SUPPORTING INFORMATION FOR

Insights into Organocatalytic Arylation of Azonaphthalenes with α-Chloroaldehydes: General Mechanism and Origin of the Selectivities

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Part 1: Computational details

All the calculations involved in the reaction were performed with the Gaussian 09 suite of programs by using density functional theory,[1] which has been identified to be a powerful and widely used method for exploring the mechanisms of organic, biological as well as transition metal-catalyzed reactions. The solution-phase structure optimization of all the stationary points was carried out at M06-2X/6-31G(d, p) level in THF solvent using the integral equation formalism polarizable continuum model (IEF-PCM). The M06-2X/6-31G(d, p) harmonic frequencies were performed at 298.15 k and 1 atm to provide the thermal corrections for Gibbs free energies and make sure that the local minima had no imaginary frequencies, while the transition states had one and only one imaginary frequency. Atom-in-molecule (AIM) quantitative analysis was plotted by using Multiwfn,[2] and the computed 3D-structures were rendered using the CYLView software.[3] Moreover, we further refined the energy by employing the single-point energy calculations at the M06-2X/6-31++G (2df, 2pd)//IEF-PCM$_{THF}$ level based on the M06-2X/6-31G(d, p)//IEF-PCM$_{THF}$ optimized structures. The energies discussed in this work were obtained by the addition of the thermal correction at the M06-2X/6-31G(d, p)//IEF-PCM$_{THF}$ level to the corresponding single-point energy at the M06-2X/6-31++G (2df, 2pd)//IEF-PCM$_{THF}$ level.

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:

$$\frac{[R]}{[S]} = \frac{\exp\left(-\Delta G^{\ddagger}_{[R]} / RT\right)}{\exp\left(-\Delta G^{\ddagger}_{[S]} / RT\right)} = \exp\left(\Delta\Delta G^{\ddagger} / RT\right) \qquad (1)$$

$$ee = \frac{[R]-[S]}{[R]+[S]} \times 100\% = \frac{\frac{[R]}{[S]}-1}{\frac{[R]}{[S]}+1} \times 100\% \qquad (2)$$

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

For analyzing the local nucleophilicity and electrophilicity, we have also performed the Parr function analysis,[4] Pioneered by Domingo and coworkers, the nucleophilic (P_k^-) and electrophilc (P_k^+) Parr functions which allow for the characterization of the nucleophilic and electrophilic sites

of a molecule, can be obtained through the analysis of Mulliken atomic spin density (ASD) of the corresponding radical cations (RC) or anions (RA) of the studies molecules, separately. According to Domingo's definition, the Parr functions can be expressed by the following equations:

$$P^{-}(r) = \rho_S^{rc}(r) \; for \; the \; electrophilic \; attacks \qquad (3)$$

$$P^{+}(r) = \rho_S^{ra}(r) \; for \; the \; nucleophilic \; attacks \qquad (4)$$

where $\rho_S^{rc}(r)$ is the ASD of the radical cation and $\rho_S^{ra}(r)$ is the ASD of the radical anion. Each ASD condensed at the different atoms of the radical cation and radical anion provides the local nucleophilic P_k^- and electrophilic P_k^+ Parr functions of the neutral system, respectively.

For the global reactivity index (GRI) analysis, the relevant parameters of GRI, i.e., electrophilicity index ω[5], electronic chemical potential μ, chemical hardness η, one-electron energies of the frontier molecular orbital HOMO (E_L) and LUMO (E_H), The HOMO energies obtained within the Kohn−Sham scheme,[6] nucleophilicity index N[7] was generally utilized to judge the nucleophilicity character.

