-2.089421	-0.805660
C	-6.471922	-1.941817	0.431274
H	-6.043365	-2.461827	1.288099
H	-6.596845	-0.886355	0.686528
H	-7.457666	-2.364982	0.216747
C	-6.182156	-1.359283	-2.007668
H	-5.501803	-1.411276	-2.862175
H	-7.134679	-1.817947	-2.286072
H	-6.357047	-0.306518	-1.767945
C	-5.274418	-3.548647	-1.138439
H	-6.200821	-4.064279	-1.407504
H	-4.588677	-3.603996	-1.989028
H	-4.824815	-4.057593	-0.284991
P	-0.681264	2.097110	-1.032225
O	0.811123	1.752433	-0.910740
C	-0.860088	3.877842	-1.284450
C	0.179401	4.584508	-1.908074
C	-2.023278	4.549860	-0.882535
C	0.049900	5.954154	-2.134653
H	1.085072	4.061523	-2.198531
C	-2.149303	5.919620	-1.115967
H	-2.810826	4.006263	-0.370022
C	-1.115160	6.619989	-1.742526
H	0.856647	6.502118	-2.611397
H	-3.047942	6.440773	-0.801082
H	-1.213755	7.686816	-1.918817
C	-1.428063	1.193096	-2.412247
C	-0.730891	0.092881	-2.934429
C	-2.713356	1.497681	-2.884639
C	-1.331908	-0.717857	-3.898047

H	0.272815	-0.123767	-2.583398
C	-3.307645	0.685438	-3.850204
H	-3.248519	2.361014	-2.500078
C	-2.621809	-0.426388	-4.348676
H	-0.796860	-1.578426	-4.285424
H	-4.305137	0.916534	-4.209778
H	-3.091911	-1.061628	-5.093002
N	-1.578525	1.697708	0.302132
C	-2.689763	0.756361	0.434264
C	-3.426881	0.980866	1.741107
C	-2.767289	0.904850	2.977186
C	-4.804865	1.227919	1.718108
C	-3.482109	1.071735	4.163906
H	-1.698461	0.726626	3.020172
C	-5.519537	1.390549	2.906744
H	-5.320673	1.292546	0.764216
C	-4.858530	1.311658	4.133802
H	-2.960289	1.013315	5.114581
H	-6.587942	1.581450	2.871628
H	-5.410679	1.439148	5.060144
H	-1.858300	-0.843693	-0.744820
C	3.705240	-4.767716	3.494075
H	3.730262	-5.755988	3.033564
H	4.698675	-4.320931	3.457173
H	3.387169	-4.858177	4.529634
H	-3.398595	0.915787	-0.380971
O	1.071601	0.180836	1.203302
H	0.987923	0.795907	0.430865
H	0.778888	0.680852	2.075086
C	0.228065	2.594970	3.230161
O	-0.381508	3.159445	2.292292

O	0.564091	3.361291	4.320595
H	0.229934	4.251177	4.131702
O	0.573893	1.382290	3.335969
H	-1.232259	2.169107	1.160630
H	4.632924	1.545335	1.201366

Vibrational frequencies

-222.3683	11.5683	17.5616
19.8772	24.1857	27.2508
29.7147	34.1107	35.4778
39.0207	41.6953	43.1393
44.5859	46.2443	48.7476
51.8566	55.6084	59.3709
64.8624	69.7983	75.3185
77.2743	83.6450	84.9675
88.2414	94.1520	97.7496
103.3133	106.5931	112.4926
112.7728	118.5457	120.4978
127.1182	133.4140	137.6214
148.6744	152.0656	165.4827
174.5699	175.5585	179.8179
189.4060	189.6906	194.4236
214.9841	218.6848	221.7736
227.0523	231.8567	234.7630
235.7446	247.4680	254.3736
259.5316	262.2583	272.0054
276.2729	281.0602	287.0695
291.1625	291.7749	306.2434
312.9772	317.0283	322.7824
329.7649	331.1994	344.7256
348.6434	357.7017	365.5486

374.2518	377.3702	385.3489
389.2958	396.3698	401.5028
407.0079	408.1521	410.5603
412.7327	427.4555	429.9923
430.9224	440.5117	443.0323
446.2042	464.6328	472.2273
480.9426	487.4169	490.9764
495.5292	507.3233	513.0223
526.0552	529.9734	536.9792
542.8972	549.3604	550.9127
559.6574	564.5913	573.1109
582.7149	591.0374	592.5988
601.4866	613.7251	622.6269
629.0458	629.5680	632.8482
638.9593	653.3791	658.1473
666.9639	675.3698	691.3776
703.0302	709.1302	715.3398
722.2404	736.8779	741.7766
746.0538	751.4024	759.6337
763.9572	769.7865	773.2936
778.7473	782.4881	784.7488
788.7076	791.9808	800.2966
802.1713	807.8119	810.9897
816.4411	831.2439	838.5411
849.7006	853.0304	855.0917
872.5656	876.6950	880.7230
887.9924	890.9407	897.9584
907.1849	912.5390	921.0803
937.7033	939.6322	946.3774
949.5555	952.5127	956.8666
957.6301	958.2589	973.8805

975.4383	982.0041	983.8767
989.3299	994.7466	998.1251
999.4436	1000.2640	1009.3500
1010.8977	1012.1346	1013.4645
1016.4053	1018.4244	1019.6561
1023.6645	1029.6457	1033.0291
1049.3613	1051.4958	1053.7989
1054.3450	1057.9418	1060.4638
1063.0211	1067.9843	1072.2224
1077.5392	1081.6165	1090.7447
1102.7397	1105.3084	1108.3321
1113.4506	1114.1796	1126.5543
1131.6531	1139.8215	1142.4352
1145.3542	1146.8739	1150.2617
1157.5402	1182.7230	1187.9241
1189.8648	1190.8365	1192.1633
1194.8758	1196.2350	1203.9234
1210.1552	1212.4208	1214.7638
1216.5953	1218.5635	1223.9324
1227.8041	1245.6617	1249.0242
1250.3621	1255.1072	1267.4794
1269.2860	1271.1091	1279.1617
1287.2058	1291.2815	1293.2789
1311.3634	1324.7188	1329.7203
1332.9552	1335.7539	1336.8475
1339.6777	1355.9676	1359.6954
1361.8926	1366.8418	1371.3686
1389.3527	1391.7137	1398.0719
1407.5785	1409.2273	1411.1428
1412.6891	1414.3793	1414.8340
1416.8572	1425.4512	1429.9073

1432.0171	1437.4960	1440.7181
1445.7223	1450.0225	1453.7001
1465.8481	1475.5863	1477.8541
1478.3295	1478.8258	1481.4809
1485.9028	1487.6735	1493.5738
1493.6060	1494.9863	1496.0639
1501.2422	1501.3728	1502.5749
1506.8592	1508.7225	1510.6844
1510.7695	1518.2154	1521.2480
1522.9961	1523.6209	1527.0197
1529.7981	1531.4368	1543.2138
1552.2090	1560.2219	1563.5831
1581.2483	1600.9235	1614.3141
1625.2591	1627.5544	1637.4071
1643.2440	1644.1173	1646.6078
1648.8379	1658.9234	1671.2101
1680.3864	1697.9180	1725.9068
1794.4727	2364.3126	3009.7734
3035.3763	3038.1114	3046.2357
3052.8036	3055.5076	3057.5609
3065.0580	3076.7402	3087.3298
3090.9796	3096.1049	3103.6672
3104.6512	3106.6116	3114.8921
3115.1610	3115.1892	3116.6590
3121.7339	3128.6675	3131.2822
3133.6433	3135.8653	3141.2487
3160.1023	3166.9442	3174.2501
3175.2812	3180.7909	3184.0196
3187.5569	3187.9893	3188.2682
3191.5194	3194.5901	3195.7606
3196.4517	3196.6648	3198.3236



3200.9728	3202.2733	3205.9138
3207.8998	3208.1751	3209.9303
3211.9438	3214.7174	3215.1466
3216.4255	3220.9283	3224.7562
3251.2104	3301.5990	3407.0325
3593.7835	3686.5963	3792.8545

### TS7RR'

Zero-point correction= 1.030222

Thermal correction to Energy= 1.094116

Thermal correction to Enthalpy= 1.095060

Thermal correction to Gibbs Free Energy= 0.928579

Sum of electronic and zero-point Energies= -3290.965980

Sum of electronic and thermal Energies= -3290.902086

Sum of electronic and thermal Enthalpies= -3290.901142

Sum of electronic and thermal Free Energies= -3291.067623

### Cartesian coordinates

C	-3.830119	-0.813433	-2.573283
C	-2.491992	-0.963129	-2.108370
C	-2.294931	-0.534725	-0.742377
C	-3.312214	0.133571	-0.045219
C	-4.590129	0.272062	-0.595138
N	-4.805710	-0.256485	-1.836487
H	-4.099528	-1.204447	-3.544374
C	-2.995102	0.790509	1.267744
C	-3.223339	0.136788	2.518092
C	-2.394002	2.041251	1.243834
C	-3.886858	-1.117712	2.607544
C	-2.783656	0.773173	3.727457
C	-1.959135	2.659786	2.443752

C	-4.089122	-1.717703	3.830663
H	-4.232949	-1.599992	1.701866
C	-3.002457	0.119713	4.970469
C	-2.143662	2.038138	3.654391
H	-1.479831	3.631852	2.390669
C	-3.638838	-1.099906	5.023120
H	-4.599307	-2.674986	3.881952
H	-2.661138	0.604969	5.880727
H	-1.808457	2.512487	4.572352
H	-3.801521	-1.589243	5.978685
C	-1.073052	-0.973753	-0.034455
H	-0.885035	-0.534627	0.939527
O	-1.592916	-1.464088	-2.852992
H	-0.194114	-1.493374	-1.741155
C	-5.711827	0.988216	0.096856
H	-5.401627	1.270235	1.101168
H	-5.977939	1.907135	-0.436146
H	-6.608176	0.367312	0.183295
C	-2.240594	2.773136	-0.064421
O	-3.206794	2.985811	-0.803781
N	-0.973546	3.173717	-0.337739
H	-0.232469	2.835736	0.282974
C	-0.615112	3.828475	-1.597153
C	0.598035	3.088379	-2.175130
H	0.828974	3.455520	-3.175821
H	1.482348	3.254946	-1.546460
O	0.348930	1.684491	-2.317529
H	-0.099818	1.370211	-1.515976
C	-0.425796	5.370405	-1.443425
C	-0.102642	5.986754	-2.818974
H	0.883032	5.685439	-3.186788

H	-0.849310	5.700161	-3.568400
H	-0.102212	7.079432	-2.748544
C	0.699392	5.703959	-0.448798
H	1.678183	5.362293	-0.795612
H	0.763751	6.787532	-0.303427
H	0.513335	5.248389	0.528501
C	-1.746382	5.975063	-0.928925
H	-2.000500	5.587040	0.061331
H	-1.655936	7.063684	-0.851364
H	-2.577541	5.745064	-1.602467
N	0.039283	-1.183979	-0.785620
C	1.259159	-1.643727	-0.164461
C	1.370796	-3.174417	-0.150257
O	0.510693	-3.928013	-0.579834
O	2.517621	-3.528299	0.413630
C	2.903300	-4.945749	0.658201
C	2.987742	-5.691033	-0.673112
H	2.002188	-5.805222	-1.124614
H	3.635113	-5.152322	-1.370110
H	3.414387	-6.683126	-0.499484
C	4.279027	-4.791999	1.303354
H	4.211855	-4.184170	2.209989
H	4.676425	-5.776040	1.565799
H	4.975102	-4.307232	0.612860
C	1.897417	-5.566858	1.626180
H	2.235367	-6.569812	1.902066
H	1.826038	-4.963473	2.535764
H	0.909471	-5.643152	1.170597
P	2.323313	1.284529	0.730792
O	0.890539	1.569005	1.147388
C	3.264970	2.819096	0.529584

C	3.004345	3.864755	1.429386
C	4.244671	2.978536	-0.461297
C	3.721975	5.056004	1.341683
H	2.229984	3.747088	2.181075
C	4.950039	4.179511	-0.553767
H	4.438049	2.170135	-1.158193
C	4.692638	5.214786	0.348320
H	3.516078	5.863539	2.037099
H	5.700173	4.305685	-1.328254
H	5.245456	6.146406	0.275591
C	3.170826	0.243296	1.953607
C	2.424358	-0.272570	3.021525
C	4.524816	-0.098688	1.813764
C	3.023149	-1.145677	3.931769
H	1.379629	0.005142	3.122934
C	5.117685	-0.971776	2.724479
H	5.107390	0.305964	0.991093
C	4.365737	-1.498954	3.779823
H	2.441999	-1.550643	4.754182
H	6.162328	-1.243584	2.611215
H	4.829489	-2.181801	4.485067
N	2.545892	0.459083	-0.725118
C	2.544781	-1.008815	-0.792111
C	2.794425	-1.494481	-2.210289
C	1.989617	-1.100789	-3.290723
C	3.838984	-2.399993	-2.440441
C	2.225641	-1.613454	-4.567596
H	1.180577	-0.392502	-3.148844
C	4.073153	-2.912983	-3.717172
H	4.471205	-2.706006	-1.612286
C	3.263590	-2.522130	-4.785381

H	1.593317	-1.301550	-5.393509
H	4.887868	-3.613272	-3.875220
H	3.441979	-2.919385	-5.780055
H	1.236800	-1.347517	0.888322
C	-6.176155	-0.274246	-2.390666
H	-6.778006	-0.972937	-1.807964
H	-6.610659	0.723400	-2.351666
H	-6.132906	-0.609023	-3.423921
H	3.367177	-1.365749	-0.173637
O	-1.614527	-2.573106	0.616110
H	-1.134803	-3.200159	0.035706
H	-2.693498	-2.789583	0.424517
C	-4.062557	-3.610009	-0.986890
O	-3.175593	-4.189179	-1.621607
O	-5.337353	-3.521328	-1.508160
H	-5.304025	-3.979063	-2.361591
O	-3.967902	-3.035687	0.155263
H	2.000518	0.883858	-1.478352
H	-1.460524	3.662256	-2.272313

#### Vibrational frequencies

-389.0714	15.0637	18.3859
23.3266	25.5397	26.9372
31.1944	32.9115	39.5164
42.1765	43.1735	44.6532
45.9505	50.4316	51.6511
55.1042	57.3469	58.1405
60.4189	66.5762	72.7449
73.9593	82.5216	83.5329
84.8586	88.2164	94.3162
105.6030	113.4035	116.0461

120.2530	124.0073	126.2238
132.5477	139.3229	146.4531
154.0250	156.1111	158.4381
170.0513	174.9823	178.1182
182.9726	188.2631	195.8578
207.5714	213.9677	220.7186
226.6621	230.5291	232.3723
234.4797	242.9121	247.0584
247.5824	255.4038	264.6060
267.1160	279.5714	288.1148
293.8786	295.3163	304.5497
309.6837	314.5791	320.1943
331.7148	338.0277	344.9148
354.5186	366.0494	368.0254
384.4808	385.9637	391.1132
399.8488	402.2399	403.4545
409.6537	411.6807	413.7355
415.1346	416.7432	419.6835
430.5338	440.1515	441.7659
455.5938	463.3784	468.9851
473.2634	482.9552	486.8121
492.3242	503.4257	514.6489
519.7437	522.1244	530.6025
535.5720	551.3735	553.0321
557.2608	563.4497	575.7556
582.2077	588.6266	600.8614
604.3046	619.6812	628.7426
629.4063	632.7519	639.3783
649.1663	662.9771	676.0310
690.3007	699.1259	702.3007
709.9589	711.6999	712.6222

715.4238	719.4917	737.0477
740.2656	743.2531	754.7179
762.4985	765.7487	769.8328
775.7706	777.9575	780.3092
791.8134	794.3682	801.3243
803.3263	804.0721	813.9966
827.6227	837.4115	843.5622
849.9255	851.0557	861.5605
873.3676	874.1185	880.6779
889.1086	897.2766	902.0395
906.4491	913.8934	931.9683
938.7550	941.9692	948.4781
950.8691	952.1628	952.5523
955.7510	957.3401	968.7031
975.9114	976.2946	980.8686
984.7109	990.3068	991.7741
996.8649	997.2693	1003.0183
1011.1247	1012.3592	1013.1798
1015.5319	1018.2755	1018.6866
1022.0161	1024.2437	1030.5877
1033.9513	1049.6018	1051.1398
1052.5479	1056.8506	1060.0325
1060.6331	1063.7957	1067.0530
1069.9161	1083.8289	1101.7565
1102.9489	1107.4484	1116.4110
1118.1332	1128.0160	1131.7680
1135.0248	1135.5204	1137.8509
1145.8761	1147.7720	1162.0668
1175.9974	1182.4437	1192.6343
1193.6936	1194.3118	1194.6292
1195.2333	1197.5630	1203.5629

1210.9353	1211.0604	1212.2085
1223.0493	1228.8731	1230.6577
1238.7945	1247.3103	1248.2922
1252.9809	1268.0774	1271.4590
1277.2624	1280.7034	1281.4790
1284.2637	1292.2108	1304.3493
1318.7517	1327.7074	1329.1697
1331.3476	1333.3853	1335.1736
1340.5803	1343.4063	1357.6419
1360.7958	1361.5413	1372.0474
1372.8268	1380.1962	1385.5660
1398.1912	1399.0620	1408.6845
1411.4965	1413.9390	1415.9049
1416.1252	1420.6654	1421.1582
1428.8008	1437.4161	1438.6454
1445.5067	1448.5263	1450.7646
1469.2618	1473.2956	1475.7446
1477.1096	1479.9963	1484.6062
1487.4172	1489.7364	1493.7551
1494.8484	1495.3917	1495.5621
1496.2037	1502.1980	1502.2467
1505.9178	1508.9387	1510.7502
1511.5579	1515.1429	1518.5568
1520.6024	1521.4369	1524.1704
1530.1836	1531.6121	1532.8500
1544.2960	1554.6181	1557.2556
1581.7008	1600.5270	1607.1652
1616.7544	1625.3246	1626.8793
1637.1552	1643.9509	1644.1514
1646.7892	1655.1262	1659.8949
1673.8818	1698.0360	1723.9567



1763.9033	1848.0720	3035.6281
3039.6008	3042.7388	3049.2986
3053.0190	3054.1868	3058.6345
3064.8761	3082.5603	3094.0134
3094.0933	3105.7113	3110.8776
3112.6150	3114.1809	3116.4822
3126.7996	3130.1010	3130.2811
3131.7778	3135.9327	3136.9640
3140.9545	3141.3842	3161.1987
3166.8275	3177.0090	3181.3373
3182.4781	3182.8722	3186.6578
3186.8721	3188.2528	3189.4595
3191.2525	3191.8748	3194.9874
3198.1220	3198.6348	3202.8245
3204.1247	3205.6918	3205.8064
3206.8287	3207.7198	3208.6772
3211.0037	3215.4942	3216.6652
3217.3595	3231.6977	3255.6373
3273.2579	3387.9797	3438.2531
3588.2386	3753.9998	3797.0375

## **M7RR**

Zero-point correction= 1.033597

Thermal correction to Energy= 1.098013

Thermal correction to Enthalpy= 1.098957

Thermal correction to Gibbs Free Energy= 0.930555

Sum of electronic and zero-point Energies= -3290.979910

Sum of electronic and thermal Energies= -3290.915494

Sum of electronic and thermal Enthalpies= -3290.914550

Sum of electronic and thermal Free Energies= -3291.082952

Cartesian coordinates

C	1.402938	-3.538395	3.574671
C	0.686684	-2.386418	3.138985
C	0.909944	-2.048078	1.753264
C	1.694642	-2.847800	0.931633
C	2.358508	-3.982752	1.434775
N	2.195402	-4.269312	2.755553
H	1.328559	-3.862902	4.603666
C	1.767396	-2.563416	-0.539450
C	0.823025	-3.225944	-1.391250
C	2.663281	-1.652592	-1.083031
C	-0.189014	-4.087033	-0.878355
C	0.878831	-3.009892	-2.807912
C	2.704524	-1.446988	-2.490293
C	-1.083830	-4.706527	-1.721712
H	-0.263156	-4.239429	0.191811
C	-0.050676	-3.676662	-3.651045
C	1.854857	-2.122439	-3.330820
H	3.438868	-0.762099	-2.900534
C	-1.013637	-4.505630	-3.121826
H	-1.853135	-5.351902	-1.310714
H	0.010308	-3.515167	-4.723745
H	1.910258	-1.970618	-4.404840
H	-1.723922	-5.004462	-3.773784
C	0.307297	-0.774515	1.221670
H	0.467781	-0.714266	0.146874
O	-0.082299	-1.731814	3.904392
H	-1.437516	-1.144519	2.258852
C	3.264137	-4.845410	0.604661
H	3.257185	-4.500107	-0.427578
H	4.299491	-4.798330	0.959978

H	2.956377	-5.896056	0.609659
C	3.615039	-0.880991	-0.202943
O	4.206877	-1.406558	0.743202
N	3.789103	0.416103	-0.578175
H	3.100785	0.808678	-1.207677
C	4.725337	1.334139	0.074180
C	4.078549	2.730436	0.156499
H	4.768140	3.408525	0.664185
H	3.926984	3.127467	-0.858269
O	2.864780	2.748334	0.888481
H	2.158458	2.443565	0.286313
C	6.129057	1.339045	-0.627061
C	7.106302	2.216449	0.182068
H	6.841266	3.277105	0.150968
H	7.140162	1.904343	1.232148
H	8.117995	2.123413	-0.226538
C	6.031248	1.865462	-2.071843
H	5.739667	2.919467	-2.110166
H	7.001821	1.775098	-2.571155
H	5.302959	1.288650	-2.652039
C	6.691828	-0.095494	-0.664548
H	6.079404	-0.749211	-1.291229
H	7.704248	-0.086217	-1.082871
H	6.731015	-0.534192	0.336107
N	-1.089719	-0.617864	1.466890
C	-1.974760	-0.472105	0.344181
C	-3.066482	-1.540283	0.315680
O	-3.210672	-2.398906	1.164990
O	-3.815413	-1.365082	-0.778162
C	-4.982645	-2.214603	-1.106269
C	-6.018144	-2.129747	0.015809

H	-5.651095	-2.602530	0.926943
H	-6.255813	-1.084899	0.233320
H	-6.934421	-2.636116	-0.301867
C	-5.500660	-1.565540	-2.389375
H	-4.718637	-1.554762	-3.153999
H	-6.359348	-2.124907	-2.770431
H	-5.811313	-0.534187	-2.198828
C	-4.502903	-3.642705	-1.362268
H	-5.342979	-4.253993	-1.704724
H	-3.730586	-3.647320	-2.135896
H	-4.092560	-4.084649	-0.453404
P	-0.421973	2.235827	-0.938021
O	0.942799	1.575323	-0.704407
C	-0.210893	4.028921	-1.048987
C	1.015030	4.529813	-1.513716
C	-1.240741	4.915055	-0.701000
C	1.207400	5.905439	-1.630362
H	1.812341	3.842675	-1.776593
C	-1.043252	6.291192	-0.820285
H	-2.179593	4.524803	-0.322421
C	0.178229	6.785803	-1.284507
H	2.158342	6.289807	-1.985745
H	-1.839214	6.976150	-0.545201
H	0.329888	7.857281	-1.373193
C	-1.186476	1.584070	-2.445967
C	-0.665510	0.410191	-3.005600
C	-2.342854	2.167820	-2.986029
C	-1.311242	-0.189444	-4.088046
H	0.234064	-0.030812	-2.589999
C	-2.981218	1.566638	-4.069599
H	-2.746098	3.080013	-2.556072

C	-2.469532	0.384530	-4.615759
H	-0.914614	-1.106798	-4.509145
H	-3.878308	2.014883	-4.484749
H	-2.973968	-0.085642	-5.454363
N	-1.596598	2.019156	0.223491
C	-2.613702	0.957374	0.238135
C	-3.620754	1.224095	1.340276
C	-3.239848	1.268382	2.690651
C	-4.969950	1.407105	1.012788
C	-4.191167	1.496637	3.685621
H	-2.204629	1.100382	2.962678
C	-5.923357	1.629953	2.008650
H	-5.275085	1.372573	-0.029330
C	-5.535259	1.677771	3.349021
H	-3.880363	1.530021	4.725754
H	-6.965270	1.769441	1.735949
H	-6.273667	1.854627	4.125371
H	-1.413724	-0.615754	-0.587446
C	2.901611	-5.430819	3.336635
H	2.576630	-6.347471	2.843008
H	3.977863	-5.310288	3.208913
H	2.669062	-5.490138	4.397013
H	-3.142347	0.987410	-0.714888
O	1.099151	0.310570	1.789134
H	1.181230	0.962848	1.066469
H	0.490987	0.999151	3.057624
C	-0.129760	2.736278	3.592360
O	-0.242938	3.216162	2.467848
O	-0.378141	3.437248	4.712218
H	-0.656284	4.324193	4.434623
O	0.222390	1.510461	3.896910

H	-1.290772	2.351529	1.140374
H	4.861697	0.963485	1.095885

Vibrational frequencies

12.2462	16.1761	21.4810
24.1650	26.2880	29.3158
33.5829	38.0349	39.7841
40.8112	42.9997	44.5748
47.4842	49.0306	53.7855
56.1173	59.5427	63.8523
68.5976	70.2241	75.1069
75.9405	77.7802	80.8698
91.0009	92.7967	100.2392
101.1678	102.5043	109.6658
113.0856	118.8383	122.4425
128.2061	136.3000	144.7167
157.1484	167.3806	168.7158
179.6190	181.8726	191.2282
194.4406	204.6819	216.7260
225.5072	227.8259	229.6060
235.3171	237.8666	240.9109
249.9880	251.8554	255.8570
262.8954	270.5134	271.4649
274.2960	278.5994	284.8609
286.9922	288.9882	308.0519
322.5927	326.2052	330.0500
333.4672	337.5279	339.8927
347.8243	359.2615	366.1730
368.5457	377.6625	385.3042
395.7972	400.1068	403.7173
407.1943	409.6302	415.5280