Part 2: The possible proton transfer processes for the formation of the Breslow intermediate

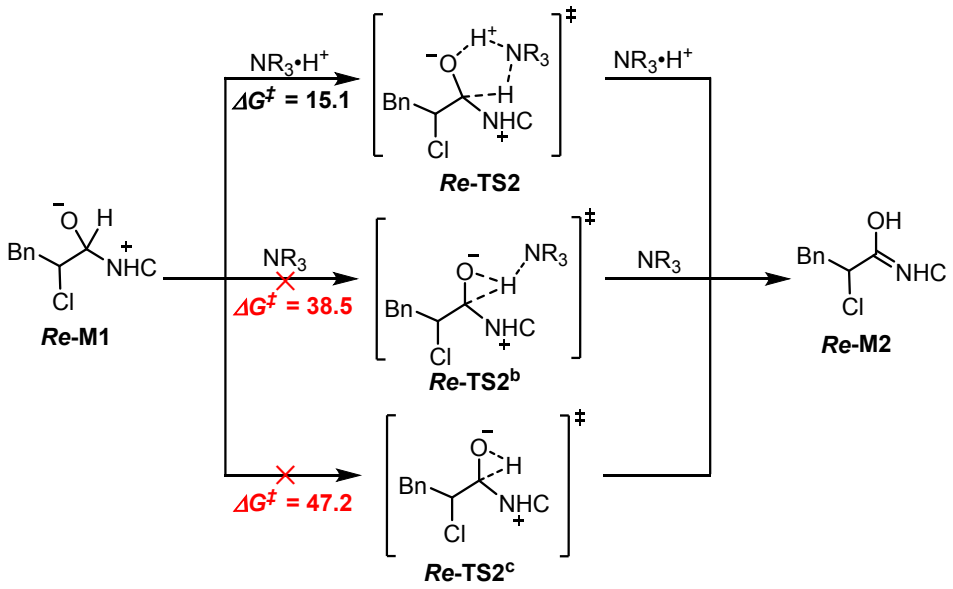


Fig. S1. The possible proton transfer processes for the formation of the Breslow intermediate (NR_3=DIPEA, unit: kcal/mol)

Part 3: The possible nucleophilic additions of R2 by M4

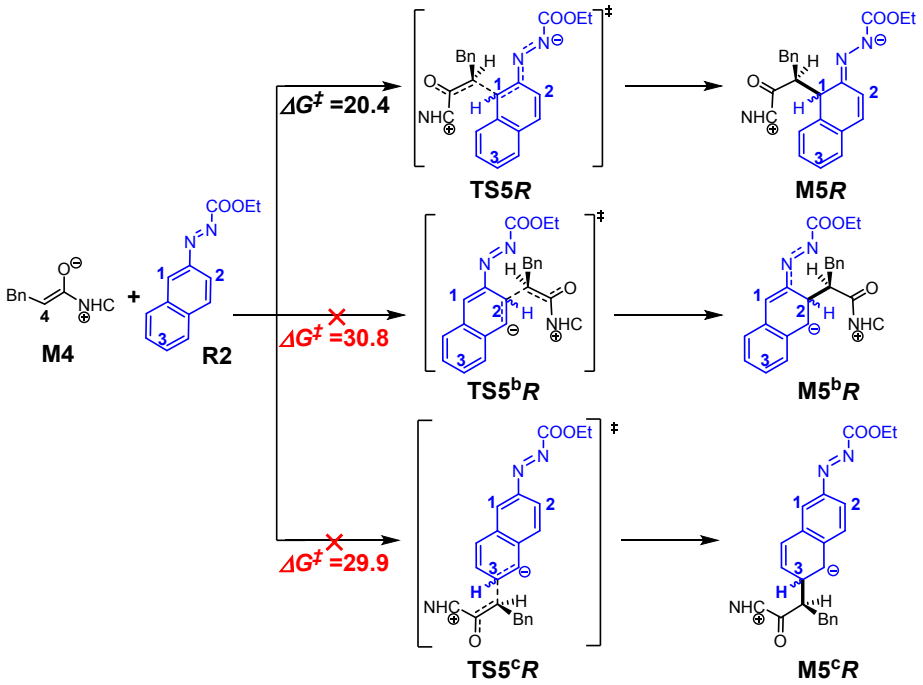


Fig. S2. The possible nucleophilic additions of **R2** by **M4** (unit: kcal/mol)