421.5034	425.3319	428.3227
442.3133	444.2722	448.5115
464.9700	473.2569	480.4598
481.6558	482.7259	495.8589
505.2393	511.6287	522.1536
527.3083	533.7054	539.7603
548.7399	552.7694	554.1331
558.4614	565.2532	574.7382
579.5481	583.2411	585.6507
598.3272	611.7269	620.6984
629.9865	631.2081	634.0037
637.7033	642.6623	650.5319
662.6126	668.0132	678.7964
692.3927	702.9298	711.9592
713.1780	722.3419	737.0347
741.1407	751.0742	756.4984
764.2678	768.6551	770.3025
775.6920	778.9556	781.3897
782.5524	787.2949	797.3430
798.3252	801.6528	810.4211
819.6933	824.1243	839.0943
850.6418	859.5944	872.5704
875.0716	876.4561	882.3427
890.8007	894.5974	897.6335
913.2940	920.2001	937.7425
940.6102	942.8200	947.4705
950.4874	952.7017	954.8705
957.9408	959.0160	973.8977
974.2203	984.4237	986.9603
987.7732	995.6303	996.1512
998.6567	1002.2690	1008.3568

1012.6451	1013.1897	1014.3093
1017.1917	1019.1292	1020.0240
1020.3586	1023.3129	1032.1455
1044.7791	1049.7633	1050.7789
1052.4170	1053.1471	1056.7937
1059.2317	1062.8778	1070.3797
1081.0359	1081.6759	1093.4858
1102.3036	1104.4159	1108.5685
1114.2584	1126.6376	1127.1681
1127.5837	1137.9386	1138.4516
1143.6015	1144.7661	1171.8756
1177.8198	1185.5901	1190.5736
1192.7423	1194.5160	1194.6419
1199.8256	1207.5228	1208.4282
1211.7111	1213.9953	1214.3216
1215.2532	1216.0899	1223.6192
1245.3074	1248.4231	1253.3236
1256.9666	1265.8949	1270.0744
1273.7507	1280.1097	1284.1141
1286.5895	1292.3480	1298.9153
1309.1961	1329.2079	1330.1959
1333.9505	1336.6468	1339.3939
1341.4286	1358.5317	1358.9498
1361.7074	1362.9545	1370.0723
1386.7810	1389.0222	1394.9732
1408.6890	1410.3846	1412.3563
1413.2101	1414.9739	1415.2218
1416.9957	1428.0076	1428.7605
1435.1630	1437.8456	1446.5432
1449.3191	1458.8905	1467.0156
1476.1764	1477.4119	1478.1269



1480.4186	1481.5922	1482.7331
1485.8489	1488.9236	1489.5174
1494.1355	1495.2843	1496.3511
1500.4668	1502.4302	1503.1012
1504.3512	1508.9630	1510.6496
1512.3964	1512.5921	1518.2931
1519.4100	1522.9891	1524.5362
1525.8653	1531.0339	1533.2199
1537.9101	1546.8254	1552.1259
1561.6453	1571.5049	1577.2626
1615.0005	1626.5147	1627.9884
1635.7821	1642.0914	1644.4947
1644.6439	1646.3121	1658.2099
1671.1165	1727.4792	1764.4298
1787.3477	2834.3359	3005.0105
3035.1852	3038.8968	3046.2019
3046.2832	3051.0577	3051.4165
3058.5334	3064.0189	3071.6896
3087.2986	3101.4184	3104.3298
3106.3203	3108.1396	3115.6465
3115.9834	3121.4177	3125.2035
3129.2640	3132.3283	3133.3391
3134.1825	3138.6807	3139.7188
3159.8298	3165.2185	3168.6138
3174.3414	3179.6709	3183.1416
3186.5940	3188.0263	3188.6279
3188.7248	3195.7540	3195.8024
3197.3249	3198.4872	3198.5586
3204.9217	3207.2007	3208.9327
3209.8353	3210.2231	3211.6906
3213.1827	3216.6683	3223.2672

3224.7204	3228.1966	3245.5515
3441.8760	3567.0841	3583.3458
3601.9003	3629.9029	3793.2377

**M7RR'**

Zero-point correction= 1.033777

Thermal correction to Energy= 1.098124

Thermal correction to Enthalpy= 1.099068

Thermal correction to Gibbs Free Energy= 0.930928

Sum of electronic and zero-point Energies= -3290.978032

Sum of electronic and thermal Energies= -3290.913684

Sum of electronic and thermal Enthalpies= -3290.912740

Sum of electronic and thermal Free Energies= -3291.080881

Cartesian coordinates

C	3.061565	-2.295708	3.055782
C	1.896073	-1.545312	2.717635
C	1.545063	-1.628072	1.322330
C	2.277185	-2.397021	0.422252
C	3.400924	-3.131785	0.842935
N	3.754524	-3.032179	2.156808
H	3.437458	-2.279835	4.069793
C	1.839142	-2.449236	-1.014731
C	0.715798	-3.283537	-1.346746
C	2.438994	-1.679003	-2.004962
C	0.002352	-4.025898	-0.363334
C	0.250364	-3.332219	-2.701656
C	1.995830	-1.781590	-3.352855
C	-1.120158	-4.751525	-0.698193
H	0.333202	-3.995582	0.667670
C	-0.893958	-4.112008	-3.018402

C	0.933518	-2.578295	-3.692953
H	2.513735	-1.195017	-4.103106
C	-1.573700	-4.799599	-2.037948
H	-1.662387	-5.290591	0.072197
H	-1.228099	-4.148629	-4.051633
H	0.589646	-2.627146	-4.722146
H	-2.455822	-5.380626	-2.288579
C	0.445353	-0.729830	0.820663
H	0.253331	-0.924904	-0.233825
O	1.251652	-0.859160	3.564558
H	-0.727678	-0.773538	2.508452
C	4.223864	-3.993573	-0.071606
H	3.791792	-3.987627	-1.070715
H	5.256304	-3.636143	-0.154964
H	4.261697	-5.032709	0.271613
C	3.555762	-0.675251	-1.788981
O	4.472530	-0.591467	-2.615908
N	3.413441	0.130586	-0.715344
H	2.581183	0.028401	-0.151673
C	4.187635	1.328866	-0.356092
C	4.027112	2.389791	-1.457777
H	4.683856	3.240160	-1.254053
H	4.321440	1.959755	-2.423359
O	2.702288	2.914934	-1.491789
H	2.060068	2.196055	-1.628334
C	5.643073	1.065572	0.151087
C	6.017083	2.221678	1.103909
H	5.975996	3.193785	0.601530
H	5.342008	2.259751	1.966503
H	7.037130	2.088508	1.479292
C	6.679722	0.997915	-0.985919

H	6.746596	1.949609	-1.523902
H	7.671831	0.786860	-0.570809
H	6.419689	0.220398	-1.704361
C	5.666782	-0.252572	0.947999
H	5.502924	-1.113092	0.294032
H	6.637543	-0.378981	1.438938
H	4.889375	-0.265894	1.720266
N	-0.775251	-0.883391	1.504024
C	-2.007304	-0.616829	0.819329
C	-3.082522	-1.612163	1.268646
O	-2.989818	-2.326803	2.246285
O	-4.116280	-1.560688	0.417283
C	-5.279905	-2.470613	0.527446
C	-5.999771	-2.240221	1.856910
H	-5.376127	-2.537513	2.699700
H	-6.263671	-1.184464	1.966892
H	-6.922390	-2.828008	1.872867
C	-6.148017	-2.036786	-0.652429
H	-5.601714	-2.150809	-1.592207
H	-7.053407	-2.648511	-0.692709
H	-6.437986	-0.987209	-0.549583
C	-4.799572	-3.913145	0.356272
H	-5.664678	-4.579960	0.296499
H	-4.222348	-4.009482	-0.568122
H	-4.174782	-4.221606	1.195064
P	-1.162983	1.918808	-1.294611
O	0.245889	1.356650	-1.513101
C	-1.209711	3.668751	-1.747876
C	-0.222786	4.170172	-2.609902
C	-2.220122	4.516994	-1.269885
C	-0.257082	5.509413	-2.998420

H	0.580539	3.523436	-2.944595
C	-2.250872	5.853728	-1.665793
H	-2.961352	4.136297	-0.574712
C	-1.272281	6.348768	-2.532288
H	0.511170	5.898857	-3.659209
H	-3.031193	6.509596	-1.292528
H	-1.295937	7.390818	-2.836609
C	-2.362877	0.963955	-2.258835
C	-1.921615	-0.209907	-2.886580
C	-3.714021	1.335338	-2.333311
C	-2.832788	-1.015986	-3.570449
H	-0.874253	-0.487936	-2.829685
C	-4.617808	0.528790	-3.022771
H	-4.059400	2.246608	-1.854777
C	-4.178045	-0.647977	-3.637745
H	-2.491478	-1.931186	-4.041981
H	-5.663760	0.813188	-3.076266
H	-4.886155	-1.276910	-4.168524
N	-1.738791	1.869344	0.269650
C	-2.591263	0.847356	0.896673
C	-2.890674	1.231805	2.331386
C	-1.862361	1.539594	3.236017
C	-4.214373	1.227035	2.788168
C	-2.157721	1.838589	4.566567
H	-0.829468	1.539856	2.907772
C	-4.509663	1.520562	4.120696
H	-5.017686	0.994454	2.094881
C	-3.481200	1.828654	5.013634
H	-1.351127	2.075898	5.253778
H	-5.541960	1.513854	4.457565
H	-3.708968	2.061052	6.049547

H	-1.848099	-0.825745	-0.243389
C	4.965630	-3.735417	2.631490
H	4.865624	-4.807255	2.459394
H	5.838628	-3.358166	2.097295
H	5.086028	-3.551051	3.695998
H	-3.532996	0.810754	0.344811
O	1.041538	0.613830	0.851424
H	0.760187	1.064073	0.010221
H	1.461001	1.553837	2.023642
C	1.245601	3.432747	2.247961
O	0.339714	3.573751	1.434657
O	1.797350	4.456362	2.918669
H	1.335690	5.262289	2.637872
O	1.815651	2.300962	2.607057
H	-1.167061	2.430636	0.901349
H	3.635958	1.717786	0.506950

Vibrational frequencies

13.1523	17.6834	21.5095
22.8976	27.2531	30.1707
32.7746	36.6868	37.3508
40.0214	43.9227	48.7049
51.1878	52.2998	54.9422
56.5782	59.6812	63.0178
65.6270	70.9223	74.8238
80.7234	81.3782	85.7531
88.3752	93.9809	95.4061
99.5331	103.9180	108.9448
112.1988	115.2584	117.1922
124.5925	128.2524	144.9889
146.7455	158.0658	172.1440

174.0226	182.7739	187.4059
189.4531	207.2133	212.0556
221.8347	225.7109	230.2109
233.8282	237.7302	241.8110
243.5989	245.2392	253.5318
259.8823	265.5635	275.3246
285.1621	292.9653	295.6049
301.2507	304.2736	311.3342
317.7360	323.0986	331.0604
337.1890	339.0703	347.0287
351.9293	360.4001	365.3042
367.5289	380.2990	388.0111
390.7083	402.5265	407.0607
407.2915	408.7521	413.4172
421.1297	429.6197	436.0856
438.2240	442.1613	448.5267
470.4537	471.5391	474.7389
485.3063	492.8847	495.3668
512.0130	514.7163	521.8967
527.6426	534.9822	542.7301
546.1743	557.7215	558.2410
560.3566	570.8289	575.4838
583.1543	588.3033	601.4231
606.7458	608.8170	628.1850
629.7766	630.3031	633.3799
634.8091	639.8638	641.3487
658.6938	669.4532	683.1687
696.4444	703.4733	709.4819
711.8763	721.0136	734.3077
741.0320	749.3691	756.2178
763.5734	769.5994	770.8906

776.8546	779.5116	783.9791
788.1812	793.6233	796.7831
801.9099	815.5364	831.8722
834.7457	837.7898	848.4682
859.3269	863.8390	870.9339
871.5078	872.4724	873.9179
887.2957	890.3905	900.5682
913.1643	932.5770	937.2893
938.9329	942.9057	945.8363
951.3309	952.7306	955.0405
968.8866	969.2847	974.5094
978.2279	981.7047	984.6329
985.5142	989.1330	994.4606
995.2938	996.6163	1003.4637
1009.4932	1011.6170	1011.8750
1013.7607	1016.4214	1018.2938
1018.3941	1021.6887	1030.6336
1036.4604	1050.4904	1051.4364
1052.1950	1056.1441	1056.8826
1058.8411	1063.3944	1070.6091
1073.4978	1077.9589	1091.4058
1093.0714	1103.4784	1108.5477
1112.8711	1116.7529	1130.1931
1134.0026	1137.1023	1141.1042
1143.0654	1147.1560	1164.8208
1179.5002	1187.2619	1190.1304
1192.4536	1194.5233	1195.6313
1196.0543	1208.9135	1209.0735
1211.9126	1215.3082	1216.3676
1218.2107	1223.3128	1233.5013
1244.2224	1246.4321	1248.3811



1249.1023	1256.1867	1269.0725
1276.8951	1277.0809	1277.6950
1289.9438	1295.1056	1320.4344
1325.1739	1328.5288	1331.2361
1333.9685	1336.0708	1337.1995
1338.9439	1358.1837	1360.3329
1362.6473	1365.4291	1377.1766
1384.6099	1393.4546	1403.2192
1405.4823	1409.2664	1412.7057
1416.3715	1416.5194	1417.2413
1423.1770	1427.4683	1431.7348
1436.7872	1439.4755	1439.6862
1445.7115	1451.3723	1458.3455
1463.6325	1475.3672	1478.0984
1479.9278	1480.0133	1480.6040
1482.8113	1489.9347	1493.6986
1494.3604	1495.5901	1497.0499
1500.3055	1500.6976	1501.9033
1503.3227	1508.3930	1510.2452
1511.3249	1516.5354	1518.1197
1523.0113	1524.9932	1525.6189
1527.6560	1530.3621	1532.5843
1539.1950	1540.1001	1550.4026
1569.2483	1574.5608	1580.4626
1609.4765	1625.4741	1627.7920
1636.4550	1643.0529	1643.7349
1644.3060	1646.8180	1659.4970
1669.3395	1718.4310	1772.4345
1795.0723	2941.4682	3032.4893
3036.3484	3039.4652	3044.0812
3045.1998	3053.7511	3056.4244

3061.7197	3062.4506	3080.7039
3089.1332	3098.2162	3098.3373
3103.0000	3104.1072	3104.2791
3107.9653	3112.3890	3124.6059
3126.5061	3127.5501	3128.6851
3134.3989	3142.0639	3160.5537
3164.1759	3168.2992	3171.7272
3173.9656	3181.9491	3181.9689
3187.9301	3189.1874	3189.3553
3190.2945	3195.1365	3196.2419
3198.0197	3198.1406	3200.8812
3204.2512	3206.2611	3207.9695
3208.7905	3211.9126	3212.8588
3219.9714	3222.2233	3222.5508
3226.1318	3229.2198	3241.1678
3246.1656	3472.5837	3588.7023
3609.1541	3685.7296	3791.3041

### **TS8RR**

Zero-point correction= 1.032110

Thermal correction to Energy= 1.094936

Thermal correction to Enthalpy= 1.095880

Thermal correction to Gibbs Free Energy= 0.933114

Sum of electronic and zero-point Energies= -3290.985716

Sum of electronic and thermal Energies= -3290.922890

Sum of electronic and thermal Enthalpies= -3290.921946

Sum of electronic and thermal Free Energies= -3291.084712

### Cartesian coordinates

C	-0.638458	4.349598	-2.806836
C	-0.441878	2.939796	-2.785815

C	0.121465	2.430803	-1.552396
C	0.349646	3.275834	-0.469456
C	0.157438	4.671762	-0.586278
N	-0.327883	5.149778	-1.765534
H	-1.040173	4.822474	-3.692418
C	0.708085	2.764076	0.896850
C	-0.314600	2.792459	1.907563
C	1.976089	2.310692	1.228519
C	-1.663749	3.150949	1.623763
C	0.023785	2.459827	3.261071
C	2.294017	1.973269	2.571912
C	-2.610663	3.196206	2.623371
H	-1.949050	3.387841	0.605431
C	-0.977528	2.515200	4.266796
C	1.355893	2.079246	3.566547
H	3.304066	1.654246	2.806764
C	-2.268695	2.877327	3.958734
H	-3.630238	3.483229	2.388123
H	-0.703975	2.263351	5.287180
H	1.617646	1.851553	4.595853
H	-3.027045	2.916680	4.734251
C	0.511000	0.966500	-1.551888
H	0.836067	0.635311	-0.562897
O	-0.762555	2.209266	-3.769791
C	0.472137	5.647723	0.513904
H	1.044822	5.153495	1.296243
H	1.069139	6.488726	0.151149
H	-0.436071	6.055620	0.973312
C	3.038784	2.141926	0.172454
O	3.310987	3.018263	-0.648764
N	3.648847	0.925916	0.234509

H	3.207271	0.238797	0.835863
C	4.593856	0.440654	-0.770984
C	4.254688	-1.027939	-1.104183
H	4.822633	-1.336915	-1.983137
H	4.541495	-1.687369	-0.275700
O	2.875960	-1.233224	-1.410006
H	2.375755	-1.209624	-0.557459
C	6.082169	0.646119	-0.333058
C	6.375585	-0.064308	1.002260
H	5.696864	0.281333	1.788516
H	6.282062	-1.151961	0.924500
H	7.399462	0.152763	1.324119
C	6.347738	2.153758	-0.159209
H	5.721370	2.581230	0.627830
H	7.395597	2.319822	0.113962
H	6.140554	2.701631	-1.083175
C	7.023677	0.105623	-1.427918
H	6.775484	0.528644	-2.408106
H	8.059249	0.377861	-1.199056
H	6.984649	-0.985003	-1.507360
N	-0.681119	0.092440	-1.893194
C	-1.604523	-0.025774	-0.745131
C	-2.948208	0.629149	-1.061046
O	-3.260960	1.033513	-2.164109
O	-3.699498	0.648211	0.038290
C	-5.121838	1.078541	0.015225
C	-5.910158	0.191957	-0.949921
H	-5.612065	0.368214	-1.983531
H	-5.751851	-0.862720	-0.710935
H	-6.975950	0.416991	-0.848592
C	-5.550620	0.835262	1.460753

H	-4.924661	1.409830	2.148325
H	-6.592500	1.137570	1.595667
H	-5.457311	-0.225421	1.710667
C	-5.194257	2.560270	-0.353614
H	-6.223608	2.911371	-0.237494
H	-4.553516	3.148952	0.307876
H	-4.879946	2.723212	-1.384804
P	0.536732	-2.171810	1.054138
O	1.566769	-1.047093	0.945855
C	1.378001	-3.772795	0.936703
C	2.750825	-3.815603	1.221341
C	0.699420	-4.951311	0.593994
C	3.439975	-5.026692	1.160889
H	3.270687	-2.899218	1.481454
C	1.392263	-6.160089	0.535768
H	-0.357623	-4.917731	0.352764
C	2.760550	-6.198688	0.818852
H	4.503527	-5.054798	1.376584
H	0.866689	-7.070053	0.263279
H	3.297134	-7.141394	0.769755
C	-0.359394	-2.051233	2.623191
C	0.069999	-1.128553	3.583594
C	-1.461331	-2.880579	2.891376
C	-0.603426	-1.027408	4.802230
H	0.915540	-0.487483	3.364186
C	-2.131808	-2.774234	4.108215
H	-1.797253	-3.596754	2.147789
C	-1.703046	-1.846453	5.063745
H	-0.271988	-0.307162	5.543131
H	-2.987400	-3.410712	4.311084
H	-2.228317	-1.763363	6.010369

N	-0.641653	-2.281908	-0.108378
C	-1.854057	-1.475086	-0.198376
C	-2.927457	-2.259374	-0.937883
C	-3.901409	-2.933375	-0.189384
C	-2.967620	-2.345784	-2.335147
C	-4.900584	-3.675559	-0.819858
H	-3.881979	-2.866062	0.894940
C	-3.968900	-3.085320	-2.967921
H	-2.222755	-1.841366	-2.938792
C	-4.938064	-3.750374	-2.214438
H	-5.650808	-4.186955	-0.224282
H	-3.990445	-3.139299	-4.052238
H	-5.717008	-4.322120	-2.709750
H	-1.178133	0.531088	0.096036
C	-0.541251	6.604314	-1.931721
H	-1.172513	6.979756	-1.126576
H	0.418868	7.121916	-1.916987
H	-1.031040	6.779585	-2.886361
H	-2.225997	-1.310818	0.814854
O	1.519967	0.800696	-2.498859
H	2.055810	0.016744	-2.228997
H	-0.227621	-0.947348	-2.594700
C	0.488743	-2.819314	-3.356966
O	0.301841	-3.545158	-2.370774
O	1.092393	-3.318950	-4.464831
H	1.291089	-4.249017	-4.275166
O	0.164110	-1.583312	-3.509774
H	-0.344389	-2.748518	-0.982683
H	-1.155354	0.593740	-2.664209
H	4.420765	1.043521	-1.669387

## Vibrational frequencies

-886.0466	14.6663	17.1644
23.1695	26.7926	29.0322
30.2736	36.3527	39.7387
42.8735	44.6772	48.9652
50.5651	52.9233	58.5844
60.4574	63.2409	65.0909
72.5600	77.6717	78.5884
81.6376	91.2270	92.9931
100.1228	101.4467	103.6215
107.4749	112.9248	121.4435
128.5872	135.2333	139.7776
141.1909	146.7668	154.9693
158.4860	160.6268	166.2533
179.3947	183.5699	189.3541
190.6137	210.2944	214.6686
219.3291	221.3160	228.7657
232.6956	236.9180	238.0979
242.4280	250.1962	254.3075
259.8610	266.2104	269.8000
278.0979	282.4623	285.2820
286.0885	288.6525	308.9679
317.5871	321.1965	332.8217
337.8021	341.3746	344.1462
349.8250	360.6232	367.3376
374.9535	384.8585	392.3047
396.1901	406.7219	410.2234
414.3172	417.0443	418.4495
421.2337	430.5083	438.7965
442.6646	444.4304	449.3518
454.3482	460.6961	468.7676

476.1245	483.8989	497.1444
501.6427	516.9341	520.7722
532.2753	537.6789	545.5142
553.5956	553.9003	560.8988
572.3891	578.3640	583.5304
592.5535	607.7744	616.5612
630.1487	630.8538	631.6202
636.6269	637.4309	646.6745
653.9600	668.6158	677.1852
689.4607	696.5503	706.4456
709.5831	714.0998	719.2260
736.3627	742.8530	746.6518
757.8487	761.0493	765.8723
770.2999	773.0562	779.2378
780.9501	783.7285	789.9980
794.6836	796.5051	797.6483
806.9670	818.4144	825.3294
831.5817	840.5539	853.3347
857.5686	867.9397	872.9586
875.3902	878.8972	886.9603
892.9784	895.9349	904.5916
913.8095	933.9424	937.9194
939.1444	940.8006	948.2111
949.0867	953.8748	957.2641
962.2672	964.2869	975.8061
975.8774	982.7746	986.1620
990.9089	993.7408	998.6524
1001.8248	1003.9294	1008.4413
1009.4374	1013.4436	1015.6687
1017.4765	1018.1690	1022.3064
1022.9128	1030.0994	1050.5446



1052.7890	1053.4562	1054.5675
1055.3910	1062.5811	1063.3469
1064.9745	1070.0054	1077.3897
1079.9075	1097.2844	1107.3450
1108.7827	1116.2723	1119.1274
1120.0461	1131.4575	1135.8123
1137.6604	1139.4128	1145.6973
1147.5273	1150.9332	1158.7695
1172.2820	1186.0511	1192.9922
1193.5573	1194.6069	1195.5657
1198.3219	1209.0682	1211.7429
1211.8921	1217.9182	1222.7599
1224.9327	1230.1485	1242.1744
1244.7235	1251.0639	1252.4271
1254.8687	1270.6296	1274.4952
1278.8076	1281.5345	1288.8420
1293.9325	1300.9383	1312.4448
1315.0020	1319.5873	1329.9232
1337.1520	1348.7361	1353.1158
1358.4792	1359.8075	1364.6222
1369.8193	1375.0296	1379.0644
1391.5225	1402.1861	1406.8133
1411.5300	1413.1777	1416.0549
1417.3090	1418.4394	1425.9882
1428.6326	1431.1892	1434.9952
1439.7363	1445.4696	1447.8510
1452.0864	1466.3302	1474.7216
1476.8033	1478.4049	1479.1543
1479.2695	1483.8347	1487.2909
1490.1315	1494.8225	1495.2766
1495.8114	1498.0647	1498.7957