As a general rule, β-substituted naphthalene compounds have three possible reaction sites. Therefore, three possible pathways of nucleophilic addition of **R2** were studied as shown in **Figure S2**. The nucleophilic addition energy barriers of reaction sites C1, C2 and C3 correspond to **TS5*R*** (20.4 kcal/mol), **TS5^{b}*R*** (30.8 kcal/mol), **TS5^{c}*R*** (29.9 kcal/mol), which indicates that reaction site C4 is the best reaction site of **R2** to be electrophilically attacked by **M4**. Additionally, the possible reactive sites have also been predicted by using the Parr function, one can find that the electrophilic Parr function (P_k^+) values of the C1 atom, C2 atom and C3 atom in **R2** are -0.058, 0.042 and 0.031, while the nucleophilic Parr function (P_k^-) values of those atoms are 0.177, 0.065 and 0.087, separately. This phenomenon shows that these reaction sites are nucleophilic and the nucleophilicity of the C1 atom is strongest. Similarly, by comparing the P_k^+(0.654) and P_k^-(0.159) of C4 atom in **M4**, it can conclude that reaction site of **M4** is electrophilic.

Part 4: Comparison of different configurations of TS5s

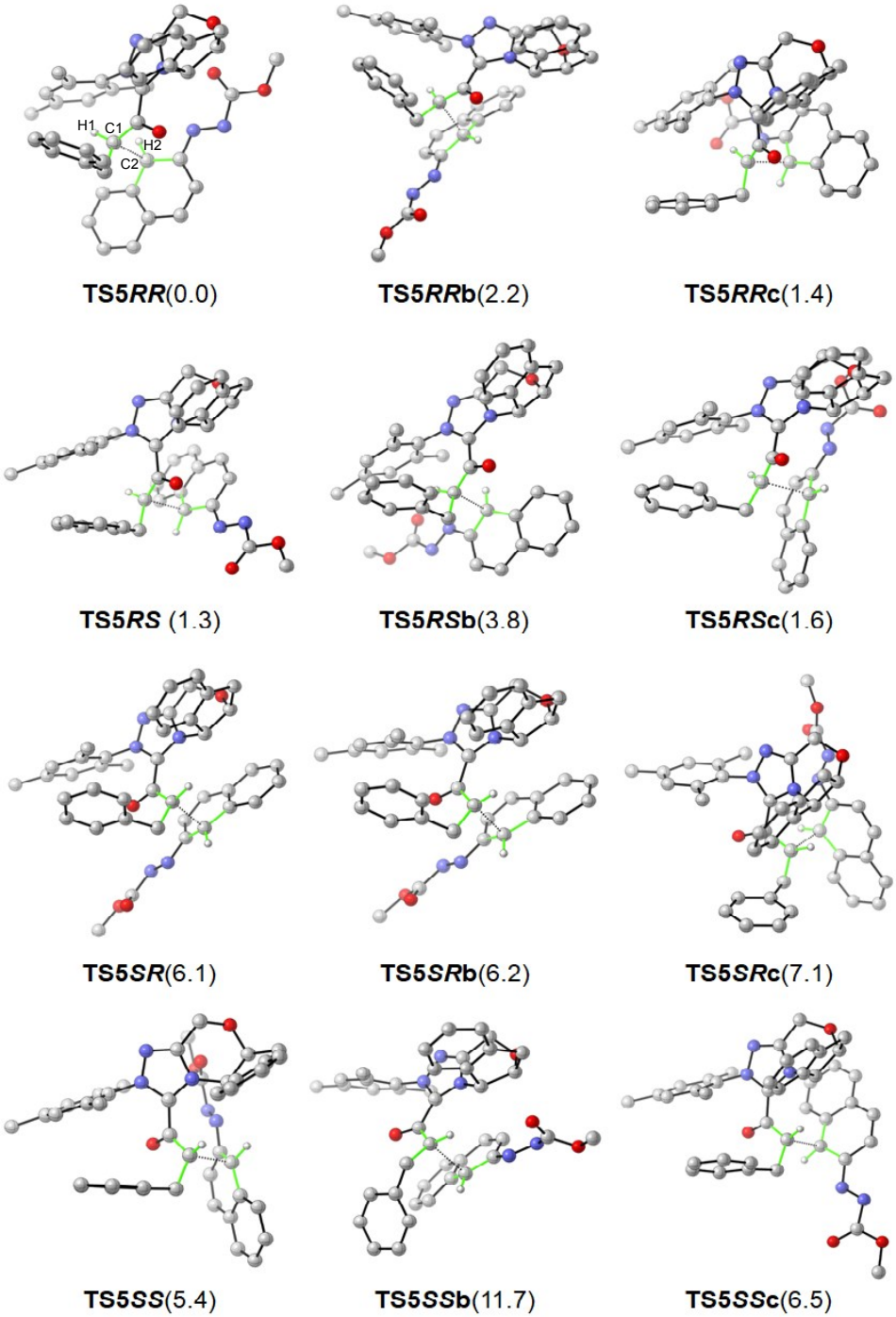


Fig. S3. Comparison of relative Gibbs free energies ($\Delta\Delta G$) at M06-2X/6-31G(d, p)//IEF-PCM$_{THF}$ level of different configurations of **TS5**s(unit: kcal/mol)

Part 5: AIM analysis for transition state TS5*R* and TS5*S*

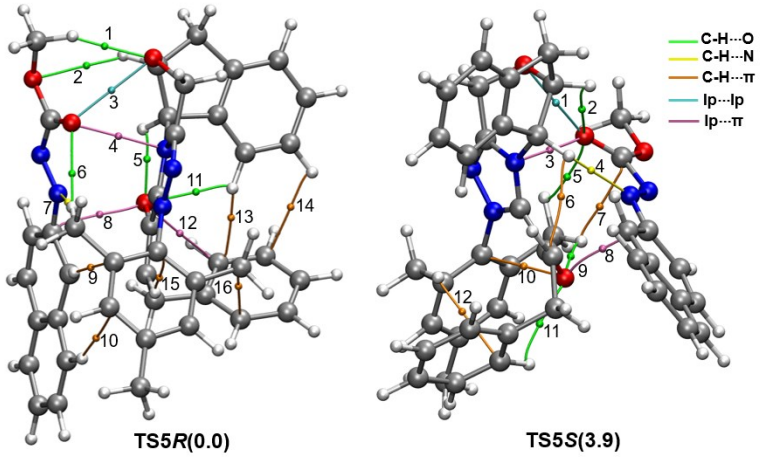


Fig. S4 Bond critical points along the bond paths for topological analysis of **TS5*R*** and **TS5*S*** (unit: kcal/mol)

Table S1 Summary of distances, type of interactions, electron densities (ρ_{bcp}), Lagrangian kinetic energies (G_b), potential energy densities (V_b), energy densities (H_b), Laplacian of electron densities (∇^2_ρ) at the bond critical points (BCPs) along the bond paths in **TS5*R*** and **TS5*S*** (the bond lengths are in Å, energies are in a.u.)

BCP indexes	Type of interactions	Distances	ρ_{bcp}*10^{-2}	G_b*10^{-2}	V_b*10^{-2}	H_b*10^{-3}	∇^2_ρ*10^{-1}
			TS5*R*				
1	C-H···O	2.40	1.0814	0.8584	-0.8209	0.3750	0.3583
2	C-H···O	2.70	0.6427	0.5366	-0.4448	0.9176	0.2513
3	LP···lp	2.99	0.9082	0.7841	-0.7533	0.3070	0.3259
4	lp···π	2.90	1.1452	0.8824	-0.8389	0.4350	0.3704
5	C-H···O	2.13	2.2607	1.9304	-1.8447	0.8569	0.8064
6	C-H···O	2.57	0.8211	0.6343	-0.5576	0.7675	0.2844
7	C-H···N	2.52	1.0964	0.7154	-0.6712	0.4411	0.3038
8	lp···π	2.88	1.4036	1.1019	-0.9564	1.4550	0.4990
9	C-H···π	2.64	0.7916	0.5448	-0.4356	1.0916	0.2616
10	C-H···π	3.32	0.2524	0.1388	-0.0957	0.4309	0.0728
11	C-H···O	2.53	0.9847	0.7727	-0.6656	1.0711	0.3519