1501.3697	1503.6974	1506.5725
1509.9816	1510.2790	1511.7231
1512.2855	1516.6483	1517.2708
1520.6569	1523.0144	1526.4551
1529.4085	1535.1810	1541.1074
1546.3215	1553.5562	1560.7414
1566.5778	1574.2732	1583.8312
1616.6476	1626.5611	1629.3314
1638.9696	1642.6013	1645.1326
1645.9500	1650.3651	1659.3543
1671.8961	1689.0493	1741.9801
1757.7110	1792.3915	3034.2588
3038.2524	3043.3912	3045.9415
3048.5206	3055.9924	3062.0886
3066.8919	3067.3174	3068.9650
3090.0518	3104.9932	3104.9986
3108.2678	3110.6912	3111.4550
3112.4609	3114.6614	3116.4719
3131.6148	3133.1218	3133.4756
3135.4884	3139.1323	3144.5729
3164.8753	3167.3570	3173.9401
3175.6536	3177.7522	3179.4170
3185.9675	3187.1362	3187.8102
3187.8710	3189.0685	3195.8213
3196.4747	3197.3234	3197.8898
3199.8618	3204.1297	3205.8342
3208.4526	3208.7599	3210.0694
3211.4497	3214.1294	3217.0165
3220.8207	3231.1807	3232.9703
3247.6244	3264.6254	3329.1209
3412.9563	3557.7862	3790.4074

## M8RR

Zero-point correction= 1.035873

Thermal correction to Energy= 1.098942

Thermal correction to Enthalpy= 1.099887

Thermal correction to Gibbs Free Energy= 0.937008

Sum of electronic and zero-point Energies= -3290.987241

Sum of electronic and thermal Energies= -3290.924171

Sum of electronic and thermal Enthalpies= -3290.923227

Sum of electronic and thermal Free Energies= -3291.086106

### Cartesian coordinates

C	0.874172	-4.235221	-2.847601
C	0.609045	-2.839771	-2.781646
C	-0.001909	-2.402953	-1.547603
C	-0.202754	-3.286738	-0.490508
C	0.059852	-4.665094	-0.649776
N	0.584163	-5.080454	-1.837473
H	1.312310	-4.658809	-3.740639
C	-0.589743	-2.822773	0.884460
C	0.431111	-2.828895	1.896993
C	-1.874320	-2.419299	1.216710
C	1.791959	-3.140197	1.613644
C	0.077645	-2.521375	3.252458
C	-2.206606	-2.104433	2.561971
C	2.737014	-3.165040	2.615788
H	2.087113	-3.358780	0.594031
C	1.077133	-2.555639	4.260857
C	-1.266654	-2.185868	3.557281
H	-3.227781	-1.824365	2.798216
C	2.380377	-2.872017	3.953368

H	3.766257	-3.416129	2.380813
H	0.792031	-2.325420	5.283134
H	-1.537603	-1.974552	4.587636
H	3.136968	-2.895434	4.731161
C	-0.485519	-0.972044	-1.522477
H	-0.797596	-0.645292	-0.527928
O	0.915073	-2.052727	-3.730438
C	-0.219389	-5.688125	0.415714
H	-0.826491	-5.246265	1.203535
H	-0.769178	-6.545906	0.019680
H	0.702706	-6.063257	0.875035
C	-2.935706	-2.286244	0.155390
O	-3.144996	-3.157978	-0.688950
N	-3.615430	-1.108654	0.231097
H	-3.223895	-0.407559	0.850087
C	-4.564989	-0.659670	-0.788376
C	-4.308149	0.833848	-1.073724
H	-4.894906	1.142179	-1.940308
H	-4.626030	1.448451	-0.222404
O	-2.942936	1.119671	-1.376309
H	-2.437760	1.122354	-0.525592
C	-6.047900	-0.974115	-0.402264
C	-6.436434	-0.298058	0.926513
H	-5.760736	-0.601362	1.732831
H	-6.418965	0.794176	0.858513
H	-7.452129	-0.590797	1.212640
C	-6.212350	-2.498314	-0.245835
H	-5.597042	-2.883494	0.571268
H	-7.257725	-2.740094	-0.024785
H	-5.918871	-3.024611	-1.158585
C	-6.987246	-0.493216	-1.526388

H	-6.677287	-0.891384	-2.499351
H	-8.008153	-0.838736	-1.333910
H	-7.022624	0.597790	-1.600060
N	0.691304	-0.046113	-1.887728
C	1.635264	0.132985	-0.754962
C	3.001586	-0.450497	-1.106083
O	3.320180	-0.794738	-2.226636
O	3.748960	-0.483229	-0.007621
C	5.171456	-0.922472	-0.030048
C	5.974438	-0.031363	-0.977754
H	5.685296	-0.193872	-2.016081
H	5.823105	1.021868	-0.729506
H	7.037173	-0.266382	-0.867779
C	5.592687	-0.706758	1.421653
H	4.953596	-1.282525	2.095904
H	6.628887	-1.027097	1.558381
H	5.514295	0.351138	1.687769
C	5.227277	-2.398712	-0.422109
H	6.254371	-2.760150	-0.319927
H	4.586736	-2.992099	0.235184
H	4.905169	-2.543375	-1.453911
P	-0.595579	2.143209	1.060394
O	-1.576364	0.974680	0.937522
C	-1.509821	3.706887	1.035319
C	-2.883921	3.670084	1.312025
C	-0.881502	4.934777	0.783224
C	-3.625374	4.851641	1.331562
H	-3.364291	2.716360	1.504695
C	-1.625078	6.113603	0.807807
H	0.176255	4.963980	0.545301
C	-2.995710	6.073049	1.080826

H	-4.690299	4.818153	1.539621
H	-1.138069	7.062641	0.606075
H	-3.572198	6.993124	1.095116
C	0.338898	2.010281	2.607311
C	-0.056440	1.066413	3.562009
C	1.431425	2.854779	2.867990
C	0.638246	0.962554	4.768352
H	-0.893446	0.412338	3.347913
C	2.124341	2.744285	4.071887
H	1.745366	3.584849	2.127809
C	1.727191	1.798003	5.022691
H	0.332148	0.227410	5.505370
H	2.972959	3.392083	4.268053
H	2.269159	1.712585	5.959636
N	0.543135	2.333365	-0.130308
C	1.802066	1.607515	-0.240008
C	2.814300	2.430524	-1.020907
C	3.887305	3.005720	-0.328497
C	2.703236	2.641000	-2.402060
C	4.840863	3.773084	-0.999638
H	3.980046	2.845774	0.742339
C	3.659268	3.405082	-3.073372
H	1.865235	2.232159	-2.956201
C	4.730595	3.970274	-2.377547
H	5.667907	4.209892	-0.448134
H	3.564500	3.559833	-4.144058
H	5.472382	4.562204	-2.905208
H	1.247002	-0.446112	0.088478
C	0.866766	-6.518557	-2.045902
H	1.497336	-6.891187	-1.239186
H	-0.070015	-7.076784	-2.068780

H	1.383553	-6.640169	-2.994550
H	2.213232	1.470592	0.762041
O	-1.490277	-0.832168	-2.460671
H	-2.048808	-0.055542	-2.200976
H	0.272044	0.851389	-2.294547
C	-0.808486	2.999129	-3.142381
O	-0.526332	3.757147	-2.181375
O	-1.668315	3.491733	-4.099770
H	-1.904911	4.384820	-3.807349
O	-0.398443	1.829975	-3.370122
H	0.220167	2.874127	-0.967749
H	1.140968	-0.526601	-2.702160
H	-4.327497	-1.224553	-1.696679

Vibrational frequencies

13.8192	22.4590	25.1573
29.2328	30.8672	32.3344
37.0114	40.5288	41.8200
46.0590	48.7022	49.4450
55.5549	57.4099	57.8355
61.5702	65.5721	70.7249
75.6070	78.5217	87.3920
90.5869	96.1328	101.2812
102.7605	106.3671	110.0405
111.4558	119.6952	122.0932
131.3898	136.0535	141.6164
143.3504	150.9974	152.6633
159.4519	162.6116	171.3194
178.5588	181.4363	191.3357
195.0674	209.5645	221.9133
222.1374	226.1853	230.6994

237.0305	238.7532	242.3846
251.1309	253.9763	260.8804
265.6554	269.9921	276.0088
281.5042	283.5115	286.6935
292.6753	307.4498	316.5409
322.7705	330.3388	333.0712
339.9097	344.0418	348.2198
356.8312	367.5825	369.8444
381.8626	390.1736	394.0076
402.5615	403.3024	408.6298
413.2608	417.1420	418.2096
419.3922	440.8305	443.7723
445.0171	447.6625	452.4977
458.8009	464.2030	474.8188
482.2597	490.6132	498.9311
514.8621	519.6333	531.7620
535.7662	543.9573	545.0679
553.2143	556.1002	569.6462
571.9937	579.3844	589.5717
597.9445	605.4763	611.1514
624.6494	629.5298	630.4497
632.3428	641.9096	654.8014
667.5281	668.3749	677.1247
695.3123	706.6364	708.9027
713.8382	718.0075	735.7641
736.8691	748.4513	756.6432
758.6077	762.4251	766.9937
770.9728	779.4236	780.2633
782.3376	789.7689	793.2039
797.2831	804.7386	806.8443
817.8783	830.2540	836.8887



850.9574	854.6737	864.7229
870.6538	871.4291	877.8474
885.4381	890.3597	896.1305
899.2238	905.9133	910.4924
918.8578	933.6022	938.1005
941.0018	947.0656	947.5989
950.3329	955.1510	961.2455
964.3835	974.5257	977.9112
979.8053	983.2079	989.5685
991.8750	993.2697	996.7551
1003.0365	1010.0068	1011.5239
1013.7429	1015.3185	1016.9421
1017.9325	1021.8348	1022.1858
1023.0049	1030.7345	1050.2924
1051.6653	1053.2677	1054.4567
1059.3640	1063.0051	1064.8811
1067.8698	1074.5147	1077.8135
1084.2867	1095.4654	1108.1307
1108.8800	1116.2983	1118.8342
1124.9227	1130.0144	1133.9337
1136.8585	1138.2542	1144.0720
1146.3928	1148.8177	1169.6497
1178.1603	1187.3018	1193.2539
1193.4548	1193.5051	1195.6213
1200.8466	1210.5310	1212.0119
1217.4557	1222.8066	1222.9464
1226.7685	1228.5344	1242.1310
1248.2413	1252.4140	1254.2266
1269.9403	1272.2740	1279.2840
1279.5821	1279.6919	1292.3545
1294.3487	1310.2066	1313.6172

1317.4417	1329.9420	1336.2809
1346.9332	1348.8777	1354.8283
1359.1292	1364.4537	1372.2791
1375.3296	1380.4142	1391.4645
1396.9473	1403.8728	1406.8369
1411.2512	1413.2703	1413.5460
1417.1281	1418.4753	1422.4428
1429.0106	1430.6852	1435.4892
1441.2510	1446.6682	1452.6813
1466.3131	1473.7372	1476.3345
1478.5398	1478.7969	1480.3057
1482.3156	1487.9857	1490.8572
1495.9714	1496.4349	1496.9864
1497.9722	1498.2565	1502.7415
1504.3622	1507.7337	1509.6727
1511.1103	1512.0720	1516.2113
1517.0209	1518.6904	1522.4250
1523.6679	1526.3048	1529.5347
1534.8877	1543.6478	1553.8674
1557.5271	1563.4598	1573.6507
1578.5051	1590.7856	1616.7086
1626.8025	1629.3386	1638.7751
1642.4584	1645.2091	1645.7215
1650.3604	1659.9130	1671.8776
1675.5087	1727.9965	1741.0662
1799.6186	2652.0864	2955.6100
3034.6766	3037.9600	3042.3959
3047.6542	3047.7847	3056.9553
3063.9146	3068.0730	3068.9039
3069.6644	3081.1456	3090.7017
3100.2698	3105.1918	3108.7399

3112.0322	3113.0010	3115.9111
3116.4887	3117.6347	3132.8905
3133.5327	3134.7634	3137.7326
3140.9881	3145.6938	3163.9435
3168.1007	3175.0674	3175.7132
3178.3096	3186.1361	3186.8483
3187.3126	3187.6583	3189.0166
3194.3762	3196.1506	3196.7723
3197.3575	3202.2048	3204.8293
3205.8441	3207.5667	3209.4255
3210.8520	3212.4312	3213.8942
3214.2486	3216.8815	3221.6634
3230.5830	3251.6784	3286.3136
3373.0061	3567.7934	3792.7246

### TS9RR

Zero-point correction= 1.003038

Thermal correction to Energy= 1.061958

Thermal correction to Enthalpy= 1.062903

Thermal correction to Gibbs Free Energy= 0.907519

Sum of electronic and zero-point Energies= -3026.431293

Sum of electronic and thermal Energies= -3026.372372

Sum of electronic and thermal Enthalpies= -3026.371428

Sum of electronic and thermal Free Energies= -3026.526812

### Cartesian coordinates

C	2.808987	-3.519628	2.854983
C	1.965948	-2.400302	2.748882
C	1.496549	-2.090738	1.440380
C	1.892136	-2.853848	0.342259
C	2.741335	-3.957621	0.510159

N	3.160670	-4.249817	1.773997
H	3.205186	-3.820319	3.814424
C	1.445218	-2.433390	-1.023047
C	0.253527	-2.973582	-1.595266
C	2.139420	-1.423080	-1.670064
C	-0.481018	-4.028485	-0.982870
C	-0.219139	-2.434749	-2.839266
C	1.659659	-0.893001	-2.893677
C	-1.624707	-4.522535	-1.571127
H	-0.121125	-4.463622	-0.055025
C	-1.403907	-2.967395	-3.413500
C	0.509337	-1.386417	-3.461953
H	2.208877	-0.088374	-3.370298
C	-2.089219	-3.990506	-2.797394
H	-2.173454	-5.326486	-1.091975
H	-1.758162	-2.554526	-4.353671
H	0.143270	-0.979306	-4.400020
H	-2.991092	-4.390216	-3.248410
C	0.616297	-0.863279	1.297712
O	1.647268	-1.678470	3.784592
C	3.241385	-4.779027	-0.638878
H	2.725165	-4.485396	-1.550807
H	4.311086	-4.606443	-0.794208
H	3.080472	-5.849031	-0.484229
C	3.411865	-0.897933	-1.047377
O	4.362896	-1.655351	-0.817870
N	3.387407	0.420140	-0.764278
H	2.508917	0.924898	-0.904916
C	4.480231	1.111129	-0.081828
C	3.893497	1.847479	1.136200
H	4.672159	2.460890	1.598485

H	3.088915	2.525055	0.820509
O	3.438633	0.925623	2.119617
H	2.481537	0.788105	2.025742
C	5.321967	1.989886	-1.060938
C	4.485788	3.149178	-1.631347
H	3.592990	2.774552	-2.143572
H	4.166588	3.842953	-0.847693
H	5.071920	3.719478	-2.359832
C	5.814579	1.105222	-2.223139
H	4.978141	0.732857	-2.821201
H	6.470156	1.681306	-2.884764
H	6.372792	0.240014	-1.851920
C	6.552912	2.552622	-0.322400
H	7.133638	1.750101	0.146385
H	7.209115	3.071051	-1.029400
H	6.279676	3.272760	0.454335
N	-0.894066	-1.354704	1.232758
C	-1.827945	-0.534003	0.393875
C	-3.080952	-1.389973	0.149356
O	-3.167079	-2.535221	0.550260
O	-3.964985	-0.696767	-0.544112
C	-5.290321	-1.258127	-0.963157
C	-6.078660	-1.692074	0.271073
H	-5.611069	-2.545524	0.762184
H	-6.158361	-0.871263	0.987528
H	-7.087660	-1.975858	-0.041154
C	-5.935123	-0.060316	-1.653321
H	-5.315998	0.281642	-2.486058
H	-6.918698	-0.344450	-2.036024
H	-6.060403	0.770216	-0.953002
C	-5.040010	-2.404010	-1.938223

H	-5.995419	-2.734435	-2.355472
H	-4.397515	-2.071299	-2.757256
H	-4.563698	-3.247868	-1.438695
P	-0.303652	2.408012	-0.329704
O	0.814571	1.571345	-0.920001
C	0.275519	4.039238	0.191094
C	1.334215	4.619285	-0.524912
C	-0.309185	4.733740	1.260681
C	1.808749	5.880656	-0.168983
H	1.786284	4.077375	-1.347436
C	0.169671	5.996781	1.611692
H	-1.120911	4.279572	1.818770
C	1.226679	6.568923	0.899689
H	2.631518	6.323628	-0.721377
H	-0.278988	6.530871	2.443394
H	1.598299	7.550358	1.178090
C	-1.668634	2.564257	-1.513303
C	-1.688678	1.687733	-2.607565
C	-2.721090	3.471404	-1.317666
C	-2.764662	1.711379	-3.496353
H	-0.863371	0.997618	-2.754232
C	-3.790995	3.492777	-2.211047
H	-2.705189	4.153492	-0.472700
C	-3.813969	2.611465	-3.297360
H	-2.782526	1.028726	-4.340179
H	-4.606215	4.193378	-2.061257
H	-4.650981	2.628748	-3.988492
N	-1.056402	1.795184	1.053097
C	-2.183654	0.865711	0.988663
C	-2.920559	0.761310	2.315652
C	-2.261105	0.505518	3.527652

C	-4.314984	0.903799	2.321693
C	-2.988219	0.372800	4.712889
H	-1.179405	0.427028	3.559520
C	-5.040151	0.771975	3.505999
H	-4.832026	1.125121	1.393669
C	-4.378146	0.499413	4.705075
H	-2.463415	0.174230	5.642169
H	-6.119471	0.887748	3.491106
H	-4.940656	0.395391	5.627634
H	-1.332881	-0.391497	-0.570658
C	4.062051	-5.405526	1.990226
H	3.549454	-6.324108	1.704331
H	4.962898	-5.281714	1.389626
H	4.329360	-5.450846	3.042581
H	-2.886738	1.267439	0.259707
H	-0.950341	-2.319479	0.880761
H	-0.383050	1.563387	1.784648
H	-1.244250	-1.398512	2.197219
H	0.758010	-0.361311	0.338778
O	0.758325	0.002455	2.344999
H	1.137548	-0.675366	3.205618
H	5.138630	0.327729	0.305856

Vibrational frequencies

-770.8959	10.4810	17.8890
21.2484	26.0357	27.7877
33.7982	39.4549	39.8351
43.1022	44.3131	48.6357
52.6512	54.9788	55.5916
58.9584	63.9623	66.7605
69.4355	73.3291	76.3104

86.2899	91.0040	97.7763
103.2408	110.3926	115.6780
119.3174	126.0478	127.5363
135.9989	145.5027	152.3466
163.6965	164.8026	171.4634
175.7613	187.3907	190.4987
199.0913	213.9083	220.8836
222.9097	224.9311	231.8620
236.3541	241.7863	245.9921
246.9459	254.1676	256.6130
265.1388	279.0569	280.7301
290.7103	294.5339	303.0911
309.4374	321.8129	325.3986
331.2365	332.6538	341.6319
352.1179	358.6649	359.3505
363.6661	383.5566	388.7825
397.3600	400.7309	405.4565
408.7763	412.1355	414.3507
419.1299	425.1402	429.5779
434.3916	440.9193	444.1410
462.2059	470.6392	475.1900
483.1897	485.3484	489.7324
493.2700	504.7527	518.8750
523.6616	534.5417	537.5253
549.7964	551.5505	556.2458
574.0938	577.1823	582.1528
599.2793	616.9908	628.3091
629.4975	629.6828	632.7089
635.7290	652.4290	666.0960
672.9669	693.6749	696.0069
704.7608	711.0126	713.3634



714.7710	722.1959	733.7352
741.3890	742.9490	755.7789
765.8825	769.3706	773.1300
774.1056	781.1602	787.0612
791.2506	797.8464	802.4652
812.1138	822.1735	827.5536
839.5797	846.7861	852.4705
857.1966	868.9571	875.4094
876.2870	876.7422	889.3841
893.0932	901.9503	910.4604
917.0114	926.2003	941.1032
943.5721	948.8613	950.2873
955.8870	957.6628	958.9520
969.1919	973.7203	976.3499
982.6626	986.1765	988.1187
998.2955	1000.0037	1000.1358
1000.5829	1010.4453	1012.9230
1013.7806	1016.0883	1019.0789
1020.5557	1021.9793	1024.0171
1032.4719	1049.3822	1051.2668
1052.6724	1055.5210	1057.8505
1059.2757	1067.9438	1070.2706
1074.0510	1083.6183	1085.1783
1100.3036	1103.8698	1106.8630
1109.4048	1118.6478	1125.4439
1133.2019	1135.7757	1136.0107
1137.4206	1148.5297	1169.4782
1176.4655	1181.3289	1190.7465
1191.7389	1194.2611	1194.8521
1195.7534	1199.0969	1210.6544
1211.7931	1213.7034	1214.5995

1221.2411	1227.0407	1235.7176
1247.8527	1253.3755	1254.9194
1257.7217	1267.6763	1274.6487
1277.4291	1279.5863	1282.9889
1293.4626	1295.7776	1323.4753
1325.9767	1330.8100	1332.1554
1335.3549	1338.0863	1348.8098
1359.6119	1360.6988	1362.6754
1368.5252	1369.9900	1381.3511
1390.2088	1392.6790	1399.8650
1408.7294	1410.9760	1416.7451
1417.8061	1418.7805	1420.3855
1421.4808	1423.0221	1426.3515
1430.3316	1435.0421	1442.4648
1443.4937	1447.9895	1462.3526
1470.3944	1475.8962	1477.3162
1477.7068	1480.2837	1481.2094
1489.3722	1491.2647	1493.6742
1494.1185	1495.8356	1496.2180
1502.3356	1504.0200	1505.7484
1508.6386	1510.6929	1510.8940
1511.3474	1513.9478	1519.9875
1521.3578	1522.7757	1524.3893
1530.8778	1531.5609	1541.6019
1553.8205	1554.0208	1593.0732
1609.6073	1617.6665	1625.6995
1626.8806	1633.0221	1636.5824
1643.8162	1643.8555	1645.3095
1658.7318	1670.8648	1671.9097
1718.2512	1790.1862	1848.8023
3028.9732	3033.5799	3036.9563

3044.4656	3058.5367	3061.9919
3063.2779	3070.4723	3085.1742
3095.3863	3098.7857	3103.1674
3106.3031	3111.3989	3113.1653
3115.9087	3118.3011	3118.8609
3122.9971	3126.1673	3136.0094
3137.4725	3137.6037	3143.3515
3149.7512	3164.2244	3170.5500
3180.0773	3182.1785	3185.9036
3188.2669	3188.7869	3188.8613
3190.1935	3191.1960	3192.9721
3195.9795	3199.7412	3200.4828
3203.8832	3205.9385	3206.3497
3208.0600	3208.9833	3210.8795
3213.0838	3216.0590	3216.7360
3216.8155	3219.1251	3226.6452
3261.0197	3379.2114	3397.3904
3435.8705	3471.1778	3699.6983

### **M9RR**

Zero-point correction= 1.007098

Thermal correction to Energy= 1.066032

Thermal correction to Enthalpy= 1.066976

Thermal correction to Gibbs Free Energy= 0.912310

Sum of electronic and zero-point Energies= -3026.431157

Sum of electronic and thermal Energies= -3026.372223

Sum of electronic and thermal Enthalpies= -3026.371279

Sum of electronic and thermal Free Energies= -3026.525946

### Cartesian coordinates

C	3.035404	-3.447326	2.779702
C	2.154760	-2.374194	2.691199

C	1.634443	-2.043777	1.419609
C	2.033520	-2.785861	0.304498
C	2.931571	-3.855726	0.437230
N	3.396010	-4.150416	1.682315
H	3.461347	-3.739368	3.728802
C	1.546345	-2.373987	-1.049237
C	0.361836	-2.946709	-1.602869
C	2.204256	-1.345523	-1.704696
C	-0.339316	-4.016441	-0.977510
C	-0.141969	-2.420581	-2.839705
C	1.696333	-0.831244	-2.922900
C	-1.483836	-4.533221	-1.544273
H	0.044576	-4.443230	-0.055311
C	-1.325681	-2.977786	-3.392730
C	0.553041	-1.357866	-3.475738
H	2.215826	-0.011307	-3.406621
C	-1.980518	-4.012175	-2.762731
H	-2.008734	-5.346098	-1.053769
H	-1.704263	-2.573665	-4.327184
H	0.164480	-0.963491	-4.410143
H	-2.882088	-4.430452	-3.196935
C	0.714559	-0.830255	1.300934
O	1.844960	-1.697575	3.795264
C	3.434401	-4.639563	-0.735387
H	2.860835	-4.382389	-1.623390
H	4.481123	-4.386762	-0.931905
H	3.358015	-5.717444	-0.575166
C	3.458097	-0.776333	-1.082575
O	4.446256	-1.494147	-0.880004
N	3.364711	0.527101	-0.758603
H	2.465902	0.997071	-0.901506

C	4.417409	1.260107	-0.058511
C	3.808434	1.865817	1.219879
H	4.544779	2.521495	1.696004
H	2.939182	2.485889	0.961904
O	3.461498	0.845952	2.145849
H	2.495206	0.701954	2.129701
C	5.145954	2.269528	-1.002038
C	4.186749	3.373841	-1.481476
H	3.317127	2.947538	-1.991596
H	3.823104	3.987333	-0.651566
H	4.695927	4.039288	-2.186804
C	5.685192	1.502524	-2.225352
H	4.872314	1.066765	-2.812963
H	6.247053	2.178826	-2.878550
H	6.352325	0.690034	-1.919426
C	6.340382	2.904549	-0.262486
H	7.004509	2.136130	0.149149
H	6.926806	3.516658	-0.955915
H	6.024136	3.555615	0.557384
N	-0.802754	-1.419568	1.249426
C	-1.774287	-0.654510	0.408347
C	-3.015737	-1.541767	0.223286
O	-3.070203	-2.675879	0.660178
O	-3.935907	-0.888834	-0.465089
C	-5.260423	-1.491610	-0.820354
C	-5.996306	-1.910945	0.451078
H	-5.496296	-2.743884	0.945066
H	-6.065151	-1.074363	1.150314
H	-7.010466	-2.219280	0.181564
C	-5.961489	-0.329458	-1.516981
H	-5.381893	0.007082	-2.379616

H	-6.949706	-0.649549	-1.857036
H	-6.085439	0.515210	-0.833523
C	-5.017916	-2.656144	-1.775678
H	-5.979687	-3.025623	-2.142477
H	-4.421755	-2.326410	-2.630185
H	-4.495366	-3.472243	-1.275892
P	-0.371095	2.398946	-0.401358
O	0.815011	1.694859	-1.029906
C	0.047072	4.081763	0.119251
C	0.982463	4.799431	-0.642817
C	-0.549793	4.682762	1.237517
C	1.322159	6.102981	-0.284523
H	1.446514	4.332776	-1.504292
C	-0.207128	5.988941	1.590786
H	-1.264641	4.121667	1.829886
C	0.727833	6.697600	0.832525
H	2.050612	6.652238	-0.872784
H	-0.665915	6.450261	2.459797
H	0.994733	7.712305	1.112005
C	-1.769964	2.445026	-1.556318
C	-1.770266	1.524166	-2.614174
C	-2.864240	3.303466	-1.371685
C	-2.866313	1.453608	-3.474933
H	-0.912413	0.874417	-2.756849
C	-3.955234	3.230647	-2.236983
H	-2.864549	4.021362	-0.556739
C	-3.957545	2.304776	-3.285398
H	-2.866967	0.736539	-4.289981
H	-4.802527	3.893905	-2.094956
H	-4.810536	2.249366	-3.954658
N	-1.017836	1.693171	0.986558

C	-2.140305	0.757681	0.964566
C	-2.854305	0.686547	2.307085
C	-2.169247	0.480497	3.514396
C	-4.249568	0.816889	2.334237
C	-2.873365	0.383872	4.716891
H	-1.085985	0.411249	3.522315
C	-4.951536	0.721931	3.536200
H	-4.785692	0.999685	1.408496
C	-4.264559	0.498630	4.731388
H	-2.330032	0.223055	5.643013
H	-6.032036	0.828157	3.537945
H	-4.808719	0.423498	5.667768
H	-1.307462	-0.530944	-0.573260
C	4.353507	-5.266921	1.864135
H	3.867178	-6.207268	1.603794
H	5.222104	-5.107239	1.226110
H	4.666806	-5.293984	2.904425
H	-2.859894	1.130990	0.237257
H	-0.822743	-2.392729	0.921253
H	-0.291131	1.424931	1.661843
H	-1.134012	-1.449406	2.219993
H	0.802572	-0.375083	0.308056
O	0.819651	0.033514	2.314247
H	1.357225	-0.867989	3.448940
H	5.149935	0.511639	0.258306

Vibrational frequencies

9.8725	18.0697	25.7159
28.1595	30.3412	34.2252
38.0188	39.3669	42.6273
44.5597	49.1766	53.8950

55.1975	58.1989	63.5313
68.6326	69.4153	74.7843
76.6797	78.5948	87.7870
92.4540	98.6613	104.6879
113.9985	118.2099	120.9655
129.1269	138.7091	143.1556
148.7065	155.0082	167.9563
170.3039	173.5373	178.7014
188.0954	190.2051	200.8995
214.2674	218.2914	219.4611
226.3827	231.9355	240.7889
243.3552	247.3079	248.9870
255.8372	259.7005	263.6270
277.3090	281.0003	289.2549
290.6716	294.4661	306.9987
308.8821	322.1017	327.9430
331.5566	344.1981	354.2192
356.4711	360.2838	364.9231
381.6173	386.5112	392.2187
398.7750	401.1199	406.3641
408.5458	412.9653	413.8540
418.0995	426.2654	431.7291
434.2062	441.5722	446.8914
459.1234	471.1881	475.3196
480.7751	482.9484	488.9525
494.2806	515.4209	523.4780
530.8948	534.0891	550.1153
552.4876	556.3457	570.1097
576.2129	577.2487	590.9997
602.6450	621.8482	629.1488
629.3781	633.2027	637.1434



643.3407	651.1800	668.5033
683.0104	695.4981	702.7394
712.1573	713.1744	716.1465
728.8809	739.9443	745.8805
748.2490	754.1581	766.0915
767.6397	771.2219	776.8327
778.2781	782.2945	788.2212
795.5557	801.3365	814.1390
826.7755	835.4012	840.1393
843.7955	852.0534	861.5237
872.9995	875.9726	877.2663
879.7278	886.9115	893.8223
899.6967	911.4458	927.0247
934.6973	940.1441	942.9852
948.4436	950.1061	956.0812
958.4478	960.9936	970.3545
974.2758	975.9502	976.8152
987.7239	987.8683	995.4904
998.1478	999.2820	999.7159
1006.0628	1012.2767	1012.9897
1013.7655	1016.0857	1019.0901
1021.8678	1023.3443	1025.9007
1033.4756	1049.2876	1050.5823
1051.3820	1054.4289	1058.6719
1059.9114	1067.1453	1070.7492
1081.7955	1084.7758	1091.7432
1101.8386	1104.9657	1107.4242
1109.1630	1120.2848	1125.4137
1129.8280	1135.6849	1136.9406
1138.0543	1148.2176	1171.3599
1181.7090	1184.0890	1193.4354

1193.7503	1194.0880	1194.7110
1198.0014	1200.2945	1211.0980
1214.3182	1215.0276	1219.2588
1222.7709	1230.4759	1248.8463
1251.5758	1253.0930	1262.6223
1268.7200	1272.8695	1276.2992
1282.6374	1283.0120	1293.6556
1296.9806	1320.1723	1325.7215
1330.5056	1330.7665	1331.4047
1340.7549	1347.7204	1357.2666
1358.2654	1361.5942	1363.2230
1371.2834	1380.9286	1383.3012
1388.5181	1393.4133	1396.1855
1405.7989	1409.1684	1410.1077
1417.5598	1418.4407	1419.7701
1420.7092	1420.9508	1422.5543
1425.3656	1437.9666	1442.1930
1447.4271	1451.6267	1469.7986
1471.5583	1475.1160	1475.6171
1477.1157	1479.2196	1479.2867
1489.0942	1493.8967	1494.0227
1495.3094	1496.2036	1498.7066
1503.5597	1503.6790	1507.7668
1510.2963	1511.6583	1513.0263
1518.2976	1519.1388	1521.6955
1523.4213	1525.5256	1528.4064
1531.8641	1535.3258	1541.7882
1554.4563	1563.2071	1610.8973
1618.7984	1625.4055	1626.2357
1628.9057	1632.3465	1636.3481
1643.8296	1644.1545	1645.8935

1659.1224	1672.2257	1676.9118
1716.6425	1788.1502	2762.3607
3025.4126	3035.0693	3038.1815
3044.9044	3058.1662	3063.1009
3066.1279	3070.0594	3075.0461
3080.2965	3092.8755	3096.0977
3103.6938	3105.4921	3108.9514
3112.0668	3116.3541	3119.2729
3124.4019	3133.4524	3135.1514
3137.2461	3140.2894	3142.8510
3150.6232	3163.5441	3170.9741
3184.5304	3184.8625	3185.2164
3186.6189	3188.1797	3188.5939
3188.7188	3191.1140	3192.9952
3193.2600	3198.4023	3200.5741
3200.6471	3206.3091	3206.6095
3207.4726	3207.5196	3208.0914
3213.9711	3214.6236	3215.1789
3215.8593	3219.9982	3222.7396
3266.1002	3339.8641	3373.0260
3392.7980	3453.8105	3571.7117

### **TS10RR**

Zero-point correction= 1.005755

Thermal correction to Energy= 1.064368

Thermal correction to Enthalpy= 1.065312

Thermal correction to Gibbs Free Energy= 0.911775

Sum of electronic and zero-point Energies= -3026.427941

Sum of electronic and thermal Energies= -3026.369328

Sum of electronic and thermal Enthalpies= -3026.368384

Sum of electronic and thermal Free Energies= -3026.521922

Cartesian coordinates

C	2.551526	-3.692922	3.059462
C	1.756944	-2.557588	2.938819
C	1.393222	-2.129769	1.640644
C	1.863769	-2.839294	0.531391
C	2.676996	-3.971469	0.698398
N	2.981408	-4.362717	1.966182
H	2.852874	-4.061684	4.029449
C	1.486968	-2.392416	-0.847722
C	0.333412	-2.961146	-1.472479
C	2.207922	-1.393411	-1.485774
C	-0.417284	-4.016471	-0.879731
C	-0.083406	-2.457472	-2.749700
C	1.786957	-0.908579	-2.751512
C	-1.525524	-4.535248	-1.512458
H	-0.100428	-4.431195	0.072144
C	-1.232072	-3.015110	-3.371699
C	0.670055	-1.423470	-3.363993
H	2.366620	-0.130144	-3.235634
C	-1.937286	-4.032265	-2.769256
H	-2.086405	-5.337448	-1.044690
H	-1.541724	-2.625317	-4.337057
H	0.355421	-1.049387	-4.333846
H	-2.812489	-4.450250	-3.254767
C	0.587158	-0.851300	1.512486
O	1.374349	-1.912750	4.038172
C	3.243285	-4.742531	-0.453732
H	2.937031	-4.283674	-1.390758
H	4.336357	-4.740771	-0.421833
H	2.901974	-5.782273	-0.450173

C	3.458743	-0.845861	-0.843591
O	4.305825	-1.602136	-0.353532
N	3.559332	0.502272	-0.875401
H	2.710956	1.017689	-1.097522
C	4.621810	1.235896	-0.187424
C	3.970957	2.228672	0.799083
H	4.745763	2.647167	1.446300
H	3.511689	3.062726	0.253333
O	3.021242	1.597167	1.644777
H	2.225404	1.456544	1.104074
C	5.620299	1.875874	-1.200611
C	4.899989	2.834880	-2.168868
H	4.115652	2.317277	-2.730827
H	4.443026	3.681445	-1.646305
H	5.612757	3.242974	-2.893296
C	6.281506	0.746188	-2.013772
H	5.537522	0.173679	-2.575251
H	6.998912	1.161753	-2.729489
H	6.817225	0.051150	-1.358590
C	6.716682	2.641517	-0.434888
H	7.190962	2.003665	0.319670
H	7.495550	2.975891	-1.128252
H	6.324650	3.530634	0.068238
N	-1.091559	-1.443405	1.198411
C	-1.913670	-0.576410	0.322141
C	-3.182778	-1.346163	-0.082913
O	-3.404525	-2.482485	0.288447
O	-3.932713	-0.593870	-0.877208
C	-5.217495	-1.080915	-1.466247
C	-6.191799	-1.460745	-0.351657
H	-5.834859	-2.322471	0.211882

H	-6.340212	-0.624214	0.335150
H	-7.157517	-1.709562	-0.800969
C	-5.702393	0.143373	-2.237000
H	-4.973858	0.431775	-2.997962
H	-6.653385	-0.084098	-2.725774
H	-5.850706	0.991760	-1.562942
C	-4.911459	-2.247115	-2.402106
H	-5.824705	-2.531662	-2.932403
H	-4.157485	-1.955222	-3.137624
H	-4.543143	-3.109535	-1.846360
P	-0.242676	2.417389	-0.074980
O	1.025690	1.679976	-0.477640
C	0.148358	4.075659	0.528346
C	1.214853	4.762314	-0.074887
C	-0.589886	4.688569	1.550445
C	1.540418	6.050394	0.345502
H	1.787044	4.284245	-0.863799
C	-0.258931	5.979124	1.967330
H	-1.404616	4.148326	2.020920
C	0.803419	6.658480	1.366507
H	2.367814	6.577707	-0.118821
H	-0.826780	6.450900	2.763160
H	1.059550	7.661201	1.694885
C	-1.400388	2.534571	-1.463380
C	-1.216339	1.657057	-2.541148
C	-2.487275	3.422244	-1.455966
C	-2.122199	1.659089	-3.602270
H	-0.366677	0.982482	-2.543846
C	-3.388414	3.420135	-2.519827
H	-2.627773	4.108584	-0.626109
C	-3.205792	2.540129	-3.591585

H	-1.980312	0.975697	-4.433643
H	-4.230363	4.104924	-2.515653
H	-3.910108	2.542860	-4.417691
N	-1.121204	1.693267	1.163895
C	-2.272472	0.816397	0.938978
C	-3.127407	0.681627	2.190944
C	-2.580898	0.364661	3.444163
C	-4.513853	0.852509	2.081608
C	-3.411534	0.203168	4.555328
H	-1.507126	0.253766	3.561464
C	-5.343044	0.690612	3.192005
H	-4.942474	1.119020	1.120870
C	-4.793484	0.360045	4.432374
H	-2.974562	-0.042995	5.518279
H	-6.414951	0.828468	3.087883
H	-5.436282	0.233212	5.298010
H	-1.339155	-0.405362	-0.593317
C	3.840301	-5.550772	2.180307
H	3.388661	-6.417954	1.699711
H	4.827922	-5.364694	1.757629
H	3.928059	-5.732054	3.248128
H	-2.889295	1.284222	0.172631
H	-1.100399	-2.388709	0.804933
H	-0.498291	1.351802	1.906934
H	-1.519293	-1.518770	2.124591
H	0.723029	-0.363909	0.541340
O	0.560265	-0.085475	2.558323
H	0.967349	-1.041763	3.683586
H	5.168037	0.492934	0.402003

Vibrational frequencies

-100.1745	17.3699	20.9321
25.0085	26.3679	31.8310
34.3027	38.7049	40.8034
42.9632	44.4746	48.6075
49.9119	56.6710	57.4545
62.5170	63.9964	71.5769
73.1262	77.0178	83.5759
91.1079	93.5188	100.0959
101.9966	108.2246	115.2282
120.8895	123.9688	127.8072
136.7151	148.2987	156.2352
160.3584	170.5248	173.9580
185.5299	187.7663	195.5309
200.5634	211.8287	228.0980
230.6391	232.7370	241.2621
248.3996	248.7257	252.5180
259.4670	263.8034	266.7938
279.5189	289.2626	294.9608
298.1907	310.1139	311.5835
317.5075	318.8934	320.2998
331.3981	337.2885	351.5965
355.9871	361.6232	367.2064
379.0373	382.4693	389.0200
393.7136	395.7009	400.8295
403.3188	407.5719	409.8338
413.2935	416.7745	424.0843
430.2418	438.7453	442.5034
447.2354	457.7624	469.7580
478.4527	486.8323	488.3707
490.8835	492.3257	517.0317
521.5668	523.9581	534.4083



551.9244	552.7266	555.8085
567.6866	573.0969	578.7824
597.3374	620.5937	625.2659
628.9851	629.6210	632.7162
637.1358	640.8531	660.6274
670.4705	689.7080	698.8708
705.6898	711.9369	712.5524
720.3835	725.2275	741.2893
742.2688	749.3584	755.7645
757.5781	764.8188	767.7338
770.8060	776.7842	782.3394
787.3424	798.4337	801.5142
807.4496	816.8333	833.2337
837.3181	844.5331	859.2791
869.0494	876.0023	876.4030
877.7773	883.9628	894.8228
900.5894	903.1945	931.1596
933.8501	939.1056	941.2917
948.3278	951.2485	952.6642
956.1600	957.9170	960.3160
968.9119	972.6726	974.1370
978.6564	982.0440	985.9881
996.6558	998.6150	999.3338
1000.3975	1012.3138	1012.4933
1013.6359	1015.4012	1018.7549
1020.0925	1021.4885	1021.9411
1030.2707	1049.4155	1050.4511
1051.4994	1054.0616	1058.8278
1059.2578	1065.6246	1070.2199
1082.0497	1083.0923	1100.9844
1101.6715	1104.9568	1106.6119

1108.8291	1116.4820	1126.3509
1129.9629	1134.7357	1135.7620
1138.4527	1146.9607	1159.3455
1179.4840	1181.6349	1190.3993
1194.1991	1194.2136	1195.4956
1197.0564	1203.0148	1210.3019
1212.3616	1216.0743	1220.4878
1221.5219	1225.2006	1235.8341
1248.3963	1253.8524	1255.3866
1265.9549	1276.5489	1277.9301
1281.0354	1281.5954	1285.0319
1292.1373	1296.8042	1322.9856
1324.8620	1326.8142	1330.0821
1333.5242	1338.6775	1347.2584
1352.8627	1358.5774	1359.6382
1363.7015	1370.6370	1379.6134
1382.2309	1393.7883	1394.6677
1406.6906	1409.4050	1409.6965
1411.4038	1413.6314	1416.3699
1417.8628	1418.4878	1422.9181
1423.3919	1439.4969	1439.7621
1445.8571	1447.5315	1468.4815
1471.0110	1476.1340	1477.6698
1478.3745	1478.4556	1480.3389
1492.7763	1494.1698	1495.0692
1496.0131	1496.0191	1500.9799
1502.2961	1504.0018	1506.6415
1508.4813	1510.9888	1512.3222
1520.7045	1522.0077	1522.8140
1523.4707	1525.7538	1528.7531
1531.6703	1537.8715	1542.9482

1553.0590	1569.3955	1594.9033
1614.7055	1625.8021	1626.7184
1628.4716	1636.8595	1642.0896
1644.0507	1644.5324	1645.4767
1659.2910	1671.0661	1677.9089
1720.0019	1788.6908	2730.5722
3033.6917	3035.7172	3039.2690
3045.7571	3057.6834	3063.0553
3063.6771	3069.6787	3076.6225
3083.8803	3096.1692	3096.8188
3103.5362	3106.1256	3109.1012
3111.5348	3115.2116	3118.3154
3121.0242	3125.3735	3134.4616
3136.6381	3139.6455	3141.7097
3149.0579	3167.4898	3170.6423
3183.0026	3185.5467	3188.1036
3188.8334	3189.4783	3190.4732
3190.8083	3191.5091	3192.9566
3195.1725	3196.1482	3198.8278
3203.4066	3204.1264	3205.3796
3207.3829	3209.6644	3210.5806
3212.4687	3213.3454	3213.9063
3216.3749	3217.6466	3220.3685
3265.4146	3337.0741	3428.9209
3501.1300	3503.7579	3700.6415

### **M10RR**

Zero-point correction= 1.005452

Thermal correction to Energy= 1.065357

Thermal correction to Enthalpy= 1.066301

Thermal correction to Gibbs Free Energy= 0.909786

Sum of electronic and zero-point Energies= -3026.432498

Sum of electronic and thermal Energies= -3026.372593

Sum of electronic and thermal Enthalpies= -3026.371649

Sum of electronic and thermal Free Energies= -3026.528164

Cartesian coordinates

C	2.889598	-3.678047	3.011411
C	2.163388	-2.492841	2.954483
C	1.757162	-2.010506	1.688626
C	2.105111	-2.735024	0.536876
C	2.864447	-3.910514	0.641486
N	3.221616	-4.341697	1.884755
H	3.213172	-4.086758	3.957826
C	1.639492	-2.279990	-0.812266
C	0.487891	-2.899297	-1.393848
C	2.286319	-1.245857	-1.473901
C	-0.194273	-3.989501	-0.781504
C	-0.004172	-2.405878	-2.647356
C	1.802682	-0.786653	-2.726317
C	-1.316258	-4.537474	-1.362779
H	0.172740	-4.395747	0.155225
C	-1.166226	-2.992484	-3.216883
C	0.686346	-1.348933	-3.294747
H	2.334172	0.008011	-3.238243
C	-1.811794	-4.032462	-2.588662
H	-1.826659	-5.361743	-0.875920
H	-1.535399	-2.602976	-4.161164
H	0.322890	-0.994848	-4.254886
H	-2.700746	-4.469518	-3.030014
C	1.051738	-0.705345	1.618166
O	1.888585	-1.874119	4.102813

C	3.323875	-4.690310	-0.552101
H	3.030069	-4.176674	-1.464257
H	4.412860	-4.789363	-0.558221
H	2.891263	-5.695586	-0.567651
C	3.526186	-0.638867	-0.869830
O	4.388963	-1.349817	-0.340801
N	3.600088	0.709043	-0.968258
H	2.740758	1.193199	-1.212263
C	4.645537	1.489527	-0.304918
C	3.971415	2.518334	0.628345
H	4.730494	2.955718	1.281849
H	3.535294	3.337800	0.041346
O	2.992517	1.919246	1.462910
H	2.208738	1.777627	0.898819
C	5.650618	2.092375	-1.333206
C	4.932692	2.986336	-2.363049
H	4.170003	2.424732	-2.912311
H	4.447979	3.849204	-1.895094
H	5.652611	3.370529	-3.093325
C	6.345039	0.933457	-2.074591
H	5.621040	0.318523	-2.617094
H	7.067181	1.323640	-2.799831
H	6.881915	0.283884	-1.375378
C	6.720198	2.915430	-0.589479
H	7.192593	2.324877	0.203804
H	7.504822	3.228230	-1.286328
H	6.304566	3.821511	-0.138168
N	-1.213273	-1.589229	1.187282
C	-2.036337	-0.767553	0.309391
C	-3.327083	-1.497300	-0.108445
O	-3.611374	-2.615168	0.276428

O	-4.039364	-0.741223	-0.947814
C	-5.307324	-1.215461	-1.564315
C	-6.336536	-1.526428	-0.476855
H	-6.021446	-2.369009	0.138069
H	-6.491472	-0.656604	0.166588
H	-7.290512	-1.773137	-0.952114
C	-5.735261	-0.012073	-2.400457
H	-4.976129	0.223987	-3.149546
H	-6.677881	-0.231420	-2.909205
H	-5.875972	0.867632	-1.766153
C	-5.005973	-2.424688	-2.448890
H	-5.906570	-2.698698	-3.006020
H	-4.215467	-2.180251	-3.163586
H	-4.686744	-3.278504	-1.851044
P	-0.378370	2.340268	-0.066774
O	0.954513	1.740660	-0.495996
C	-0.121979	3.991646	0.626931
C	0.919901	4.777766	0.109456
C	-0.945912	4.501792	1.640179
C	1.135323	6.062660	0.604369
H	1.558125	4.377469	-0.671611
C	-0.727546	5.790356	2.130479
H	-1.739188	3.883950	2.048316
C	0.310898	6.568957	1.614040
H	1.944714	6.666864	0.206693
H	-1.362919	6.182745	2.918310
H	0.480627	7.569534	1.999964
C	-1.537399	2.444562	-1.453822
C	-1.318058	1.601943	-2.552201
C	-2.648750	3.301233	-1.435169
C	-2.210380	1.609973	-3.624493

H	-0.450526	0.951613	-2.562282
C	-3.537366	3.304153	-2.509562
H	-2.817149	3.962265	-0.590267
C	-3.317520	2.460987	-3.603390
H	-2.039950	0.955193	-4.473334
H	-4.397573	3.965784	-2.496842
H	-4.011326	2.468420	-4.438293
N	-1.197610	1.486176	1.117033
C	-2.372117	0.632628	0.918163
C	-3.178830	0.515894	2.202580
C	-2.578220	0.243027	3.441310
C	-4.571549	0.654363	2.144701
C	-3.358851	0.100981	4.590202
H	-1.499114	0.145973	3.522293
C	-5.352752	0.509980	3.292078
H	-5.042391	0.881996	1.193646
C	-4.747697	0.229999	4.518873
H	-2.879262	-0.109249	5.541369
H	-6.430717	0.623098	3.227127
H	-5.352383	0.119261	5.413746
H	-1.478896	-0.585252	-0.617485
C	4.020753	-5.581961	2.028562
H	3.494239	-6.408487	1.552886
H	4.994367	-5.440638	1.559012
H	4.153063	-5.793724	3.086044
H	-3.002743	1.121704	0.176789
H	-1.159189	-2.527076	0.797308
H	-0.600344	1.230848	1.901965
H	-1.666970	-1.692858	2.093186
H	0.869304	-0.289015	0.626944
O	0.871552	-0.018952	2.637650

H	1.428239	-1.025670	3.862652
H	5.191789	0.780427	0.324529

Vibrational frequencies

16.2790	20.7031	23.5258
26.7407	32.7459	37.1852
39.4536	41.3012	44.1580
45.4084	48.4997	49.5306
52.9494	54.3340	57.9573
59.5148	65.2534	66.5263
72.7257	76.1929	78.8646
88.7537	90.1556	96.8187
103.1565	113.6693	121.9223
124.5051	127.2651	144.0411
144.4183	147.3250	156.8962
160.0704	166.9200	173.1202
185.9794	193.7379	199.0092
203.7224	206.6642	224.9360
227.3784	231.6834	243.0383
247.3409	249.3013	258.4625
261.1495	265.6618	274.3135
279.7395	286.4709	291.6710
292.5875	304.6709	308.6773
310.9433	319.5434	323.2087
325.6074	326.5418	345.0603
348.5407	355.6181	362.5597
363.5842	370.8898	373.7797
389.1196	393.3846	394.6823
400.1504	403.6190	405.9219
409.0686	412.5017	417.6189
422.2424	424.1729	439.0101



440.0831	443.4382	454.7566
464.8037	473.6676	480.6441
489.5855	489.7084	495.1192
510.9525	520.7297	523.8338
532.7390	545.0946	548.6611
552.6925	564.8296	570.5788
578.3528	593.4914	612.5953
618.5805	629.4655	630.2010
634.5182	638.7555	639.0690
647.7795	656.5691	671.7942
686.8399	701.1900	710.6176
712.7462	714.7261	728.7261
732.7502	740.7669	746.9404
755.4201	755.9864	766.6066
769.6449	777.2953	781.0179
781.6038	789.9244	796.2214
800.8628	805.1874	813.0731
820.0430	838.1760	855.1941
857.4062	872.3358	873.2927
875.0239	877.4957	880.6161
893.5191	901.4015	905.1778
913.2998	927.3614	936.8081
939.1943	941.6801	945.3013
951.2925	953.3181	956.7267
959.5728	965.4985	971.7151
977.7694	980.2810	985.7927
991.6335	995.8943	996.6929
1000.7835	1011.3598	1012.6090
1012.9507	1014.3378	1015.5017
1019.2261	1019.9993	1020.7943
1024.3973	1031.8308	1033.6963