12	lp···π	3.14	0.8086	0.6374	-0.5284	1.0902	0.2986
13	C-H···π	2.79	0.6616	0.4078	-0.3127	0.9505	0.2011
14	C-H···π	3.00	0.4586	0.2837	-0.2041	0.7960	0.1453
15	C-H···π	2.46	1.4028	0.9951	-0.8224	1.7278	0.4672
16	C-H···π	2.89	0.5389	0.3206	-0.2412	0.7948	0.1601
				TS5*S*			
1	lp···lp	3.01	0.7999	0.7302	-0.6801	0.5005	0.3121
2	C-H···O	2.61	0.8480	0.7147	-0.5839	1.3073	0.3382
3	lp···π	2.87	1.2041	0.9799	-0.9130	0.6687	0.4187
4	C-H···N	2.68	0.8930	0.6017	-0.5171	0.8454	0.2745
5	C-H···O	2.68	0.7602	0.5856	-0.4641	1.2154	0.2829
6	C-H···π	2.96	0.7647	0.5491	-0.4226	1.2648	0.2702
7	C-H···π	2.67	0.7489	0.5582	-0.4013	1.5697	0.2861
8	lp···π	3.26	1.3805	1.1236	-0.9641	1.5941	0.5132
9	C-H···O	2.53	0.9640	0.7620	-0.6727	0.8925	0.3405
10	C-H···π	2.85	1.3535	1.0761	-0.9871	0.8905	0.4661
11	C-H···O	2.65	0.7936	0.6258	-0.5087	1.1708	0.2972
12	C-H···π	2.89	0.6358	0.4396	-0.3450	0.9462	0.2137

Part 6: The relative Gibbs free energy profiles for all the possible pathways involved in the two RC-first and two PT-first mechanisms

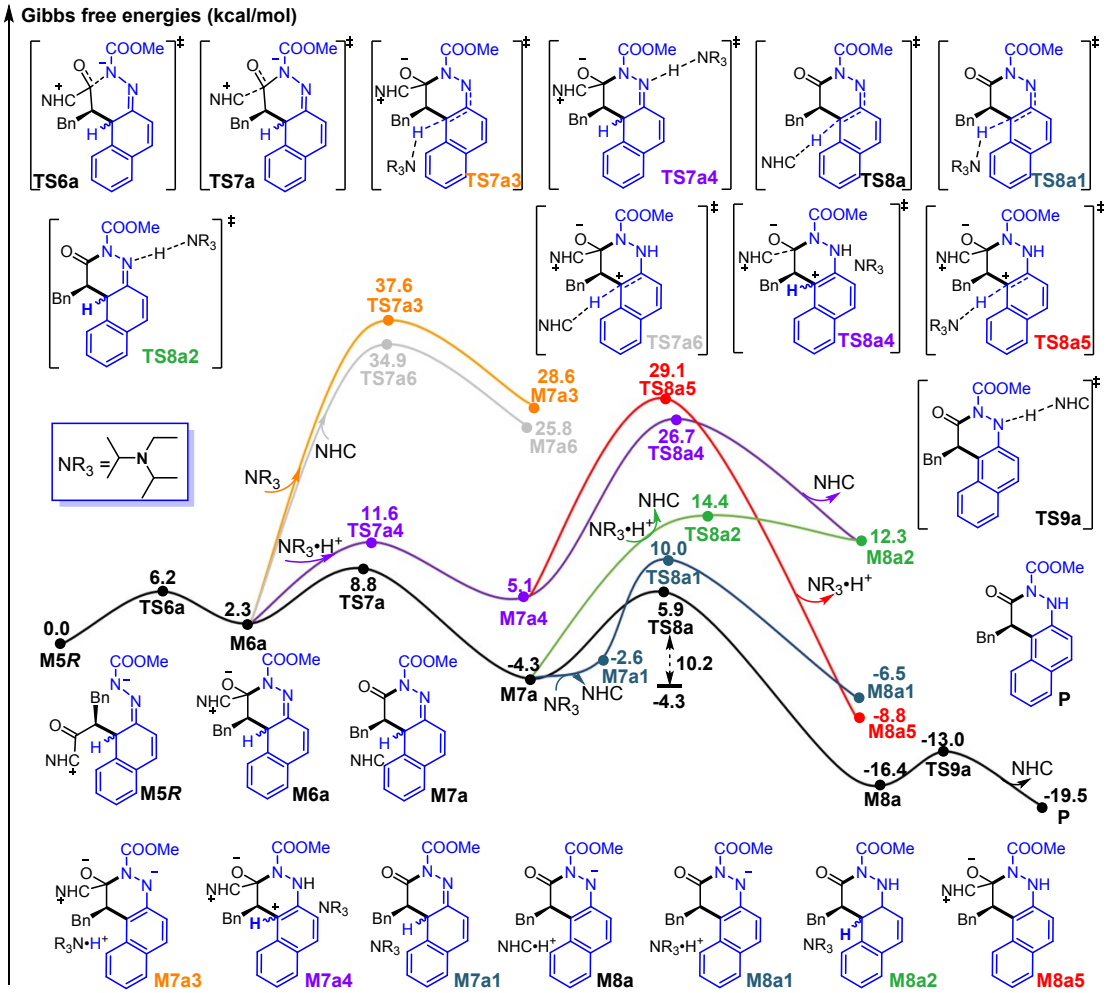


Fig. S5. The Gibbs free energy profiles of the possible pathways for the RC-first mechanism associated with [4 + 2] cyclization reaction

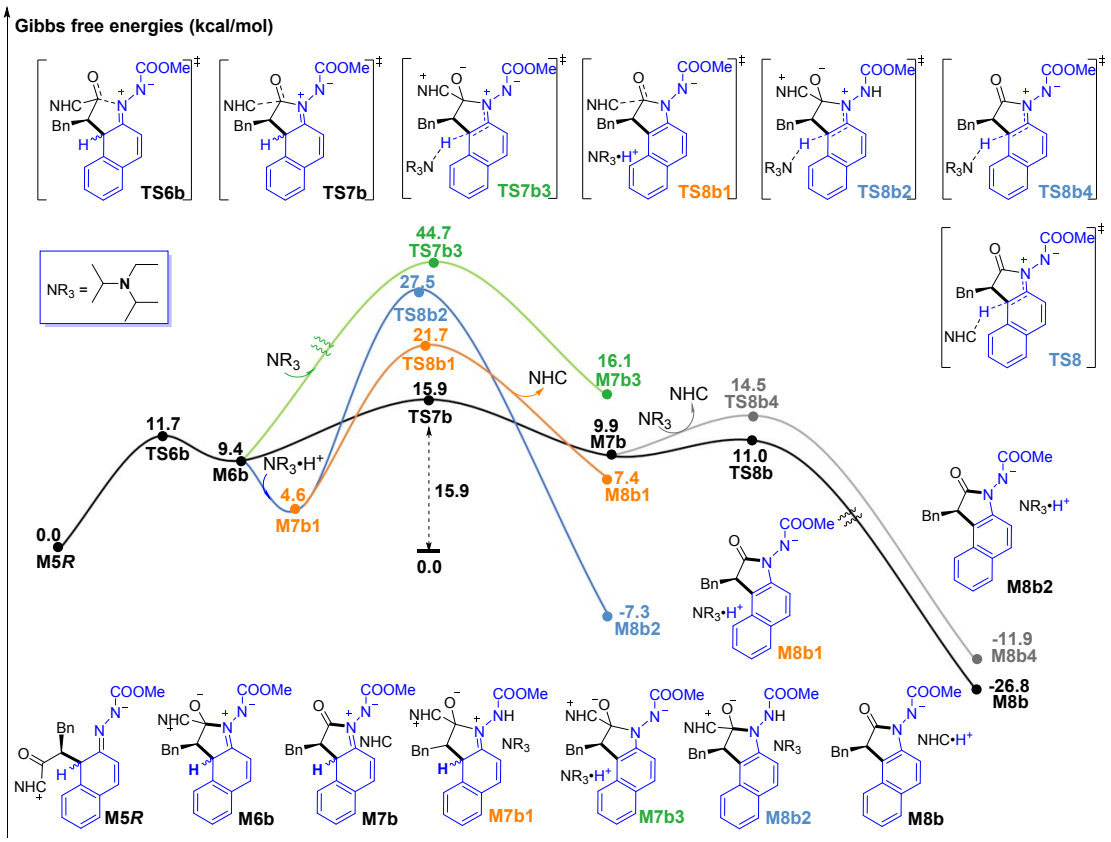


Fig. S6. The Gibbs free energy profiles of the possible pathways for the RC-first mechanism associated with [3 + 2] cyclization reaction