1049.8259	1051.4276	1054.0610
1056.9238	1058.7750	1061.9115
1066.6630	1070.8378	1080.8853
1087.4697	1101.3048	1103.2463
1107.7828	1109.0298	1117.4161
1129.5030	1133.2592	1134.7241
1138.0974	1138.7434	1149.1461
1156.1654	1160.5534	1181.0432
1183.9897	1193.0713	1194.1280
1194.8626	1195.4635	1196.7626
1205.9099	1210.5694	1213.7943
1216.3454	1222.5192	1225.9478
1230.8409	1248.0422	1252.8804
1256.1186	1267.8286	1278.4871
1278.6491	1279.5966	1279.9311
1292.6362	1293.2488	1317.7032
1320.1370	1325.1670	1329.6839
1333.7115	1337.5991	1355.8573
1356.6267	1359.1920	1363.4959
1369.0272	1371.7620	1379.2183
1384.1497	1389.0227	1396.5051
1409.0521	1409.7719	1413.3252
1413.4776	1416.4664	1418.3640
1426.6339	1427.2427	1429.3328
1440.1204	1441.7783	1445.3325
1461.4233	1468.0548	1469.7883
1476.1309	1477.8046	1478.2654
1480.0648	1482.0153	1490.3286
1494.0872	1494.4489	1495.4391
1497.1692	1497.4226	1502.6733
1503.3802	1505.9449	1507.9461

1509.3994	1513.2060	1513.8278
1517.0343	1520.3321	1522.3611
1523.5862	1525.2325	1530.2722
1531.8134	1533.0782	1542.2055
1554.3974	1591.7601	1611.9990
1615.3592	1626.4371	1627.4154
1637.1217	1644.0273	1645.1355
1646.2102	1651.8583	1659.2136
1665.2741	1671.6308	1700.2707
1719.6782	1785.9209	3032.8793
3034.3282	3038.4124	3044.1623
3056.0038	3060.3292	3064.5386
3066.2253	3066.8184	3084.7395
3097.3725	3104.0477	3106.4677
3109.5604	3111.8383	3113.7281
3116.6553	3122.4493	3126.2190
3131.9891	3132.4680	3137.5682
3142.0021	3146.3620	3151.0951
3166.2269	3171.2890	3182.9484
3185.3654	3188.6418	3188.8588
3188.9389	3189.2321	3191.8108
3192.2790	3194.9756	3196.4997
3197.1450	3197.3906	3204.1307
3204.5251	3204.9280	3209.7007
3211.2288	3211.6750	3212.8847
3213.1507	3214.2305	3216.5675
3221.3966	3221.8404	3263.8307
3268.5978	3492.5490	3496.6970
3528.3195	3572.2189	3614.6193

**M4'**

Zero-point correction= 0.657136

Thermal correction to Energy= 0.695831

Thermal correction to Enthalpy= 0.696775

Thermal correction to Gibbs Free Energy= 0.584918

Sum of electronic and zero-point Energies= -1744.719425

Sum of electronic and thermal Energies= -1744.680730

Sum of electronic and thermal Enthalpies= -1744.679786

Sum of electronic and thermal Free Energies= -1744.791643

#### Cartesian coordinates

C	-1.270558	0.437062	-3.425247
C	-0.291243	-0.024212	-2.583405
C	-0.652565	-0.526847	-1.279032
C	-2.042730	-0.467192	-0.948141
C	-2.991825	0.016710	-1.834944
N	-2.594295	0.456577	-3.068159
H	-1.017995	0.814543	-4.406227
C	-2.454967	-0.877711	0.430205
C	-2.835638	-2.230649	0.694502
C	-2.389747	0.032162	1.476743
C	-2.896210	-3.212204	-0.333897
C	-3.166364	-2.619335	2.035127
C	-2.702741	-0.364122	2.803597
C	-3.272533	-4.506220	-0.052291
H	-2.642656	-2.924280	-1.348433
C	-3.553831	-3.962964	2.290368
C	-3.089863	-1.654814	3.073480
H	-2.647595	0.370178	3.601182
C	-3.606717	-4.886555	1.271270
H	-3.314443	-5.242846	-0.848764
H	-3.805963	-4.248240	3.307922

H	-3.340614	-1.951056	4.087938
H	-3.902903	-5.910403	1.477842
C	0.323822	-0.998586	-0.374316
O	0.987492	0.023161	-3.000096
C	-4.447744	0.130251	-1.485886
H	-4.643015	-0.343252	-0.526009
H	-4.739231	1.182146	-1.403216
H	-5.084967	-0.343525	-2.237695
C	-1.990390	1.461400	1.213666
O	-2.631832	2.164574	0.415230
N	-0.919568	1.875882	1.924195
H	-0.464400	1.163062	2.476764
C	-0.225469	3.181113	1.875688
C	-1.203005	4.374666	1.832238
H	-1.991578	4.177899	2.576803
H	-0.655438	5.257127	2.174605
O	-1.748814	4.698696	0.568291
H	-2.188792	3.871245	0.279432
C	0.940244	3.187962	0.830024
C	0.454344	2.904290	-0.603373
H	-0.106027	1.970365	-0.652407
H	-0.185834	3.707328	-0.968971
H	1.315242	2.802853	-1.273426
C	1.956932	2.097418	1.229241
H	2.811186	2.106499	0.544300
H	2.338227	2.255433	2.245128
H	1.517601	1.098199	1.173079
C	1.637969	4.560000	0.874022
H	1.962274	4.814119	1.890138
H	2.526993	4.546392	0.234842
H	0.978521	5.353927	0.512968

C	3.971289	-1.093513	-0.458602
O	4.258532	-0.627609	-1.559991
O	4.877275	-1.485787	0.477054
C	2.620241	-1.295468	0.043970
N	1.617871	-0.939245	-0.721036
C	6.322694	-1.341319	0.264613
C	6.910783	-1.881097	1.569939
H	6.614534	-2.923118	1.722046
H	8.002875	-1.830257	1.539532
H	6.557934	-1.292240	2.421651
C	6.770018	-2.197709	-0.924131
H	6.451454	-3.234822	-0.780910
H	6.345367	-1.822948	-1.855136
H	7.861858	-2.180634	-0.997588
C	6.681314	0.137211	0.083106
H	6.265235	0.528998	-0.844839
H	6.291711	0.723095	0.921409
H	7.769660	0.249910	0.061093
C	-3.572942	0.975194	-4.036506
H	-3.040662	1.336001	-4.914153
H	-4.264377	0.186493	-4.340556
H	-4.136584	1.802016	-3.601528
H	0.025945	-1.376214	0.603672
H	0.248437	3.258547	2.862644
H	2.479209	-1.695821	1.049041
H	1.544127	-0.323023	-2.225214

Vibrational frequencies

7.6323	20.9085	24.3525
28.0912	31.1609	45.5748
52.4770	56.2269	58.8817

64.4381	76.6981	97.2588
103.9772	111.6486	114.3522
123.3415	127.4669	142.5721
150.3607	164.1900	168.1515
180.6135	193.6506	196.5994
220.3826	224.7462	233.9126
241.7360	245.7141	252.0626
256.1848	265.2380	284.6775
291.1888	295.8552	306.7707
321.1856	323.7245	331.9584
334.7031	341.1737	355.3560
366.0623	373.2169	381.4738
386.6057	392.8093	396.1595
403.3456	411.0860	421.9982
437.4488	440.6310	450.3952
455.5680	471.0055	479.0199
480.0238	512.6072	526.2213
535.4347	548.1836	557.6899
566.4204	593.0640	600.0991
601.2591	644.1210	647.7448
657.0646	688.8322	699.7947
729.2917	730.5482	740.4042
750.1600	760.6841	761.7034
767.5951	774.2988	793.5459
795.4592	806.6659	816.0660
827.6276	837.0898	850.9338
856.2822	861.9825	878.0937
889.2740	893.1456	913.7782
926.4793	931.8661	934.9778
936.5255	941.9241	950.6754
957.2036	971.0831	975.3625

978.3677	983.2835	1006.1880
1009.2398	1024.6240	1029.3159
1049.0310	1054.2072	1057.2551
1061.4019	1068.9128	1073.5049
1081.7424	1095.9599	1117.3469
1133.7016	1138.9225	1143.5306
1157.5557	1182.0378	1188.3545
1204.2295	1215.3417	1225.1273
1233.5527	1246.5126	1252.6327
1262.6271	1267.0098	1272.8064
1284.6206	1286.4253	1292.5325
1293.5744	1311.7376	1317.9013
1335.9088	1349.5925	1351.7042
1376.4286	1383.3387	1387.4957
1405.4540	1406.0758	1409.6051
1410.4779	1411.7229	1414.4012
1417.7793	1421.9113	1425.2754
1433.2705	1446.1458	1465.6367
1468.3609	1470.9235	1478.7603
1478.8412	1488.6785	1490.9061
1494.8024	1495.2063	1495.5738
1498.0517	1499.3944	1501.1552
1504.7943	1507.6558	1509.9117
1512.7744	1517.2282	1518.8696
1525.0696	1529.1421	1533.8789
1536.2114	1552.1628	1561.0993
1569.8222	1571.5855	1585.5368
1613.2823	1645.1284	1672.4054
1694.7735	1703.6632	1720.7653
2841.1798	2983.1830	3032.5890
3035.6053	3039.3494	3048.9088



3051.3229	3056.7497	3057.2237
3059.8397	3076.0194	3098.6140
3100.2325	3104.2280	3120.2042
3121.3228	3121.5657	3123.0173
3126.2374	3127.9307	3133.7982
3134.1607	3134.6485	3140.9060
3151.9540	3165.0813	3168.1118
3176.4883	3181.2829	3183.1384
3187.2586	3187.5808	3192.7868
3204.9089	3205.4625	3214.5551
3253.2857	3529.3869	3626.3849

### **M05RR**

Zero-point correction= 0.960523

Thermal correction to Energy= 1.019145

Thermal correction to Enthalpy= 1.020089

Thermal correction to Gibbs Free Energy= 0.865913

Sum of electronic and zero-point Energies= -2949.546616

Sum of electronic and thermal Energies= -2949.487994

Sum of electronic and thermal Enthalpies= -2949.487050

Sum of electronic and thermal Free Energies= -2949.641226

### Cartesian coordinates

C	-1.958281	-3.152966	-3.114436
C	-0.855969	-2.650743	-2.400013
C	-1.136058	-2.210818	-1.041201
C	-2.450678	-2.340575	-0.527302
C	-3.469610	-2.924921	-1.282052
N	-3.194107	-3.294773	-2.568238
H	-1.831109	-3.474341	-4.138945
C	-2.744898	-1.851127	0.859563

C	-2.314430	-2.622921	1.989235
C	-3.359842	-0.621807	1.064428
C	-1.663377	-3.880496	1.844817
C	-2.527734	-2.115149	3.313220
C	-3.558091	-0.128027	2.381265
C	-1.238215	-4.589546	2.945895
H	-1.502158	-4.276247	0.848398
C	-2.080950	-2.874253	4.429466
C	-3.161900	-0.855804	3.476057
H	-4.027525	0.841723	2.508250
C	-1.445880	-4.082905	4.252513
H	-0.740756	-5.545412	2.813523
H	-2.246386	-2.477881	5.427414
H	-3.318453	-0.470346	4.479464
H	-1.104779	-4.651778	5.111931
C	-0.066723	-1.722487	-0.233026
H	-0.230282	-1.381180	0.779322
O	0.314374	-2.592090	-2.926272
C	-4.844100	-3.199745	-0.742959
H	-4.879128	-2.953472	0.316224
H	-5.596275	-2.584945	-1.242520
H	-5.114039	-4.254295	-0.858586
C	-3.841183	0.218207	-0.097839
O	-4.655375	-0.219384	-0.919698
N	-3.335731	1.472397	-0.114680
H	-2.542551	1.659836	0.507051
C	-3.461773	2.332076	-1.286592
C	-2.112746	2.327805	-2.044839
H	-2.260764	2.732673	-3.051022
H	-1.382058	2.967342	-1.534740
O	-1.604970	1.006006	-2.168652

H	-0.935513	0.905068	-1.462879
C	-4.000078	3.745844	-0.916753
C	-4.109897	4.603420	-2.192758
H	-3.128279	4.838978	-2.615553
H	-4.699457	4.093693	-2.963480
H	-4.604712	5.554034	-1.966522
C	-3.089110	4.459671	0.102427
H	-3.522839	5.428236	0.374242
H	-2.968672	3.872776	1.017027
H	-2.089560	4.649927	-0.300960
C	-5.404837	3.582044	-0.305591
H	-5.369489	2.967771	0.598887
H	-5.824898	4.558407	-0.040507
H	-6.088272	3.100899	-1.014546
N	1.190927	-1.806962	-0.664367
C	2.311345	-1.490829	-0.001909
C	3.580081	-1.745865	-0.628995
O	3.732348	-2.233499	-1.749742
O	4.586751	-1.351913	0.198587
C	5.989619	-1.693638	-0.064262
C	6.493229	-0.968426	-1.315040
H	5.926339	-1.275098	-2.193395
H	6.397407	0.114103	-1.191186
H	7.551839	-1.199706	-1.470009
C	6.697022	-1.171990	1.187908
H	6.316801	-1.676682	2.080913
H	7.773600	-1.350800	1.115777
H	6.528471	-0.096847	1.299987
C	6.142708	-3.213425	-0.180514
H	7.204510	-3.472185	-0.233839
H	5.712922	-3.702098	0.699315

H	5.641848	-3.588367	-1.073147
P	0.380894	1.969881	1.156919
O	-1.099710	1.969223	1.454182
C	1.130759	3.625347	1.208217
C	1.503477	4.181894	2.442039
C	1.246386	4.394301	0.038997
C	1.995671	5.485486	2.502771
H	1.420658	3.595204	3.351857
C	1.733772	5.699405	0.105698
H	0.963573	3.973908	-0.920300
C	2.110465	6.244663	1.335584
H	2.290723	5.906514	3.458792
H	1.823008	6.287963	-0.802001
H	2.494295	7.259075	1.384258
C	1.264540	0.915870	2.341477
C	0.518170	-0.094569	2.968987
C	2.651505	0.985383	2.547198
C	1.156730	-1.048869	3.760709
H	-0.557466	-0.126128	2.830345
C	3.286290	0.030137	3.342754
H	3.236488	1.780213	2.095582
C	2.542347	-0.991961	3.938742
H	0.572015	-1.834816	4.228341
H	4.360441	0.079692	3.488801
H	3.041988	-1.739714	4.546889
N	0.684918	1.383687	-0.424371
C	1.909329	1.226850	-0.829059
C	2.313269	0.908144	-2.195339
C	1.404772	0.565259	-3.214398
C	3.688981	0.960474	-2.488430
C	1.877160	0.282570	-4.492720

H	0.342655	0.536055	-3.010935
C	4.153308	0.686721	-3.770130
H	4.390471	1.209111	-1.698199
C	3.245516	0.345139	-4.776348
H	1.174136	0.009697	-5.273691
H	5.216954	0.729348	-3.981433
H	3.603014	0.124430	-5.777743
H	2.246647	-1.173265	1.026586
C	-4.254653	-3.885299	-3.406687
H	-4.545942	-4.860423	-3.011973
H	-5.124079	-3.227847	-3.426959
H	-3.875036	-4.007289	-4.418543
H	2.755610	1.400655	-0.155051
H	1.229044	-2.146134	-1.671544
H	-4.200421	1.849260	-1.933062

Vibrational frequencies

14.8526	19.3616	23.1195
26.8212	29.4560	35.3146
36.8436	40.0713	40.6430
46.1156	47.1946	48.8656
54.7317	59.7712	60.8366
69.8374	70.3549	72.2344
74.9548	81.9698	84.0553
88.5561	102.2857	109.5193
110.1018	116.7745	122.1582
126.5902	131.7953	140.7778
146.9588	153.4175	157.9810
165.1967	167.6862	178.3859
185.5073	197.2940	200.7392
208.5421	214.5953	222.4345

228.4860	237.3567	242.1342
243.9525	247.2247	256.8329
266.4291	270.0550	278.4608
281.3697	283.0151	291.5344
293.4782	296.1064	303.6894
310.8711	318.6389	319.5597
331.8221	341.1616	348.1874
363.3650	366.9992	376.7845
379.6605	383.7090	385.6683
386.7313	392.2989	403.0662
406.1275	408.4772	409.1535
415.2102	419.6186	420.7894
437.4715	442.5568	448.4118
454.6548	467.3913	479.6792
482.8082	485.6067	494.2829
518.3607	523.3419	526.7756
530.6324	534.6397	543.6243
554.0267	556.5283	563.0777
572.6102	591.0922	607.9136
621.8778	627.1021	630.3873
631.1460	642.8742	647.1539
661.0825	670.5149	696.5889
697.5494	702.1393	710.7513
715.1072	719.5187	736.8071
738.0865	740.4073	748.0346
765.6715	765.9695	767.2520
767.7737	768.9070	769.9544
774.6573	792.1452	793.6790
808.9274	814.8164	821.3455
823.2211	842.2720	848.7626
850.8390	858.4218	869.9624

874.9480	876.2560	886.2437
887.6992	891.8269	914.9213
916.9787	933.2933	933.3698
936.3834	937.9852	945.5739
947.4192	950.8431	960.9054
967.4615	972.0065	977.6248
979.1671	979.2334	981.6721
984.2013	993.1822	1002.1562
1005.3352	1007.6109	1012.2036
1013.9175	1014.4031	1018.3794
1019.3448	1027.3735	1030.6938
1039.4461	1050.6785	1051.7772
1052.2433	1056.0471	1056.1183
1058.4381	1064.9374	1069.1490
1081.7918	1083.7186	1094.8529
1110.3433	1114.9719	1119.5461
1123.5577	1126.7548	1137.8229
1138.1477	1144.2357	1147.0138
1154.6397	1163.9674	1182.4546
1182.8849	1187.2244	1194.7575
1196.6086	1197.1307	1205.4889
1218.3921	1219.1417	1220.3328
1221.9178	1225.0712	1236.2081
1245.6012	1252.1453	1253.2515
1254.3900	1269.3593	1272.9017
1275.7007	1279.7465	1286.9677
1288.1062	1295.8109	1327.2384
1327.4766	1331.7777	1334.6957
1352.1118	1354.2728	1356.2536
1362.0268	1363.4277	1365.1485
1377.1503	1387.3059	1396.5381

1401.2802	1407.7248	1407.9316
1408.3534	1410.9717	1417.7479
1420.3418	1421.4463	1424.6196
1433.0245	1434.8822	1436.9754
1445.6699	1462.2644	1463.9076
1469.9003	1473.6315	1477.8723
1478.8774	1479.8942	1480.6716
1487.7399	1492.8356	1493.9941
1495.0908	1496.6572	1498.2594
1500.8437	1501.6690	1505.9122
1508.4275	1508.9896	1511.9444
1512.6458	1518.2308	1519.3663
1524.0216	1526.4578	1526.9458
1533.2939	1540.5903	1546.9653
1550.6853	1567.1595	1581.6053
1606.4161	1608.6154	1619.6786
1623.3223	1626.4898	1640.4531
1641.9190	1645.1984	1646.2988
1656.9823	1670.7027	1673.7029
1713.7323	1720.3466	2776.2019
3031.3020	3035.0941	3038.8286
3045.7295	3047.8094	3052.0816
3058.0574	3059.0662	3069.4676
3079.5491	3083.7404	3096.1952
3100.0149	3104.4627	3107.4546
3112.7925	3118.5200	3119.9005
3122.5185	3126.4250	3129.0053
3130.6633	3132.9781	3163.0411
3164.3053	3174.0637	3178.6821
3182.2709	3186.6362	3187.1401
3188.2195	3190.9410	3192.7240



3194.2055	3194.3115	3195.4558
3197.6898	3201.9197	3202.8417
3205.4598	3206.2080	3208.9968
3209.8540	3213.2186	3213.5447
3216.3850	3217.4955	3218.2267
3241.9402	3250.2291	3256.6588
3297.4276	3345.0537	3577.9781

### **M05RR''**

Zero-point correction= 0.919395

Thermal correction to Energy= 0.975746

Thermal correction to Enthalpy= 0.976691

Thermal correction to Gibbs Free Energy= 0.829475

Sum of electronic and zero-point Energies= -2909.797867

Sum of electronic and thermal Energies= -2909.741515

Sum of electronic and thermal Enthalpies= -2909.740571

Sum of electronic and thermal Free Energies= -2909.887786

### Cartesian coordinates

C	1.837229	-3.509458	3.379942
C	0.731800	-3.009384	2.627496
C	1.082538	-2.456654	1.336597
C	2.440780	-2.448850	0.932789
C	3.416590	-3.008705	1.761370
N	3.103640	-3.524419	2.973321
H	1.619948	-3.931148	4.362480
C	2.803376	-1.903700	-0.412703
C	2.643616	-2.753240	-1.560246
C	3.221199	-0.589712	-0.594103
C	2.170752	-4.091716	-1.445281
C	2.945206	-2.252288	-2.869094

C	3.529828	-0.112230	-1.899672
C	1.994506	-4.881664	-2.559610
H	1.943179	-4.481310	-0.459715
C	2.756133	-3.093210	-3.999557
C	3.408494	-0.918069	-3.003389
H	3.868204	0.911314	-2.014825
C	2.286006	-4.378917	-3.851538
H	1.628276	-5.897901	-2.449399
H	2.985676	-2.698555	-4.985627
H	3.649306	-0.538035	-3.992165
H	2.139956	-5.011004	-4.722232
C	0.052919	-1.970253	0.469978
H	0.280467	-1.574925	-0.512618
O	-0.480006	-3.058881	3.063082
C	4.867246	-3.050843	1.348053
H	4.998981	-3.538271	0.374631
H	5.263117	-2.033703	1.264818
H	5.446671	-3.601186	2.093163
C	3.411445	0.368541	0.561372
O	4.018777	0.050195	1.591555
N	2.922349	1.610637	0.331748
H	2.302365	1.753167	-0.472248
C	3.178429	2.756224	1.201376
C	1.865289	3.540063	1.367483
H	2.041117	4.428230	1.979150
H	1.510019	3.880573	0.384698
O	0.864336	2.782814	2.030786
H	0.544254	2.093325	1.410925
C	4.376596	3.620587	0.680263
C	4.727223	4.701989	1.722189
H	3.926120	5.436022	1.848695

H	4.934680	4.253683	2.700611
H	5.622845	5.249600	1.409533
C	4.037954	4.286647	-0.667385
H	4.922395	4.788951	-1.074077
H	3.704144	3.546539	-1.402113
H	3.249601	5.039199	-0.566845
C	5.611774	2.717122	0.493371
H	5.458920	1.989119	-0.307991
H	6.484557	3.323912	0.229013
H	5.838467	2.162037	1.408250
N	-1.218115	-2.026917	0.826703
C	-2.282883	-1.564517	0.116549
C	-3.590655	-1.697379	0.662260
O	-3.867514	-2.167111	1.772549
O	-4.511461	-1.170946	-0.210131
C	-5.947804	-1.245858	0.040249
C	-6.319350	-0.399676	1.262382
H	-5.829056	-0.783735	2.156622
H	-6.012739	0.639474	1.106607
H	-7.403962	-0.415622	1.409976
C	-6.543074	-0.640392	-1.233669
H	-6.258602	-1.233687	-2.107915
H	-7.634748	-0.615796	-1.168416
H	-6.178401	0.381386	-1.376084
C	-6.389362	-2.705419	0.196241
H	-7.481950	-2.758708	0.233816
H	-6.045627	-3.292720	-0.661087
H	-5.979987	-3.140251	1.107804
P	-0.446292	1.771460	-1.354888
O	1.010288	2.029464	-1.682963
C	-1.451878	3.288560	-1.417080

C	-2.011331	3.737489	-2.622890
C	-1.571092	4.078287	-0.260293
C	-2.697868	4.951614	-2.668546
H	-1.919717	3.137158	-3.522873
C	-2.252669	5.293932	-0.313976
H	-1.123301	3.749318	0.673123
C	-2.820102	5.729208	-1.514591
H	-3.136511	5.288597	-3.602683
H	-2.342744	5.900358	0.582075
H	-3.355122	6.673361	-1.551030
C	-1.159913	0.543386	-2.482620
C	-0.281900	-0.433653	-2.980138
C	-2.536606	0.431918	-2.728780
C	-0.777583	-1.521121	-3.698491
H	0.782442	-0.338285	-2.792620
C	-3.027092	-0.650835	-3.460604
H	-3.226811	1.174709	-2.342632
C	-2.151432	-1.630357	-3.936409
H	-0.091825	-2.280066	-4.063425
H	-4.093712	-0.737262	-3.640875
H	-2.539761	-2.478805	-4.491632
N	-0.604590	1.170027	0.220224
C	-1.770576	0.956207	0.774684
C	-1.891684	0.664236	2.200974
C	-0.784186	0.254180	2.965843
C	-3.143388	0.806058	2.826704
C	-0.930918	0.002244	4.325982
H	0.177303	0.123788	2.484774
C	-3.281113	0.571630	4.191511
H	-4.002646	1.106551	2.236274
C	-2.173705	0.168139	4.944696