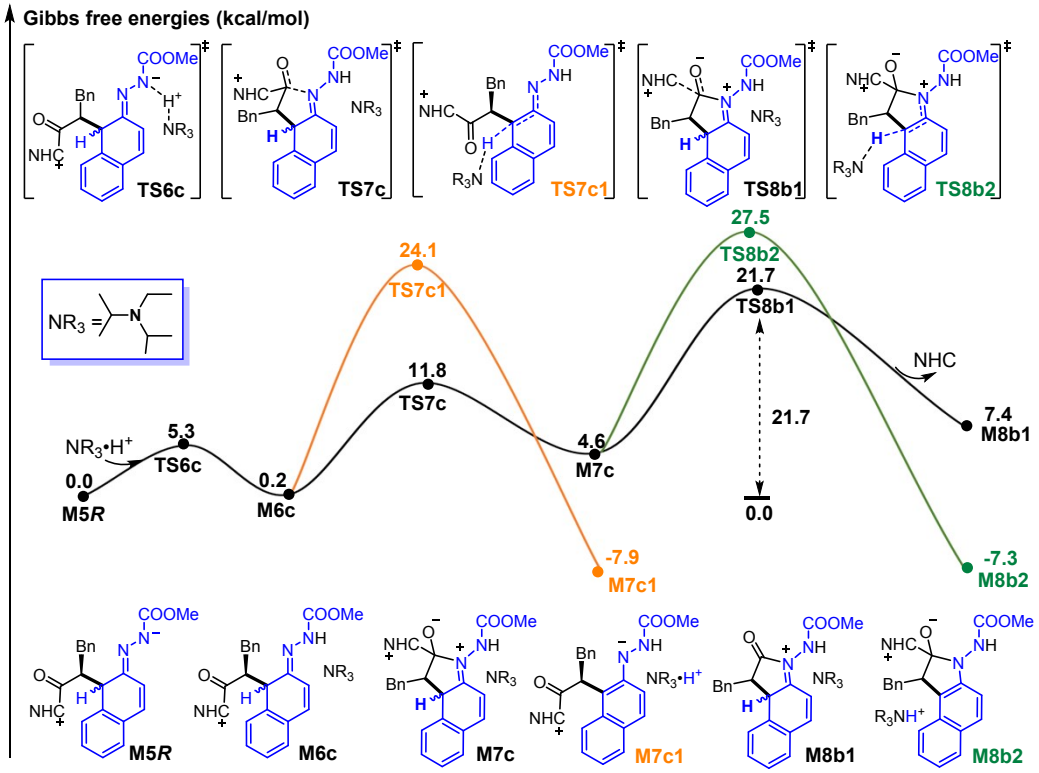


Fig. S7. The Gibbs free energy profiles of the possible pathways for the PT-first mechanism associated with [3 + 2] cyclization reaction