H	-0.075481	-0.333730	4.903343
H	-4.249731	0.694758	4.666470
H	-2.281450	-0.024692	6.008055
H	-2.127250	-1.269579	-0.906896
H	-2.712757	1.139479	0.248642
H	-1.329822	-2.412034	1.805265
H	3.454167	2.353956	2.181395

Vibrational frequencies

19.3230	24.9799	29.9421
31.9922	36.1301	40.8111
43.2290	44.6477	50.2870
52.8479	56.1640	59.4716
61.7416	64.5560	67.8822
70.8028	78.5962	80.5062
87.0012	90.3451	95.6275
98.8131	106.5679	107.9984
111.0840	132.7366	140.3395
143.6237	145.0022	148.2350
153.6496	160.6495	166.4714
176.7497	185.9553	192.4994
198.8181	203.1450	209.8916
220.9900	228.5391	231.4068
235.9738	243.7655	249.7985
263.2656	266.1526	269.7269
279.7630	283.0014	285.0789
288.5610	297.3441	303.7472
306.0303	317.9810	322.5919
333.0964	340.7561	351.9161
355.0302	362.8546	365.3391
372.7631	376.6189	382.2168

385.8871	390.2682	393.4224
399.8199	402.1561	411.8012
418.7271	421.3479	424.8362
437.5247	446.5264	451.7125
459.3719	468.8720	481.8026
486.6346	490.1911	509.9739
513.5262	523.1551	528.9546
530.3609	532.3288	542.6664
545.3173	550.8975	566.3026
572.6863	606.2073	607.2948
618.3197	629.5797	631.0151
631.9982	653.9616	674.6881
686.5616	695.1337	700.3251
704.0286	714.8063	716.4474
719.4912	724.0220	727.9666
739.2806	745.9514	760.6741
766.8882	767.9092	768.4291
769.1426	769.7255	774.9564
784.2527	792.4812	801.1606
809.0772	823.0097	833.2213
845.9282	847.9600	860.9607
870.1566	872.9578	881.6890
882.0461	884.4453	886.9875
893.5925	904.3258	909.9152
920.9621	929.2296	932.7637
935.6616	943.6692	944.6663
953.4773	954.3094	958.2722
964.4273	967.0965	972.3342
973.8861	979.1693	979.1928
984.8530	999.8111	1001.0852
1003.8130	1007.6544	1011.6344

1014.1215	1014.9807	1021.1370
1022.9720	1031.0660	1033.6762
1039.8412	1049.6709	1050.9656
1053.0426	1053.1368	1056.3850
1061.9237	1063.7429	1067.2547
1086.9679	1105.6168	1106.9924
1111.5163	1115.1258	1116.7825
1118.8839	1119.5667	1136.5311
1137.3549	1166.7507	1169.6414
1178.5602	1182.3155	1191.6151
1194.5464	1196.6809	1198.2558
1205.3591	1211.6642	1215.2355
1222.1481	1224.2419	1226.2808
1239.1459	1247.5419	1250.4799
1255.6568	1263.5977	1268.7293
1270.0293	1270.7581	1281.5517
1284.7230	1290.6139	1316.4027
1324.6007	1325.5250	1328.8780
1333.1507	1340.0143	1341.3707
1354.7114	1361.7686	1369.2203
1372.4940	1380.7486	1390.1470
1395.7381	1399.2692	1404.5915
1408.5458	1409.1838	1412.4553
1413.0603	1416.4303	1426.1342
1430.8289	1433.3354	1433.5431
1444.5216	1463.6876	1472.2525
1477.4151	1479.7698	1480.5403
1483.4087	1488.2558	1488.9030
1493.2588	1494.0579	1495.4402
1497.7148	1499.2971	1500.8822
1501.2235	1505.2730	1512.0345

1514.8784	1516.6498	1517.8303
1518.4274	1522.7671	1527.7250
1531.3717	1534.7307	1536.7932
1547.6052	1553.2820	1573.4402
1605.1390	1614.6673	1615.2210
1622.6105	1626.5016	1633.9430
1642.4293	1645.7209	1646.7419
1654.3374	1657.5193	1670.4774
1694.6166	1713.5380	2861.7843
3020.4647	3033.6879	3033.7909
3038.5004	3045.4393	3045.6272
3048.1371	3054.5952	3079.5793
3082.4336	3098.6969	3101.4892
3104.8720	3108.4944	3113.6047
3115.2419	3116.0540	3118.4297
3119.0734	3123.8699	3126.8606
3128.7637	3130.3158	3134.4975
3165.5978	3168.9383	3179.9492
3183.0264	3185.3534	3185.7776
3187.9895	3190.6207	3190.8017
3194.5748	3196.1538	3197.0744
3203.1787	3204.4456	3204.7856
3204.8187	3212.8161	3213.1813
3213.4389	3214.2570	3216.8732
3219.3852	3226.8574	3232.3596
3309.9235	3341.1090	3508.1011

### **M5RR''**

Zero-point correction= 0.921627

Thermal correction to Energy= 0.977358

Thermal correction to Enthalpy= 0.978303



Thermal correction to Gibbs Free Energy= 0.829804

Sum of electronic and zero-point Energies= -2909.810718

Sum of electronic and thermal Energies= -2909.754986

Sum of electronic and thermal Enthalpies= -2909.754042

Sum of electronic and thermal Free Energies= -2909.902541

Cartesian coordinates

C	2.433703	-2.527843	3.984902
C	1.259842	-2.270934	3.185787
C	1.544491	-1.925885	1.807478
C	2.896740	-1.857637	1.361403
C	3.925479	-2.151491	2.243571
N	3.673528	-2.480506	3.544757
H	2.272367	-2.792196	5.030555
C	3.195574	-1.502626	-0.060385
C	3.217187	-2.545389	-1.044840
C	3.404224	-0.186406	-0.450944
C	2.945787	-3.903217	-0.713576
C	3.504479	-2.222838	-2.412022
C	3.684264	0.118131	-1.811588
C	2.950479	-4.883607	-1.680962
H	2.727222	-4.157384	0.317636
C	3.509102	-3.259009	-3.385049
C	3.751982	-0.869942	-2.761982
H	3.844621	1.153383	-2.090926
C	3.233925	-4.561011	-3.030873
H	2.735477	-5.912501	-1.408801
H	3.726533	-3.001440	-4.418048
H	3.973047	-0.624399	-3.796864
H	3.233805	-5.343380	-3.783690
C	0.475181	-1.676434	0.908080

H	0.668905	-1.402493	-0.121685
O	0.083543	-2.357772	3.669424
C	5.371944	-2.076168	1.825392
H	5.568975	-2.676381	0.930139
H	5.632402	-1.038151	1.593373
H	6.011747	-2.434419	2.634813
C	3.379375	0.954546	0.542790
O	4.038683	0.917586	1.592309
N	2.634232	2.005542	0.145532
H	2.002107	1.889628	-0.661757
C	2.554541	3.263410	0.882651
C	1.073055	3.677420	0.981857
H	1.006142	4.648991	1.483192
H	0.662295	3.804734	-0.029462
O	0.306299	2.756025	1.728840
H	0.005775	2.025665	1.117390
C	3.488440	4.353629	0.256746
C	3.536229	5.588977	1.178107
H	2.565874	6.087580	1.256619
H	3.858926	5.314413	2.189047
H	4.249464	6.323443	0.788059
C	2.996278	4.767368	-1.143814
H	3.726785	5.428336	-1.623439
H	2.855005	3.892405	-1.786281
H	2.044250	5.305635	-1.098651
C	4.918133	3.789058	0.137514
H	4.964253	2.969088	-0.584537
H	5.606808	4.571152	-0.200809
H	5.272529	3.405468	1.098991
N	-0.781142	-1.785491	1.275270
C	-1.870785	-1.336491	0.452653

C	-3.164357	-1.966165	0.931402
O	-3.282330	-2.579051	1.977072
O	-4.127980	-1.704071	0.045286
C	-5.522618	-2.173529	0.219121
C	-6.114936	-1.598446	1.506517
H	-5.622742	-2.012171	2.386588
H	-6.006637	-0.511136	1.522555
H	-7.180683	-1.841802	1.548728
C	-6.212142	-1.591919	-1.013993
H	-5.743776	-1.969259	-1.927501
H	-7.268414	-1.874065	-1.019294
H	-6.141129	-0.500417	-1.011672
C	-5.538728	-3.702332	0.196719
H	-6.574429	-4.054309	0.200404
H	-5.051010	-4.071401	-0.710268
H	-5.025482	-4.110917	1.067956
P	-0.585576	1.279057	-1.537129
O	0.800153	1.792297	-1.920020
C	-1.859173	2.550078	-1.907359
C	-2.326866	2.794398	-3.207144
C	-2.320774	3.353475	-0.852218
C	-3.244985	3.818104	-3.448240
H	-1.981477	2.176581	-4.031551
C	-3.235299	4.379769	-1.094523
H	-1.954912	3.168067	0.153578
C	-3.700620	4.611687	-2.391572
H	-3.605819	3.995819	-4.457219
H	-3.587876	4.995149	-0.271716
H	-4.416401	5.406831	-2.579133
C	-0.996874	-0.167908	-2.589977
C	0.058736	-1.048613	-2.881082

C	-2.307966	-0.549116	-2.914755
C	-0.190136	-2.291007	-3.464023
H	1.074191	-0.753002	-2.638632
C	-2.557717	-1.791161	-3.504327
H	-3.138456	0.115502	-2.697660
C	-1.502041	-2.666077	-3.772734
H	0.637882	-2.963612	-3.669173
H	-3.577420	-2.077314	-3.745899
H	-1.700292	-3.635381	-4.220704
N	-0.718853	0.848332	0.027450
C	-1.969826	0.263558	0.448131
C	-2.426572	0.757925	1.810866
C	-1.590250	0.702529	2.935046
C	-3.725397	1.258510	1.965143
C	-2.053477	1.116158	4.183704
H	-0.570725	0.352931	2.830297
C	-4.190217	1.681083	3.213107
H	-4.375590	1.322830	1.096768
C	-3.355587	1.603830	4.329324
H	-1.394038	1.061164	5.045286
H	-5.200295	2.068845	3.310439
H	-3.712450	1.927275	5.302890
H	-1.698987	-1.634442	-0.582830
H	-2.801203	0.448920	-0.246976
H	-0.917403	-2.029199	2.275221
H	2.911636	3.057593	1.897082

#### Vibrational frequencies

12.4805	15.1916	21.0840
26.6271	28.0744	32.9869
36.0233	37.6878	42.5459

47.4818	51.8802	54.7115
58.1445	63.1131	65.4573
68.0974	73.0213	82.2326
86.1882	87.4301	93.4404
98.6617	107.6086	109.5393
117.8091	125.0948	132.6677
138.8552	145.3329	155.7021
158.3530	172.1769	177.0153
183.7058	193.5298	195.7906
206.0471	215.2750	223.5749
223.7293	227.4016	233.4497
243.6861	248.0186	262.0671
264.2881	269.3056	273.3263
278.7424	282.6066	285.5750
286.5491	299.8151	307.4823
314.9326	318.8509	331.1445
342.2492	347.9070	357.9477
366.6486	369.8297	372.4150
380.5901	391.5185	394.6779
397.1050	400.7612	404.2937
412.0372	419.7317	423.4058
424.1575	437.6772	444.4530
448.8881	453.0120	457.1462
472.1647	482.6290	485.8725
508.7990	510.7033	518.5590
525.3235	527.7947	532.9671
541.1314	546.3359	554.9734
565.7663	571.4564	585.6127
599.5433	607.8259	630.1445
631.6833	632.7721	648.2077
654.0140	677.3565	687.4852

695.5666	705.0281	712.5011
717.3145	718.8567	728.1529
733.6155	747.9975	755.5604
766.9175	767.9429	768.5356
775.5282	780.5646	785.1613
788.8203	796.9846	808.8925
810.6318	819.7178	823.5061
835.5081	846.6739	855.5400
858.0873	879.8040	883.2221
884.9260	891.2795	895.5823
906.4435	909.7630	911.2133
917.6272	922.5735	926.8192
936.4776	938.5215	940.4850
944.5733	945.3515	947.9621
953.5779	954.6444	966.6407
968.4283	971.9683	974.6418
977.8454	980.3575	996.1016
996.5235	1000.7709	1000.8539
1004.8299	1011.8536	1013.6510
1015.6851	1018.0233	1019.6767
1023.6604	1026.1042	1035.4584
1049.4198	1051.0029	1052.2250
1056.3199	1056.5436	1060.9543
1062.3373	1068.6103	1096.7936
1101.3162	1103.0349	1103.6839
1109.2347	1111.3730	1115.3941
1117.2633	1129.7199	1137.7637
1141.0431	1149.2877	1174.9170
1183.4760	1188.4540	1189.8944
1191.8766	1192.1723	1195.4119
1207.1479	1212.1083	1213.6225

1215.4655	1216.9444	1222.2768
1230.1855	1248.2130	1249.0314
1250.9120	1261.3828	1270.2690
1276.7913	1278.2528	1289.6172
1291.4295	1294.9012	1321.5897
1322.2743	1328.8779	1329.6160
1338.6077	1344.9786	1346.6222
1354.6216	1358.8404	1362.9477
1363.8163	1367.1688	1385.5586
1392.2465	1399.2501	1408.4708
1409.7978	1410.5344	1412.8437
1415.0378	1418.0706	1422.7754
1426.7974	1428.8075	1431.1728
1436.9399	1445.3241	1461.8162
1465.6176	1470.9270	1475.3597
1479.2544	1486.5863	1489.0332
1493.8540	1494.1524	1495.3560
1497.4592	1498.1124	1499.3129
1502.0343	1505.8295	1508.0699
1510.5558	1515.4212	1517.8968
1521.1390	1522.2854	1526.0872
1528.1846	1530.8878	1536.9981
1551.7113	1566.7022	1569.7867
1609.9755	1620.6228	1625.0810
1628.9572	1636.6370	1636.9786
1641.7964	1644.1844	1646.9211
1657.3606	1670.7978	1686.3215
1708.6978	1780.9707	3004.8235
3013.0749	3032.7731	3036.3843
3039.0201	3042.9642	3050.8397
3057.0031	3065.4145	3067.7547

3081.1443	3099.7115	3101.7488
3104.5213	3110.8087	3116.3911
3118.4622	3122.6064	3125.9381
3127.3506	3129.5811	3134.8764
3137.7882	3139.0616	3139.8750
3142.9116	3154.6273	3159.9312
3168.3379	3173.3679	3176.9783
3179.0767	3180.1899	3180.9406
3182.9882	3185.6317	3188.7529
3190.2160	3190.8019	3191.2201
3197.0427	3197.9906	3202.7611
3204.6803	3204.9156	3206.1104
3213.7157	3215.7853	3216.3168
3218.3668	3230.6078	3241.2709

#### **TS5RR'**

Zero-point correction= 0.960919

Thermal correction to Energy= 1.018079

Thermal correction to Enthalpy= 1.019023

Thermal correction to Gibbs Free Energy= 0.868677

Sum of electronic and zero-point Energies= -2949.539571

Sum of electronic and thermal Energies= -2949.482411

Sum of electronic and thermal Enthalpies= -2949.481467

Sum of electronic and thermal Free Energies= -2949.631813

#### Cartesian coordinates

C	2.594766	-2.327905	3.489617
C	1.449956	-2.103759	2.746878
C	1.581251	-1.830457	1.350714
C	2.879819	-1.814832	0.799137
C	4.001222	-2.108228	1.582332



N	3.824671	-2.337484	2.914346
H	2.536195	-2.517932	4.551795
C	3.070100	-1.446661	-0.640502
C	2.844753	-2.422589	-1.663410
C	3.421014	-0.147815	-0.984129
C	2.448451	-3.757284	-1.369579
C	3.015456	-2.046363	-3.036672
C	3.565327	0.214849	-2.348763
C	2.227717	-4.667544	-2.379104
H	2.319105	-4.054651	-0.334628
C	2.787456	-3.012672	-4.053715
C	3.384561	-0.711016	-3.346617
H	3.823963	1.240038	-2.590309
C	2.398816	-4.294627	-3.734890
H	1.921690	-5.680222	-2.135516
H	2.919241	-2.716971	-5.090738
H	3.505672	-0.427509	-4.388091
H	2.222355	-5.022966	-4.520233
C	0.395732	-1.613212	0.545535
H	0.506149	-1.388543	-0.512065
O	0.269823	-2.145081	3.369926
C	5.390646	-2.189165	1.024460
H	5.354321	-2.136994	-0.061503
H	5.992259	-1.346735	1.373922
H	5.881768	-3.123578	1.309130
C	3.669981	0.894531	0.082697
O	4.512242	0.710141	0.972448
N	2.928142	2.012867	-0.056190
H	2.135129	1.961695	-0.711288
C	2.820226	2.984999	1.026168
C	1.481925	2.745551	1.773122

H	1.527141	3.240442	2.750199
H	0.649506	3.192323	1.214911
O	1.244996	1.361764	1.967062
H	0.569162	1.112538	1.288592
C	3.034989	4.442534	0.522288
C	2.914842	5.415706	1.711519
H	1.896838	5.447865	2.111981
H	3.591765	5.132752	2.526036
H	3.176054	6.431594	1.395973
C	2.011238	4.833139	-0.562774
H	2.226455	5.842428	-0.930848
H	2.041917	4.146380	-1.412532
H	0.985968	4.835167	-0.179605
C	4.454180	4.548102	-0.067605
H	4.576750	3.866808	-0.914712
H	4.651641	5.567648	-0.416763
H	5.212331	4.294429	0.682256
N	-0.775931	-1.780762	1.098076
C	-1.922340	-1.506671	0.411898
C	-3.165834	-2.053194	0.993237
O	-3.270831	-2.561622	2.099544
O	-4.179383	-1.858555	0.119458
C	-5.521909	-2.427168	0.326365
C	-6.182081	-1.826520	1.569483
H	-5.621526	-2.079813	2.468700
H	-6.238756	-0.738626	1.485729
H	-7.200412	-2.217293	1.659681
C	-6.257423	-1.998401	-0.943932
H	-5.758038	-2.402246	-1.829354
H	-7.287957	-2.363887	-0.924306
H	-6.275059	-0.907498	-1.023998

C	-5.417463	-3.952418	0.410027
H	-6.420989	-4.387873	0.426722
H	-4.886865	-4.341538	-0.464246
H	-4.886431	-4.258500	1.312035
P	-0.685516	1.516357	-1.398353
O	0.753307	1.848063	-1.750915
C	-1.786793	2.954062	-1.642008
C	-2.114734	3.379434	-2.938976
C	-2.241458	3.694519	-0.540578
C	-2.887969	4.524309	-3.130723
H	-1.774219	2.809379	-3.798812
C	-3.011320	4.842781	-0.734568
H	-1.997104	3.364670	0.463916
C	-3.335702	5.257886	-2.028153
H	-3.142562	4.843084	-4.137029
H	-3.360955	5.409553	0.123165
H	-3.938032	6.148982	-2.177902
C	-1.297593	0.212508	-2.521086
C	-0.354707	-0.717948	-2.987038
C	-2.658252	0.007889	-2.796393
C	-0.766366	-1.851756	-3.686847
H	0.698740	-0.545194	-2.794229
C	-3.069166	-1.127051	-3.498835
H	-3.398244	0.729953	-2.465231
C	-2.126474	-2.061548	-3.934804
H	-0.026729	-2.568017	-4.031160
H	-4.124628	-1.281952	-3.701228
H	-2.450473	-2.947534	-4.472639
N	-0.873948	1.031300	0.181480
C	-2.070631	0.520877	0.568246
C	-2.544538	0.719522	1.966704

C	-1.686372	0.702462	3.077238
C	-3.917326	0.921769	2.174772
C	-2.201621	0.865944	4.362509
H	-0.621406	0.576265	2.936637
C	-4.429998	1.091685	3.460923
H	-4.585070	0.944469	1.318725
C	-3.572311	1.059071	4.561979
H	-1.528111	0.844394	5.214737
H	-5.495633	1.248098	3.600721
H	-3.966352	1.186763	5.565960
H	-1.887206	-1.519591	-0.675478
C	4.989632	-2.608604	3.781925
H	5.437541	-3.566271	3.513018
H	5.725685	-1.813074	3.668328
H	4.655346	-2.644330	4.815904
H	-2.905768	0.544851	-0.138547
H	3.630839	2.748372	1.721453
H	-0.434083	-2.028386	2.635472

Vibrational frequencies

-374.8934	16.7051	19.8711
23.5121	33.4154	35.9819
37.4299	38.2199	39.1809
40.7413	45.6454	47.5017
49.7761	53.1624	58.5534
62.1127	65.2789	73.2831
78.0736	83.2482	87.8407
90.0887	92.7776	104.7384
109.7431	120.2843	125.9092
133.5046	139.6007	145.0271
153.6424	158.2248	158.8834

164.5260	182.1925	184.9856
191.9162	198.5580	203.6674
211.6166	217.7209	222.7480
231.8814	232.3500	245.1472
248.2867	250.3298	258.3645
263.0444	275.2864	281.8877
286.3495	293.2523	294.4856
295.4927	301.0162	312.1837
317.5325	320.5785	334.3511
346.9403	354.6232	364.6891
366.6648	374.9693	379.1855
384.1807	389.7039	398.3606
400.5572	405.3301	408.6162
410.3358	410.8920	418.0767
418.3277	421.4724	436.6482
440.7627	443.1700	456.0863
462.0835	472.4292	482.1659
483.2533	503.5869	522.2068
523.2880	528.4798	532.3045
535.6842	547.8717	551.9146
557.1435	565.1643	572.0218
575.5599	599.8117	613.3205
629.5245	631.2703	632.0707
641.1498	650.6445	658.0433
668.5569	696.5478	699.9934
704.9983	712.2134	720.0194
731.9460	736.7318	746.2670
748.4370	764.3895	766.5011
767.2157	768.8658	769.8296
774.9020	776.8555	780.8699
795.9004	798.1581	818.9554

821.4718	838.8656	847.8800
853.4890	858.7495	871.7546
872.1862	874.9420	883.5337
886.5104	892.0515	902.7442
909.8848	914.8636	923.7112
925.8731	935.3364	938.1160
938.4314	948.5406	948.9184
949.5851	954.2225	958.9165
967.4123	971.9830	973.0170
978.5984	979.4733	981.7309
992.1849	992.7094	1000.8438
1002.4568	1003.6453	1012.5358
1014.0395	1014.7063	1015.1188
1018.9172	1021.8424	1030.3135
1033.2637	1050.1966	1051.2135
1051.6045	1056.7060	1057.9124
1058.5690	1064.8682	1069.5759
1083.4311	1090.8780	1091.7409
1096.2855	1104.5771	1110.3239
1117.4285	1119.7140	1128.5991
1134.2555	1138.0869	1145.4762
1148.6334	1159.8493	1174.2601
1181.5111	1188.0668	1191.7358
1193.2054	1194.2088	1205.0484
1213.5151	1214.5165	1216.9848
1221.1021	1223.2740	1227.1129
1243.3005	1246.9587	1254.0139
1262.3273	1273.5442	1275.1397
1280.6790	1284.9620	1288.0402
1291.8055	1301.7930	1317.1204
1324.7020	1331.9414	1336.0174

1343.4396	1349.6879	1352.8105
1358.4659	1360.2604	1360.9662
1371.3313	1373.0068	1378.8959
1390.6135	1408.7710	1410.4372
1411.7230	1412.7638	1415.4006
1416.4761	1417.5655	1422.6858
1430.3693	1435.4601	1446.7253
1453.8542	1456.4773	1464.9331
1468.0243	1472.6782	1472.9330
1476.5387	1480.5396	1481.5892
1493.4179	1494.2493	1495.1874
1496.1851	1499.2576	1502.0301
1503.4449	1504.1160	1506.1115
1508.9020	1509.8475	1512.1023
1515.9883	1519.6412	1520.3286
1522.5336	1524.1369	1525.5808
1528.7521	1532.3372	1543.7005
1549.8702	1553.1609	1586.3455
1608.9786	1615.4230	1623.0677
1624.3996	1626.2069	1636.3356
1642.8991	1644.9136	1646.7128
1655.6567	1668.1051	1671.7795
1713.2773	1754.1943	2701.0478
3023.5717	3030.7270	3033.8626
3043.7596	3049.8436	3054.8462
3062.9592	3067.5629	3068.8915
3069.2201	3089.8078	3090.2680
3098.9971	3102.8890	3107.2474
3112.0091	3118.5572	3124.6520
3127.6171	3131.6230	3131.9024
3136.3937	3138.6036	3155.6719

3159.9142	3172.7321	3174.5427
3177.6877	3180.8218	3181.6496
3183.5843	3183.9143	3184.6382
3184.8910	3187.9694	3189.1250
3193.0101	3193.6861	3194.2238
3196.9790	3200.3034	3201.7440
3205.3965	3206.0772	3206.1170
3209.3160	3212.0538	3212.3153
3215.5901	3218.0368	3244.3082
3254.0688	3261.4382	3328.6029

### TS5RR''

Zero-point correction= 0.919379

Thermal correction to Energy= 0.974984

Thermal correction to Enthalpy= 0.975928

Thermal correction to Gibbs Free Energy= 0.829658

Sum of electronic and zero-point Energies= -2909.797244

Sum of electronic and thermal Energies= -2909.741639

Sum of electronic and thermal Enthalpies= -2909.740695

Sum of electronic and thermal Free Energies= -2909.886964

### Cartesian coordinates

C	1.974696	-3.208668	3.596911
C	0.854747	-2.771449	2.817996
C	1.194092	-2.299629	1.492390
C	2.551827	-2.300900	1.078729
C	3.536349	-2.790058	1.935416
N	3.233589	-3.230904	3.183229
H	1.767729	-3.567661	4.606004
C	2.904599	-1.828420	-0.295982
C	2.783268	-2.748873	-1.391190



C	3.283433	-0.515249	-0.548050
C	2.349293	-4.091947	-1.202045
C	3.087427	-2.315718	-2.723519
C	3.589116	-0.103014	-1.875643
C	2.213878	-4.951497	-2.269572
H	2.119333	-4.430067	-0.198020
C	2.941254	-3.228007	-3.803821
C	3.508288	-0.976551	-2.930848
H	3.890707	0.924421	-2.046335
C	2.509641	-4.517227	-3.585130
H	1.877126	-5.970347	-2.103765
H	3.172234	-2.885388	-4.808802
H	3.747571	-0.647119	-3.937995
H	2.396619	-5.204274	-4.418257
C	0.156424	-1.879394	0.605142
H	0.374712	-1.545903	-0.402023
O	-0.348557	-2.812155	3.265798
C	4.987497	-2.830086	1.525365
H	5.127861	-3.365562	0.579144
H	5.364182	-1.811397	1.388465
H	5.575936	-3.329290	2.298674
C	3.431395	0.510748	0.555164
O	4.074755	0.279660	1.587704
N	2.860169	1.703395	0.272489
H	2.223868	1.765731	-0.531710
C	3.028502	2.899633	1.093919
C	1.662435	3.598127	1.218774
H	1.777855	4.525157	1.786753
H	1.295406	3.868284	0.219142
O	0.708999	2.809688	1.911007
H	0.383336	2.108262	1.301126

C	4.165667	3.823946	0.539675
C	4.435998	4.968885	1.536649
H	3.583801	5.647756	1.632764
H	4.671852	4.576102	2.532443
H	5.291246	5.566213	1.202392
C	3.783807	4.409849	-0.833762
H	4.634140	4.948574	-1.265874
H	3.493075	3.620210	-1.534456
H	2.950452	5.115665	-0.759845
C	5.461856	3.003351	0.388966
H	5.360383	2.233311	-0.380625
H	6.289598	3.658938	0.097096
H	5.726507	2.504112	1.325699
N	-1.109524	-1.925894	0.971676
C	-2.168201	-1.430021	0.249835
C	-3.493260	-1.701959	0.747561
O	-3.753378	-2.173654	1.854817
O	-4.416221	-1.279952	-0.161371
C	-5.855603	-1.472292	0.038597
C	-6.340336	-0.636407	1.226225
H	-5.851420	-0.955146	2.146588
H	-6.122969	0.422285	1.056192
H	-7.423402	-0.747886	1.337495
C	-6.445647	-0.947739	-1.272080
H	-6.074905	-1.533137	-2.118665
H	-7.536958	-1.016530	-1.250055
H	-6.164451	0.098348	-1.425478
C	-6.170517	-2.961446	0.213580
H	-7.254836	-3.108762	0.212322
H	-5.744332	-3.534030	-0.615975
H	-5.761897	-3.340131	1.150234

P	-0.487616	1.608215	-1.424053
O	0.960286	1.923112	-1.754818
C	-1.554950	3.078439	-1.596202
C	-2.073694	3.462533	-2.841838
C	-1.767999	3.900275	-0.476058
C	-2.808965	4.642487	-2.964241
H	-1.911945	2.836860	-3.714495
C	-2.498113	5.081965	-0.604747
H	-1.352841	3.620960	0.488199
C	-3.022951	5.451921	-1.845925
H	-3.214388	4.928418	-3.930061
H	-2.659356	5.712770	0.264252
H	-3.596052	6.369273	-1.941842
C	-1.120742	0.314010	-2.534544
C	-0.196491	-0.658884	-2.950491
C	-2.482791	0.142054	-2.823821
C	-0.630261	-1.798924	-3.626193
H	0.857071	-0.519856	-2.731215
C	-2.912702	-0.995110	-3.510422
H	-3.209818	0.880274	-2.501354
C	-1.990639	-1.968768	-3.902999
H	0.092545	-2.551208	-3.928029
H	-3.968891	-1.126018	-3.724050
H	-2.331714	-2.858295	-4.424060
N	-0.658344	1.077236	0.155105
C	-1.860478	0.796854	0.664067
C	-2.035424	0.735383	2.125095
C	-0.964791	0.434232	2.984513
C	-3.305894	0.970540	2.676967
C	-1.166095	0.377695	4.361719
H	0.017512	0.249530	2.567708

C	-3.501628	0.925366	4.055045
H	-4.137778	1.195807	2.017161
C	-2.430191	0.627372	4.902951
H	-0.333535	0.131786	5.013872
H	-4.487499	1.119524	4.467298
H	-2.580987	0.586868	5.977776
H	-2.022416	-1.306921	-0.811253
H	-2.777218	1.001210	0.102611
H	-1.225577	-2.250348	1.966843
H	3.325711	2.560425	2.091424

#### Vibrational frequencies

-152.1944	15.8678	23.5575
27.5097	33.4777	36.7354
38.1764	39.5901	43.5376
47.4876	52.0660	54.0399
57.4175	61.8263	65.1554
65.6721	69.8465	75.7999
80.8896	92.2532	94.0842
96.3414	100.4239	105.1693
107.6703	118.7377	137.2143
140.6471	143.3584	147.6684
152.9132	154.3828	159.3379
171.5214	183.1040	190.2529
197.6015	202.0568	214.4811
219.3344	225.6325	230.3063
232.4009	241.6226	247.3133
259.1266	266.1450	271.8849
280.8059	283.3556	287.6895
289.4401	295.5001	297.2357
304.9173	317.0760	319.2998

334.0143	341.8140	351.0328
362.3462	365.6817	369.9610
375.0415	381.8231	388.4018
388.7256	393.4884	397.1411
399.0283	411.6813	419.3937
420.5225	427.1772	431.8271
438.7361	447.4399	452.4517
459.0837	469.7437	485.2370
488.5003	496.3523	512.4096
522.8729	526.6060	530.1625
533.1836	540.1674	543.2437
549.4543	555.1339	565.3021
572.0446	604.2696	607.0640
624.8761	630.1520	631.4599
633.4751	654.8208	676.3555
687.4746	699.8985	705.2095
710.9401	715.9323	719.6457
735.9041	739.4599	743.9800
753.1595	762.5248	767.7767
768.4403	768.5801	772.1460
774.6545	776.1168	783.5353
793.0330	798.8589	809.1460
812.7301	822.8403	845.5370
856.4261	859.4406	866.0111
877.7354	878.5530	882.2919
884.5978	885.7361	890.7779
903.1034	903.8638	909.2156
920.5711	933.9455	936.9187
940.1197	944.0020	945.8333
951.9570	952.8725	962.2798
966.6237	969.6480	973.6569

977.2485	979.8420	980.3483
986.4807	998.1663	1001.3120
1004.0198	1006.0435	1011.7151
1014.1899	1015.4096	1022.8614
1023.3539	1027.8812	1032.4724
1043.5516	1050.2777	1050.7935
1052.4292	1053.6300	1055.9568
1060.7535	1062.5991	1070.6917
1091.3159	1099.7717	1105.1790
1106.8887	1113.9737	1115.7080
1116.3168	1117.6878	1136.7105
1138.2069	1159.4797	1171.4583
1176.6100	1182.3642	1190.2440
1192.3728	1194.7639	1194.8860
1205.5639	1210.9592	1216.6668
1220.2364	1221.3880	1223.6067
1238.4176	1243.9794	1246.5340
1248.4821	1258.9767	1266.9124
1270.2807	1273.5624	1285.9758
1286.5917	1291.8463	1318.4032
1325.0730	1329.4680	1330.1767
1333.2942	1337.3070	1339.2466
1353.7411	1358.7188	1362.7375
1366.8714	1370.4155	1377.7682
1387.9324	1400.4799	1406.5883
1409.0479	1409.8747	1413.2472
1414.7873	1416.4685	1427.4796
1432.3494	1432.6690	1435.5113
1445.1171	1463.7487	1465.5385
1472.5591	1476.7662	1480.1063
1480.6164	1484.1254	1484.2190

1494.8186	1495.2593	1496.8878
1497.5880	1499.2481	1502.0189
1505.2271	1506.9301	1511.5449
1512.8693	1516.4663	1520.1728
1520.8626	1523.4657	1527.0190
1528.5459	1529.8993	1534.1647
1538.8634	1549.3207	1556.5432
1608.3197	1621.6106	1622.8437
1626.0535	1627.3743	1632.4468
1642.8167	1645.3038	1646.7680
1654.7983	1667.6280	1670.6817
1711.7991	1712.3038	2925.9532
3023.1572	3032.8042	3036.4819
3037.0029	3044.0687	3048.6590
3051.6704	3057.7261	3071.2158
3077.4889	3099.2357	3101.0601
3101.1005	3106.3349	3112.3359
3114.8573	3118.4816	3119.6109
3122.2401	3126.6898	3127.3928
3131.3311	3133.8339	3136.2786
3165.3045	3170.5609	3179.5954
3180.0241	3183.4434	3185.4939
3186.3968	3188.8780	3189.7527
3190.8496	3194.5574	3195.4232
3199.9214	3201.9715	3202.6130
3204.8985	3207.9111	3211.0924
3211.3639	3212.1771	3215.7777
3218.0656	3230.8513	3233.5779
3283.9053	3297.5983	3424.5770

**TS51RR**

Zero-point correction= 0.989755

Thermal correction to Energy= 1.048634

Thermal correction to Enthalpy= 1.049579

Thermal correction to Gibbs Free Energy= 0.896355

Sum of electronic and zero-point Energies= -2988.814839

Sum of electronic and thermal Energies= -2988.755960

Sum of electronic and thermal Enthalpies= -2988.755016

Sum of electronic and thermal Free Energies= -2988.908239

#### Cartesian coordinates

C	2.830196	-2.080505	3.341690
C	1.573349	-1.933653	2.700382
C	1.636183	-1.711852	1.267673
C	2.887156	-1.701437	0.612332
C	4.074377	-1.923388	1.313356
N	3.998598	-2.082053	2.672362
H	2.867033	-2.216970	4.413552
C	2.953450	-1.442631	-0.861787
C	2.689262	-2.503614	-1.786281
C	3.235973	-0.168356	-1.331146
C	2.363618	-3.822081	-1.360947
C	2.749151	-2.233290	-3.193407
C	3.270349	0.090883	-2.725221
C	2.105028	-4.816686	-2.277706
H	2.318618	-4.038512	-0.299177
C	2.482240	-3.284240	-4.112505
C	3.049253	-0.916513	-3.632348
H	3.472894	1.101231	-3.063707
C	2.164494	-4.548051	-3.667244
H	1.854612	-5.815706	-1.934422
H	2.527616	-3.068687	-5.176336



H	3.083332	-0.713138	-4.698785
H	1.958417	-5.341690	-4.378665
C	0.413894	-1.552504	0.531062
H	0.420849	-1.378669	-0.535952
O	0.489172	-1.999808	3.366597
C	5.422738	-1.995362	0.658006
H	5.301848	-2.022174	-0.423148
H	6.019625	-1.110890	0.894536
H	5.972710	-2.890752	0.960822
C	3.551196	0.953808	-0.366274
O	4.573381	0.914443	0.335460
N	2.659538	1.960544	-0.373731
H	1.813161	1.850191	-0.950927
C	2.711939	3.042560	0.605487
C	1.716050	2.715207	1.736747
H	1.688381	3.532405	2.471457
H	0.716910	2.582817	1.315109
O	2.003913	1.484459	2.390365
C	2.510759	4.447040	-0.043972
C	2.863971	5.537135	0.988615
H	2.173640	5.544150	1.837267
H	3.879158	5.401515	1.378860
H	2.814608	6.525767	0.519972
C	1.066861	4.658172	-0.539045
H	0.978261	5.636758	-1.024082
H	0.776861	3.893740	-1.263660
H	0.345113	4.635721	0.283639
C	3.476563	4.576766	-1.238114
H	3.231937	3.859847	-2.026439
H	3.420471	5.584301	-1.664187
H	4.512329	4.396166	-0.928210

N	-0.748274	-1.714256	1.127439
C	-1.977263	-1.456806	0.555677
C	-3.124629	-1.979987	1.311583
O	-3.065195	-2.398012	2.460803
O	-4.239483	-1.859712	0.565736
C	-5.545171	-2.389547	1.004228
C	-6.028632	-1.649986	2.253045
H	-5.350538	-1.813003	3.090288
H	-6.098479	-0.576806	2.058375
H	-7.024542	-2.013856	2.523762
C	-6.440416	-2.082935	-0.196370
H	-6.064908	-2.585921	-1.092131
H	-7.459716	-2.427492	-0.001728
H	-6.466059	-1.006311	-0.387887
C	-5.430039	-3.898696	1.232129
H	-6.423540	-4.314155	1.424785
H	-5.019900	-4.383918	0.341384
H	-4.785342	-4.117897	2.083635
P	-0.915328	1.333874	-1.622697
O	0.487348	1.649399	-2.117425
C	-2.073580	2.713372	-1.939261
C	-2.516565	2.979219	-3.244441
C	-2.464983	3.564414	-0.895326
C	-3.338925	4.076570	-3.500410
H	-2.226546	2.321934	-4.059480
C	-3.285294	4.663949	-1.153196
H	-2.127534	3.361394	0.115726
C	-3.722867	4.920922	-2.454534
H	-3.681354	4.272007	-4.512194
H	-3.584350	5.317321	-0.338975
H	-4.363426	5.774908	-2.653906

C	-1.577678	-0.093675	-2.549940
C	-0.652306	-1.048388	-3.000549
C	-2.951004	-0.363933	-2.657950
C	-1.088839	-2.265239	-3.524731
H	0.407663	-0.827569	-2.933895
C	-3.387284	-1.580614	-3.186593
H	-3.679840	0.369858	-2.327620
C	-2.458139	-2.534811	-3.610668
H	-0.360618	-2.997700	-3.859305
H	-4.451128	-1.785078	-3.261028
H	-2.801038	-3.483901	-4.011719
N	-0.954239	1.018313	-0.001266
C	-2.081877	0.568750	0.591635
C	-2.257630	0.850166	2.043599
C	-1.156432	0.916056	2.910082
C	-3.546734	1.045929	2.558207
C	-1.350657	1.167201	4.267660
H	-0.155908	0.771081	2.524006
C	-3.738323	1.302212	3.916136
H	-4.399400	1.002969	1.886889
C	-2.638686	1.361446	4.776389
H	-0.490275	1.211481	4.929667
H	-4.742429	1.456941	4.300308
H	-2.784660	1.559812	5.834310
H	-2.024090	-1.571048	-0.519560
C	5.240758	-2.254744	3.455495
H	5.714719	-3.201546	3.193913
H	5.923066	-1.431767	3.243653
H	4.991721	-2.254904	4.513844
H	-3.033334	0.573465	0.045265
H	-0.665008	-1.874142	2.161356

H	3.725521	3.024202	1.014845
C	3.143767	1.513039	3.237248
H	3.123590	2.382220	3.911826
H	3.110499	0.601337	3.838983
H	4.074553	1.518821	2.658622

Vibrational frequencies

-368.0581	19.9692	24.0949
28.2284	33.4275	35.7969
37.9370	40.7255	42.3396
45.3311	47.4331	51.6462
54.1488	55.5170	56.6468
62.9043	66.3464	72.5246
74.6243	79.1267	86.3146
88.9505	92.9179	94.9856
102.6835	104.6381	113.4317
124.9829	130.1989	135.3378
140.7254	148.3025	153.5688
156.1047	160.7408	165.0554
173.3096	188.0177	189.8804
195.7269	202.3010	218.8013
221.9623	225.1471	230.2447
231.5346	239.2655	244.9772
247.3471	263.9219	265.2133
270.4794	275.9863	280.8291
284.5671	292.4213	297.3809
301.1954	311.1600	317.5478
325.3475	334.0668	338.4728
342.7900	359.7720	363.2296
370.0027	375.8906	380.5324
386.2891	388.1890	396.4311

407.2275	408.3249	410.4155
411.8596	418.3456	423.5538
427.1269	436.7537	442.2778
443.8275	450.6379	457.1433
460.6567	471.5147	484.0600
485.4320	500.2537	520.1335
520.7287	533.0465	534.2968
536.2244	546.8184	555.4645
558.3998	567.9708	570.6434
574.8489	592.0464	611.0992
630.0012	631.4580	632.0946
642.6828	651.5087	663.2054
673.9993	700.6428	702.0845
713.1417	717.0795	721.1664
731.3450	736.1819	744.8690
747.9933	760.7719	766.6654
768.3641	769.0400	770.5484
775.9684	779.0854	794.4158
795.7197	812.3287	821.6208
842.8266	844.9610	845.0787
859.6984	866.8552	868.3731
873.1791	880.4660	885.1704
886.6769	890.1056	891.6267
910.9762	917.6408	931.1015
936.0429	937.6463	938.2025
940.8924	944.0303	947.7121
949.3717	949.7944	955.0339
966.4398	976.7581	977.2381
981.4952	981.9592	989.4359
994.0486	1002.3685	1003.2756
1009.9125	1012.7603	1014.2074

1014.4911	1015.1404	1025.0155
1028.4610	1037.8320	1041.3727
1050.6117	1051.6904	1053.6806
1055.4453	1057.1362	1063.4409
1066.0297	1069.5389	1079.8991
1082.6670	1098.8322	1105.0461
1105.9447	1110.7204	1114.4707
1115.9752	1120.9460	1132.6067
1133.9060	1143.8958	1145.1466
1154.2066	1154.7644	1179.8890
1182.2792	1188.2526	1188.9107
1189.1779	1193.7912	1193.9249
1202.9698	1210.8151	1213.5179
1214.7916	1216.0188	1226.3083
1231.2368	1237.0959	1239.9739
1246.4819	1249.4966	1256.6933
1264.9395	1272.5863	1276.6097
1278.1177	1290.3309	1296.5028
1312.6055	1325.0904	1328.1278
1331.9784	1336.6126	1343.7130
1345.0544	1352.6881	1357.0751
1360.6937	1361.4985	1365.2676
1366.8630	1391.2109	1404.3609
1408.9575	1411.3533	1412.9023
1414.1739	1414.6034	1421.0250
1423.9988	1427.7037	1436.2225
1439.4081	1441.9984	1450.9447
1454.9119	1460.7088	1467.5827
1473.0471	1476.5811	1478.6652
1479.9620	1481.7330	1484.3202
1487.0744	1491.0123	1492.8790

1494.8823	1496.1479	1496.5410
1501.0682	1501.9028	1504.7847
1506.2206	1507.7150	1508.5416
1511.5377	1512.9419	1518.7840
1522.9189	1523.1253	1525.5721
1526.6370	1532.6832	1532.9557
1537.1069	1551.0089	1554.1222
1579.1904	1611.2445	1622.8219
1625.6121	1626.3108	1628.6344
1636.6972	1642.6155	1644.9374
1647.1391	1655.2956	1671.5994
1673.4607	1706.2301	1744.5227
2981.8883	2994.0195	3014.2859
3032.8822	3033.2139	3036.2900
3043.7726	3051.1974	3056.3350
3063.1344	3063.4601	3077.5375
3090.5183	3091.0257	3100.6608
3103.3804	3106.3965	3114.3453
3122.7926	3123.7043	3124.7102
3126.1585	3129.1728	3130.4284
3131.4319	3137.6015	3142.8118
3163.0772	3171.5389	3174.6306
3176.3664	3177.7373	3180.8232
3183.4688	3183.8284	3184.3397
3187.1611	3188.4341	3192.9893
3193.0626	3193.2360	3196.3303
3201.4553	3201.6691	3204.2019
3205.8482	3205.8935	3209.1280
3211.5866	3212.1752	3215.5377
3218.5184	3232.1206	3245.1184
3254.6009	3259.6209	3260.4495

## TS51SS

Zero-point correction= 0.989344

Thermal correction to Energy= 1.048531

Thermal correction to Enthalpy= 1.049476

Thermal correction to Gibbs Free Energy= 0.893599

Sum of electronic and zero-point Energies= -2988.810540

Sum of electronic and thermal Energies= -2988.751352

Sum of electronic and thermal Enthalpies= -2988.750408

Sum of electronic and thermal Free Energies= -2988.906285

### Cartesian coordinates

C	3.530636	-3.692008	1.095874
C	2.193918	-3.249626	0.887269
C	2.073857	-1.884444	0.417312
C	3.230295	-1.145199	0.084139
C	4.504987	-1.667819	0.288088
N	4.604579	-2.932907	0.813812
H	3.708042	-4.682117	1.492447
C	3.061503	0.195247	-0.558516
C	3.038014	0.276730	-1.987432
C	2.800468	1.320982	0.205168
C	3.245075	-0.857194	-2.823373
C	2.771557	1.542351	-2.604597
C	2.532132	2.565790	-0.418648
C	3.185151	-0.743480	-4.194724
H	3.439264	-1.823166	-2.370555
C	2.720078	1.624584	-4.022432
C	2.529700	2.676116	-1.786977
H	2.305318	3.427351	0.199889
C	2.919458	0.508317	-4.802316



H	3.339435	-1.620652	-4.815685
H	2.503388	2.586419	-4.476771
H	2.298433	3.625265	-2.259465
H	2.870160	0.581783	-5.884302
C	0.782212	-1.270772	0.345637
H	0.669938	-0.214333	0.151478
O	1.201203	-4.003561	1.134285
C	5.763033	-0.902852	-0.002234
H	5.510915	0.054909	-0.453364
H	6.324153	-0.698682	0.915580
H	6.423416	-1.439211	-0.690232
C	2.742469	1.209592	1.708721
O	3.719076	0.829685	2.370294
N	1.537380	1.534113	2.221712
C	1.234905	1.530276	3.650539
C	0.217326	0.406161	3.996193
O	0.806071	-0.686605	4.690063
C	0.812283	2.953284	4.141443
C	0.766960	2.957553	5.682109
H	0.028416	2.255566	6.080980
H	1.743283	2.694262	6.104407
H	0.500511	3.954805	6.047765
C	-0.560567	3.366766	3.573615
H	-0.797937	4.391375	3.879949
H	-0.575874	3.323741	2.480889
H	-1.365815	2.722205	3.942078
C	1.871848	3.974538	3.684415
H	1.885968	4.074843	2.595927
H	1.655998	4.960195	4.110029
H	2.875096	3.676498	4.008916
N	-0.317851	-1.952570	0.568650

C	-1.603501	-1.423970	0.484443
C	-2.656704	-2.389027	0.826364
O	-2.483784	-3.599842	0.909569
O	-3.831411	-1.742806	0.942158
C	-5.097640	-2.443452	1.234366
C	-5.430517	-3.409271	0.095234
H	-5.476361	-2.869930	-0.855815
H	-4.685778	-4.202197	0.021622
H	-6.410438	-3.860836	0.276806
C	-4.992283	-3.148325	2.588264
H	-4.687533	-2.435055	3.359893
H	-5.969732	-3.555769	2.862832
H	-4.267507	-3.961709	2.551144
C	-6.103261	-1.294237	1.287481
H	-7.104820	-1.683770	1.490128
H	-5.834835	-0.585755	2.075718
H	-6.119461	-0.753598	0.337468
P	-1.367363	1.646954	-0.808911
O	-0.708260	1.775833	0.564703
C	-3.169396	1.885161	-0.581859
C	-3.671893	2.162729	0.696738
C	-4.059848	1.743321	-1.657575
C	-5.046345	2.304373	0.896626
H	-2.976534	2.260112	1.524467
C	-5.433422	1.880920	-1.456044
H	-3.678727	1.520712	-2.650760
C	-5.927133	2.162933	-0.178322
H	-5.430172	2.519963	1.889419
H	-6.117907	1.767009	-2.291308
H	-6.996560	2.267965	-0.021619
C	-0.805362	2.970809	-1.917713

C	-0.538762	4.235194	-1.371733
C	-0.635030	2.759315	-3.291277
C	-0.106024	5.276497	-2.191633
H	-0.650277	4.391195	-0.302960
C	-0.200548	3.802836	-4.111204
H	-0.816890	1.772286	-3.702986
C	0.064349	5.060372	-3.563363
H	0.105484	6.251852	-1.763776
H	-0.060384	3.631654	-5.174335
H	0.405551	5.869872	-4.201822
N	-1.075967	0.251455	-1.621858
C	-1.837693	-0.853257	-1.423692
C	-1.437032	-2.069684	-2.185397
C	-0.146652	-2.172424	-2.726786
C	-2.325683	-3.144720	-2.333867
C	0.249976	-3.331845	-3.391793
H	0.529614	-1.331872	-2.628682
C	-1.931121	-4.301765	-3.004391
H	-3.327693	-3.072505	-1.922519
C	-0.639213	-4.401146	-3.531101
H	1.253047	-3.395911	-3.804261
H	-2.629887	-5.125678	-3.116294
H	-0.331534	-5.303891	-4.050839
H	-1.712889	-0.431050	0.904454
C	5.943728	-3.502654	1.078270
H	6.493051	-3.600459	0.141252
H	6.491421	-2.849708	1.757875
H	5.825745	-4.482637	1.533855
H	-2.921950	-0.745947	-1.296252
H	-0.176649	-2.969514	0.731942
H	2.169812	1.275046	4.157326

H	-0.558719	0.778386	4.667362
H	-0.281351	0.065939	3.076120
H	0.765856	1.716246	1.568076
C	1.587123	-1.544206	3.866142
H	0.970014	-2.035217	3.101131
H	2.412168	-1.013861	3.373407
H	2.006552	-2.315197	4.518135

Vibrational frequencies

-409.7558	9.6994	21.9314
26.2592	26.5680	29.4736
32.3488	33.3561	37.9105
39.8091	45.4827	45.9902
51.6686	54.3709	57.0531
62.9071	66.6979	68.0456
70.6332	75.3028	82.2937
84.0989	90.2183	91.6205
97.1541	102.9005	109.3348
114.9718	130.0161	131.4847
138.6886	140.5783	151.7926
156.9410	161.7137	165.1020
180.1249	185.0737	189.2292
194.6342	206.3802	222.7339
228.8685	231.0257	235.7619
238.7951	241.1765	245.9343
252.1521	257.0923	260.6093
265.5096	269.2552	274.8359
282.7733	288.3120	291.7648
303.0968	307.0029	317.1550
319.8662	327.5109	332.1298
338.0653	344.5904	360.6858

373.2843	376.4068	382.8978
390.2339	399.9608	401.1347
408.1833	409.4261	410.4169
419.0062	420.2523	424.5086
432.9855	438.0452	440.0469
442.7357	445.6078	458.8283
459.6655	465.5239	473.4279
479.3393	485.2097	497.9263
516.5061	520.1020	535.1059
536.2811	543.9649	550.4493
560.2337	572.4536	579.7638
582.8970	598.0802	614.9426
629.3966	629.6269	633.0426
642.2162	650.0047	666.3587
675.2447	698.1222	704.3368
708.4071	711.3888	715.9553
733.3238	747.0094	749.4587
750.3023	762.2023	763.4956
764.4893	769.1324	771.2864
773.7709	782.0645	795.7594
797.5880	811.9268	814.2185
846.2860	850.3473	851.6593
852.3691	865.6787	870.0109
870.7420	871.4591	884.7072
887.7756	891.0957	902.3403
906.6560	916.1365	932.0598
935.1095	939.1801	942.0270
943.8145	945.1438	945.2899
947.7689	954.1502	966.7901
969.8825	971.9883	977.0070
981.7181	987.8703	988.2160

989.1204	990.0076	1003.1931
1005.9936	1009.5372	1011.1959
1012.4058	1013.8356	1015.1164
1025.9339	1028.3087	1037.5680
1045.1934	1048.7479	1050.0030
1050.0976	1056.2095	1059.7134
1062.5083	1065.6320	1073.4126
1078.9115	1083.3629	1093.4295
1102.8070	1106.7730	1109.9670
1116.5105	1127.7139	1131.5418
1133.3496	1145.4513	1146.1126
1148.6491	1155.8471	1183.9934
1185.4950	1186.7962	1191.7070
1192.0491	1192.3670	1195.6259
1201.5690	1205.9230	1206.4532
1208.8039	1213.7533	1223.9916
1230.5841	1231.8734	1238.2667
1248.5343	1250.7854	1251.6490
1263.0613	1267.4451	1274.6192
1275.5540	1292.1435	1297.3447
1314.1072	1317.4024	1327.2702
1329.1398	1330.9969	1339.6639
1343.4125	1346.7767	1355.5603
1356.4574	1357.8280	1361.8303
1366.6562	1382.0712	1405.1790
1408.5555	1412.1039	1413.8301
1414.8607	1420.6680	1421.0542
1426.1361	1429.3746	1432.8825
1436.6454	1441.0329	1441.4914
1449.2114	1460.8309	1468.6089
1474.3555	1476.1084	1479.1964

1480.0818	1485.0627	1486.6483
1489.1844	1491.9577	1494.2837
1495.9802	1496.8931	1498.3669
1499.9089	1501.9534	1503.0892
1507.4478	1507.7876	1509.8180
1512.5738	1513.2400	1519.4509
1521.8576	1522.3466	1526.2789
1528.6035	1532.7556	1533.0845
1534.5153	1547.4414	1554.5888
1582.7557	1614.8775	1624.8827
1625.5659	1626.6426	1634.2186
1636.4012	1643.6948	1645.0255
1648.9109	1655.1662	1670.0611
1673.1409	1712.1363	1738.5703
3004.7296	3013.2146	3035.2116
3036.7615	3038.7061	3043.2606
3052.6137	3054.3584	3054.7661
3060.4448	3079.7366	3089.8821
3093.0084	3101.3437	3104.1912
3108.8058	3110.9915	3112.4725
3118.5442	3122.5529	3123.3560
3124.8384	3126.6485	3129.3079
3136.7067	3139.1484	3154.7257
3161.9302	3165.5404	3173.1431
3177.8413	3178.4620	3178.6279
3182.1147	3184.6424	3186.8019
3187.8737	3189.3814	3194.5282
3195.5803	3197.7774	3199.5770
3199.7669	3200.9860	3202.8290
3203.8761	3206.3764	3207.1706
3209.1852	3210.1041	3212.6275

3214.1766	3215.1573	3226.6948
3253.5953	3271.2153	3312.8884

### TS52RR

Zero-point correction= 0.989907

Thermal correction to Energy= 1.048428

Thermal correction to Enthalpy= 1.049372

Thermal correction to Gibbs Free Energy= 0.896227

Sum of electronic and zero-point Energies= -2988.801263

Sum of electronic and thermal Energies= -2988.742741

Sum of electronic and thermal Enthalpies= -2988.741797

Sum of electronic and thermal Free Energies= -2988.894942

### Cartesian coordinates

C	-2.032996	-3.792613	-2.360835
C	-0.910884	-3.126621	-1.811029
C	-1.161046	-2.396440	-0.579627
C	-2.432952	-2.475181	0.030472
C	-3.456033	-3.249716	-0.528479
N	-3.222897	-3.855372	-1.734181
H	-1.934368	-4.311204	-3.304233
C	-2.713660	-1.789633	1.334962
C	-2.258364	-2.402110	2.549034
C	-3.455049	-0.614141	1.389051
C	-1.482075	-3.595648	2.558776
C	-2.600959	-1.804267	3.806504
C	-3.816240	-0.056758	2.643568
C	-1.050633	-4.149906	3.743470
H	-1.226335	-4.070197	1.618484
C	-2.141069	-2.402774	5.010337
C	-3.405593	-0.635441	3.818198



H	-4.429442	0.837699	2.665390
C	-1.378576	-3.548307	4.982589
H	-0.454931	-5.057459	3.728024
H	-2.404433	-1.936979	5.955877
H	-3.690407	-0.201224	4.772222
H	-1.030226	-3.995899	5.908246
C	-0.077300	-1.671792	0.030670
H	-0.219543	-1.029860	0.895352
O	0.225298	-3.187890	-2.389145
C	-4.792362	-3.464970	0.121248
H	-4.783835	-3.058534	1.129762
H	-5.582822	-2.948948	-0.429273
H	-5.039595	-4.528440	0.186587
C	-3.901340	0.046030	0.103450
O	-4.622368	-0.574603	-0.689723
N	-3.450337	1.309491	-0.133057
C	-3.498041	1.794876	-1.527633
C	-2.052608	1.921899	-2.064110
H	-2.101403	2.014368	-3.156890
H	-1.559857	2.828044	-1.693241
O	-1.327720	0.760050	-1.699224
H	-0.458207	1.009209	-1.296700
C	-4.421816	3.030900	-1.744476
C	-4.451708	3.366493	-3.250657
H	-3.493470	3.762624	-3.600641
H	-4.694728	2.482761	-3.851512
H	-5.213899	4.127235	-3.450348
C	-3.971726	4.283866	-0.967672
H	-4.615515	5.130014	-1.232086
H	-4.048213	4.141338	0.113405
H	-2.941432	4.570806	-1.198617

C	-5.844619	2.650196	-1.291685
H	-5.857654	2.383170	-0.230668
H	-6.532342	3.489510	-1.442098
H	-6.221850	1.791931	-1.857199
N	1.143022	-1.833809	-0.433174
C	2.290790	-1.197303	-0.003053
C	3.539466	-1.867410	-0.387722
O	3.623673	-2.744096	-1.239186
O	4.569708	-1.307339	0.278283
C	5.953479	-1.808081	0.158251
C	6.473576	-1.598807	-1.265294
H	5.868623	-2.146834	-1.987355
H	6.463182	-0.536466	-1.523751
H	7.507816	-1.951424	-1.325577
C	6.709065	-0.924661	1.150485
H	6.316894	-1.059928	2.162217
H	7.771568	-1.183667	1.147095
H	6.601439	0.129964	0.882957
C	6.003475	-3.277995	0.582569
H	7.046148	-3.604943	0.635457
H	5.553988	-3.399067	1.572748
H	5.471351	-3.910794	-0.128089
P	1.153558	1.828147	0.989709
O	0.426872	0.947162	1.991611
C	0.395410	3.477680	0.858259
C	-0.208793	4.033094	1.995862
C	0.401650	4.200027	-0.343198
C	-0.810444	5.289399	1.928940
H	-0.231804	3.463954	2.920184
C	-0.202232	5.458075	-0.408540
H	0.858126	3.763687	-1.225829

C	-0.810710	6.001449	0.725538
H	-1.286418	5.709639	2.809759
H	-0.204086	6.008566	-1.344467
H	-1.286951	6.975765	0.671617
C	2.863395	2.136298	1.573359
C	3.344978	1.412110	2.671666
C	3.714256	3.038066	0.915129
C	4.660071	1.585627	3.107756
H	2.681052	0.717282	3.176392
C	5.028953	3.207760	1.348562
H	3.348870	3.605281	0.063322
C	5.502963	2.480488	2.445250
H	5.027298	1.020669	3.959243
H	5.683199	3.904773	0.833599
H	6.527072	2.612310	2.781317
N	1.201310	1.266500	-0.580325
C	2.302624	0.594172	-0.992307
C	2.443538	0.200339	-2.419637
C	1.350992	-0.139580	-3.232990
C	3.736545	0.147116	-2.964643
C	1.558879	-0.522338	-4.558524
H	0.344601	-0.098626	-2.836300
C	3.941481	-0.232843	-4.289537
H	4.584637	0.410819	-2.340913
C	2.849155	-0.570965	-5.092481
H	0.706114	-0.787553	-5.177046
H	4.949219	-0.263153	-4.693325
H	3.002471	-0.869347	-6.125509
H	2.245615	-0.791034	1.000471
C	-4.304585	-4.623715	-2.387772
H	-4.543180	-5.506263	-1.792790

H	-5.190994	-3.997624	-2.486394
H	-3.968162	-4.933011	-3.374368
H	3.266407	0.848204	-0.541905
H	1.174227	-2.430871	-1.302888
H	-3.956471	0.972962	-2.080787
C	-2.576132	2.002959	0.816500
H	-2.063947	2.806776	0.301552
H	-3.146647	2.456996	1.630959
H	-1.816674	1.343431	1.235817

Vibrational frequencies

-383.4539	13.0406	21.2324
22.6932	28.7746	36.1657
36.6150	38.7422	42.1792
43.2628	45.8612	51.0469
52.9743	54.1606	57.5776
62.8945	67.6934	69.1382
71.1532	75.2186	78.5808
86.5612	92.6555	100.0404
108.3986	112.2260	120.0123
134.7114	139.3494	144.7246
152.5482	154.3742	162.7056
163.8943	183.2841	184.6731
189.3142	191.1350	198.4097
209.2429	211.1463	222.2679
226.1199	233.9735	241.4516
242.1084	244.6048	251.4821
258.0297	261.0418	264.4832
275.8846	283.8153	290.8299
296.8679	302.6298	306.6292
309.8784	315.0122	326.2634

333.5603	335.2574	344.3076
350.2122	353.2990	362.7884
364.3026	380.6994	386.5190
393.3022	403.9253	405.7570
408.6406	410.1969	413.8495
414.1240	416.7393	422.8462
424.5413	427.4021	435.0966
444.0637	448.7294	452.5584
458.2712	469.3127	474.3224
485.6110	493.2106	499.3289
521.8101	533.3216	533.9936
544.3503	552.7460	556.3627
557.6799	569.7114	580.3638
587.7645	606.8474	611.6379
629.4995	629.5470	632.7588
643.0012	656.7682	662.0954
671.8559	700.1492	702.0579
710.8924	711.5719	714.2882
728.7034	731.7438	739.5799
747.9796	750.1536	761.5918
762.5774	765.3950	768.8544
770.5152	773.0680	780.3952
789.6402	795.8067	796.3634
809.6558	824.5856	842.2299
842.5698	852.1707	866.0695
867.2285	871.8729	875.4401
886.4621	887.9500	889.1813
910.1113	922.3664	937.1279
939.3434	940.6806	942.9585
943.8295	945.4987	947.2814
950.3215	961.9127	968.9299

970.6576	979.0036	980.9642
986.9215	987.0225	992.4394
995.6559	1004.0450	1006.0493
1012.6625	1012.7946	1013.8258
1014.5637	1015.1789	1016.6220
1027.7908	1032.6325	1035.8802
1049.2662	1050.4213	1057.0498
1058.1053	1058.4684	1064.8540
1065.3401	1070.1016	1080.4872
1089.5388	1094.6703	1096.5037
1100.5990	1103.6851	1108.3209
1118.4872	1120.8155	1126.9983
1131.7399	1135.3404	1145.1769
1145.7372	1153.9931	1162.7114
1177.7265	1183.1222	1191.5899
1192.0623	1192.4920	1193.5971
1207.7526	1207.9709	1209.8602
1214.2484	1219.5179	1224.6270
1227.7208	1236.9892	1237.8884
1245.8353	1248.3006	1256.9349
1262.7179	1274.4263	1275.7095
1281.1638	1287.7501	1290.2480
1297.5831	1319.8120	1327.9144
1329.7406	1335.8424	1343.5374
1350.3409	1352.3386	1356.0194
1357.0288	1359.3156	1372.0004
1380.2350	1397.1908	1403.2865
1407.4338	1409.6776	1413.5213
1413.6440	1416.7288	1419.8460
1423.2450	1428.0810	1436.4217
1436.6991	1439.2335	1446.9849

1454.2243	1459.8721	1466.4354
1473.8228	1475.4186	1476.3328
1480.6338	1481.8847	1484.1207
1486.7395	1491.7942	1493.9858
1494.1797	1496.1991	1496.3561
1498.1158	1501.4367	1504.4281
1509.8699	1510.4377	1511.5667
1512.2268	1515.7445	1516.7884
1521.4103	1523.2500	1524.2522
1528.4378	1531.2340	1538.6290
1543.0186	1547.6795	1551.0935
1554.5530	1575.8015	1608.1725
1624.2623	1624.9655	1626.3204
1636.0588	1643.5672	1643.9318
1646.4679	1656.5881	1671.4821
1681.0422	1692.4190	1740.9833
2880.2583	3021.3556	3033.0897
3037.6188	3045.8320	3052.3540
3055.1187	3061.0530	3063.8320
3065.4701	3070.7613	3071.3200
3090.0264	3101.9998	3106.6511
3109.2093	3111.4175	3112.8613
3118.6374	3124.6970	3125.9908
3129.7810	3130.8680	3134.0531
3138.0482	3150.1772	3163.1074
3170.7533	3174.0813	3178.6155
3180.2107	3183.4297	3184.2846
3186.2001	3186.6158	3187.9052
3188.1752	3191.5046	3193.1299
3195.7535	3199.2206	3199.3976
3199.8796	3200.7309	3203.9790

3206.4738	3207.3696	3208.6768
3209.2107	3210.6751	3211.0512
3212.6470	3220.3219	3230.1012
3230.2648	3255.9527	3307.4710

## TS52SS

Zero-point correction= 0.989143

Thermal correction to Energy= 1.048398

Thermal correction to Enthalpy= 1.049342

Thermal correction to Gibbs Free Energy= 0.894470

Sum of electronic and zero-point Energies= -2988.799270

Sum of electronic and thermal Energies= -2988.740015

Sum of electronic and thermal Enthalpies= -2988.739071

Sum of electronic and thermal Free Energies= -2988.893943

## Cartesian coordinates

C	-3.075640	-1.233286	3.533297
C	-1.899999	-1.404613	2.753524
C	-1.745482	-0.456399	1.665180
C	-2.705354	0.558605	1.473222
C	-3.825706	0.665806	2.299453
N	-3.972031	-0.254983	3.304875
H	-3.271544	-1.908930	4.354333
C	-2.538485	1.539162	0.354369
C	-1.870139	2.780419	0.586344
C	-3.031580	1.238085	-0.904395
C	-1.305499	3.118126	1.847730
C	-1.765679	3.721869	-0.489181
C	-2.920230	2.173114	-1.964785
C	-0.667464	4.324518	2.031876
H	-1.376581	2.409533	2.666194



C	-1.109472	4.960310	-0.260590
C	-2.309197	3.386775	-1.758057
H	-3.320634	1.916464	-2.940528
C	-0.569209	5.255701	0.969665
H	-0.232204	4.562859	2.997564
H	-1.018207	5.661115	-1.083804
H	-2.224661	4.103504	-2.569823
H	-0.051734	6.196466	1.124139
C	-0.613586	-0.557176	0.788582
H	-0.473216	0.117339	-0.046972
O	-1.072623	-2.335304	3.013293
C	-4.892757	1.705518	2.116314
H	-4.594204	2.405898	1.339650
H	-5.835048	1.248277	1.799144
H	-5.075461	2.272375	3.033821
C	-3.787346	-0.055341	-1.086218
O	-4.917379	-0.151425	-0.585140
N	-3.180897	-1.066545	-1.765653
C	-3.881208	-2.365649	-1.820454
C	-2.966022	-3.487051	-1.302941
O	-2.361861	-3.163608	-0.055013
H	-3.059242	-2.898280	0.560051
C	-4.578074	-2.677178	-3.192614
C	-3.637461	-3.337307	-4.221463
H	-2.754761	-2.727343	-4.429062
H	-3.296576	-4.323392	-3.890779
H	-4.170065	-3.478189	-5.168029
C	-5.141404	-1.370128	-3.781193
H	-5.752859	-1.587633	-4.663218
H	-5.763145	-0.848161	-3.047733
H	-4.340834	-0.690088	-4.087872

C	-5.755692	-3.638002	-2.919924
H	-6.490741	-3.180823	-2.248608
H	-6.265462	-3.887170	-3.856530
H	-5.422054	-4.577151	-2.467259
N	0.286324	-1.493503	0.974135
C	1.497299	-1.573083	0.298783
C	2.243311	-2.814547	0.559295
O	2.009313	-3.581054	1.485736
O	3.260635	-2.914715	-0.316849
C	4.228599	-4.029096	-0.283770
C	5.018591	-3.991280	1.025708
H	5.525950	-3.027849	1.133530
H	4.363637	-4.149686	1.882739
H	5.780343	-4.776572	1.012672
C	3.494279	-5.356711	-0.484793
H	2.881966	-5.313509	-1.390470
H	4.226122	-6.161406	-0.602369
H	2.852468	-5.584063	0.366416
C	5.131687	-3.714959	-1.475768
H	5.919771	-4.469000	-1.555912
H	4.554467	-3.710569	-2.404518
H	5.593985	-2.731273	-1.358929
P	1.918364	1.441665	-1.057291
O	0.732233	0.904634	-1.846083
C	3.466275	0.839208	-1.841124
C	3.385697	-0.083971	-2.891953
C	4.727793	1.227753	-1.364005
C	4.547475	-0.608424	-3.462185
H	2.406535	-0.383918	-3.251925
C	5.888748	0.702031	-1.931269
H	4.801295	1.941902	-0.548098

C	5.799297	-0.217202	-2.981804
H	4.476701	-1.324194	-4.275931
H	6.861333	1.006466	-1.555924
H	6.703231	-0.627206	-3.422490
C	2.006054	3.256564	-1.142590
C	1.507423	3.900421	-2.283942
C	2.605755	4.016365	-0.129269
C	1.619486	5.284529	-2.416697
H	1.021094	3.312755	-3.056438
C	2.716557	5.401409	-0.262642
H	2.968540	3.519432	0.764771
C	2.228328	6.035770	-1.407484
H	1.228464	5.777568	-3.301909
H	3.178281	5.985504	0.528051
H	2.314771	7.113577	-1.509896
N	1.951774	1.089009	0.551603
C	2.544016	-0.048768	0.995061
C	2.523671	-0.262687	2.472222
C	1.561132	0.374009	3.270356
C	3.439354	-1.134237	3.077791
C	1.507660	0.129428	4.642154
H	0.871651	1.065114	2.798562
C	3.392067	-1.372865	4.451156
H	4.191212	-1.625930	2.468705
C	2.421147	-0.745843	5.237126
H	0.754129	0.623782	5.248984
H	4.110918	-2.047471	4.907152
H	2.380292	-0.934203	6.306047
H	1.461418	-1.248128	-0.734886
C	-5.159019	-0.187943	4.184432
H	-5.154384	0.751837	4.737399

H	-6.065527	-0.254987	3.582753
H	-5.125940	-1.019906	4.883380
H	3.469225	-0.396085	0.517179
H	0.102851	-2.102650	1.802960
H	-4.689601	-2.252884	-1.093906
H	-3.553294	-4.412986	-1.238517
H	-2.137576	-3.680295	-1.988136
C	-1.846919	-0.952645	-2.352257
H	-1.185294	-1.715037	-1.935577
H	-1.892522	-1.074040	-3.437831
H	-1.399935	0.013564	-2.136864

#### Vibrational frequencies

-398.9800	15.5202	20.2776
25.1402	28.2242	29.8805
32.8242	40.1330	41.1281
45.3651	47.4605	49.7338
50.6858	55.1827	61.6258
64.1316	66.8199	70.3441
71.6431	76.5058	78.8745
85.3337	89.6640	94.4249
107.1855	112.0679	119.6438
125.2395	126.1422	135.3614
139.5474	147.1992	148.7801
153.2792	157.6365	163.2917
176.2372	186.6846	187.0120
197.7009	203.1436	223.4413
226.5169	233.0152	234.8700
243.7730	244.2866	247.6408
255.3195	256.7644	261.0824
271.4056	273.5251	284.3176

293.1956	298.9223	307.5160
309.3084	315.0501	318.3763
322.5302	331.0039	333.4589
341.7231	344.8848	348.7985
363.7548	365.6601	377.6759
385.2217	391.4874	401.1924
404.5977	407.1102	408.8880
409.1601	410.8566	422.5730
425.6980	428.5888	431.5149
438.2116	445.9309	447.9721
455.1912	459.7586	466.6090
473.2064	484.5889	487.1620
499.0380	521.1946	533.8082
534.7991	539.7308	552.5704
553.9761	558.7447	567.6002
580.2941	587.3822	603.6925
607.9972	629.8818	630.2681
633.3387	644.3944	655.6269
663.1940	671.3310	702.5112
703.5611	708.5304	712.5408
718.4255	721.9480	731.3924
743.6882	748.0670	750.4897
762.2665	762.7534	767.0059
768.2287	770.5045	780.1927
782.5824	793.4088	797.7935
810.5125	823.6201	846.0276
847.5399	847.7475	866.6169
870.6834	872.0678	872.7726
880.9942	886.0715	889.0943
907.1453	922.7367	935.3219
936.1481	939.9528	941.1635

942.9253	944.8632	948.3141
949.9843	961.2556	966.8633
969.2838	975.1004	977.3588
984.1594	987.2265	989.9546
990.3679	999.7810	1006.5070
1008.5464	1010.8087	1012.6862
1013.0500	1013.8204	1015.3653
1023.1830	1033.0969	1040.1289
1049.4198	1050.7360	1053.2581
1055.1024	1058.2873	1064.4017
1065.4968	1072.5434	1073.8534
1078.8813	1080.5173	1097.7899
1098.8118	1102.0969	1108.1556
1113.5231	1115.4853	1129.7621
1134.5803	1136.4153	1146.4700
1154.5604	1154.9010	1160.4785
1182.5354	1184.3992	1188.5047
1189.7865	1191.0219	1191.1144
1193.6002	1203.9771	1204.9381
1205.7438	1208.9533	1216.1051
1230.0027	1232.3201	1237.3899
1246.7978	1249.1333	1256.6946
1264.3840	1266.8932	1269.8773
1275.2662	1275.8834	1291.4088
1298.3851	1309.4389	1326.1716
1328.0843	1329.3079	1340.0724
1351.9580	1353.6322	1355.2369
1357.9191	1362.2052	1366.3323
1387.4293	1396.8048	1406.1453
1410.0183	1411.1923	1415.1497
1416.9073	1417.5314	1421.5638

1428.0042	1431.3103	1435.9258
1438.0293	1440.3450	1440.8054
1445.9764	1455.1877	1460.0025
1469.4720	1473.6070	1476.0560
1480.7824	1481.4077	1484.2756
1488.6179	1488.8553	1492.9450
1495.2648	1495.8387	1497.0057
1502.0233	1502.2088	1503.3134
1504.8564	1507.8535	1509.1844
1510.1074	1514.0985	1518.2446
1522.2282	1522.4695	1523.1689
1525.6863	1531.4166	1534.3370
1535.2698	1535.3091	1550.6013
1555.8653	1580.7023	1615.0158
1624.7660	1626.8837	1632.8883
1635.4597	1643.5948	1645.4456
1645.6098	1656.1922	1673.2105
1676.0160	1682.8226	1742.5123
3027.2519	3030.0767	3036.1315
3041.6268	3048.6265	3052.3298
3053.8706	3055.1025	3059.9128
3059.9914	3063.0731	3089.5635
3092.6000	3106.2620	3108.6361
3111.6718	3114.2193	3117.0409
3119.4435	3123.2477	3125.0233
3125.5163	3127.9433	3134.0789
3135.9141	3138.4941	3163.5471
3166.2009	3176.3216	3177.2747
3177.3776	3179.4108	3184.0531
3186.0044	3186.4174	3186.5207
3188.0319	3189.0952	3193.5115

3195.2875	3197.4806	3199.5193
3199.8123	3202.9081	3203.6654
3203.8974	3204.0734	3204.3275
3207.5853	3209.2084	3209.6539
3210.4277	3217.0371	3217.9422
3226.4027	3255.2179	3808.8985