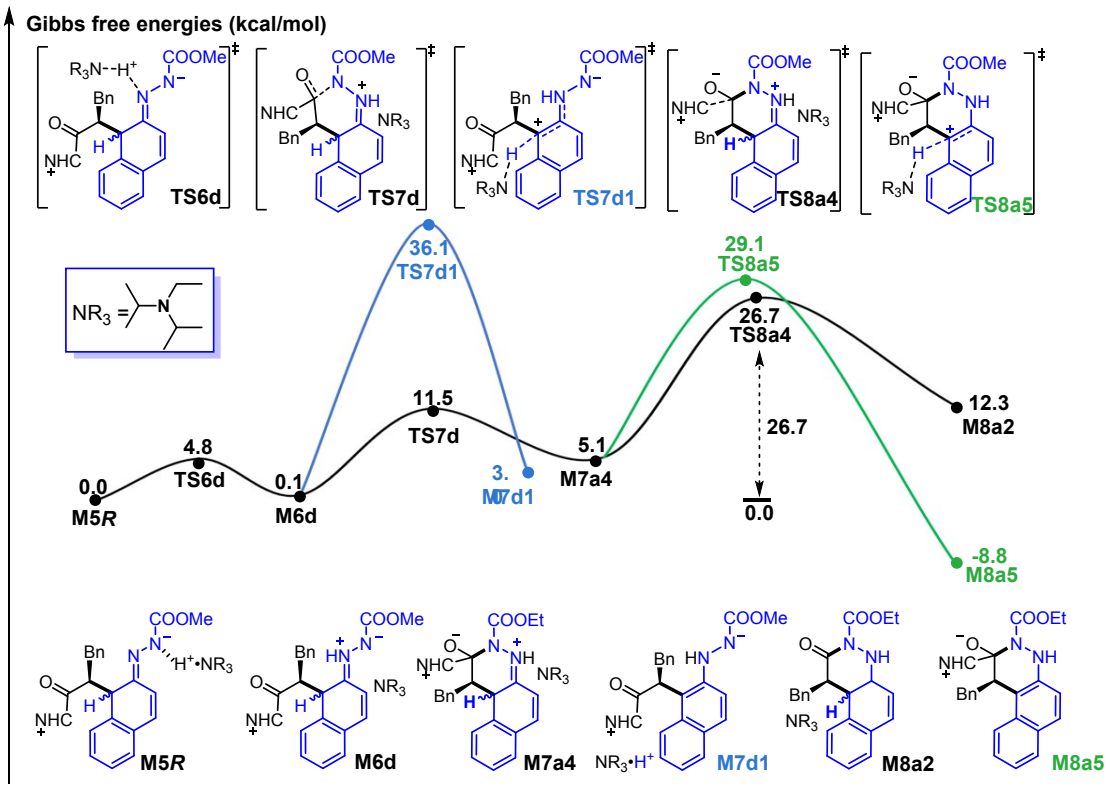


Fig. S8. The Gibbs free energy profiles of the possible pathways for the PT-first mechanism associated with [4 + 2] cyclization reaction

Part 7: Test results of the different computational methods

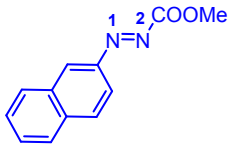
We have compared the relative Gibbs free barrier differences ($\Delta\Delta G^{\ddagger}$) of **TS5*R*** and **TS5*S***, which are computed by the Gibbs free energies at the M06-2X/6-31G(d, p)//IEF-PCM$_{THF}$ plus the refined single-point energies at the M06-2X/6-31++G(2df, 2pd)//IEF-PCM$_{THF}$(L1), M06-2X-D3/6-31++G(2df, 2pd)//IEF-PCM$_{THF}$(L2), B3LYP[8]/6-31++G(2df, 2pd)//IEF-PCM$_{THF}$ (L3) and ωB97X-D[9]/6-31++G(2df, 2pd)//IEF-PCM$_{THF}$ (L4) levels, respectively. As shown in **Table S2**, there are same trend and small energy differences between the relative Gibbs free energies of **TS5*R*** and **TS5*S***, indicating the selected method should be proper and reliable in this kind of reaction system.

Table S2. Comparison of relative Gibbs free energy barrier differences ($\Delta\Delta G^{\ddagger}$) of **TS5*R*** and **TS5*S*** calculated by using the different levels (L1-4) (unit: kcal/mol).

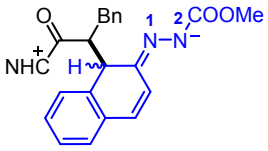
Levels	L1	L2	L3	L4
$\Delta\Delta G$	3.9	4.0	3.5	4.8

Part 8: Energy of HOMO (E_H), global nucleophilicity (N), Parr function (P_k^-) and the local nucleophilicity N_k of N1 and N2 atoms in Reactant R2 and intermediate M5*R*

Table S3 Energy of HOMO (E_H), global nucleophilicity (N), Parr function (P_k^-) and the local nucleophilicity N_k of N1 and N2 atoms Reactant **R2** and in intermediate **M5*R***



R2



M5*R*

	Atom	E_H(a.u.)	N^a(eV)	P_k^-	N_k(eV)
R2	N1	-0.27759	2.752	0.525	1.445
	N2			0.395	1.087
M5*R*	N1	-0.22318	4.232	0.418	1.769
	N2			0.019	0.052

a E_H(TCNE) = -0.37872 a.u. (calculated at the M06-2X/6-31G(d, p)/IEF-PCM$_{THF}$ level).

Part 9: Tests of the influence of explicit solvent in proton transfer process

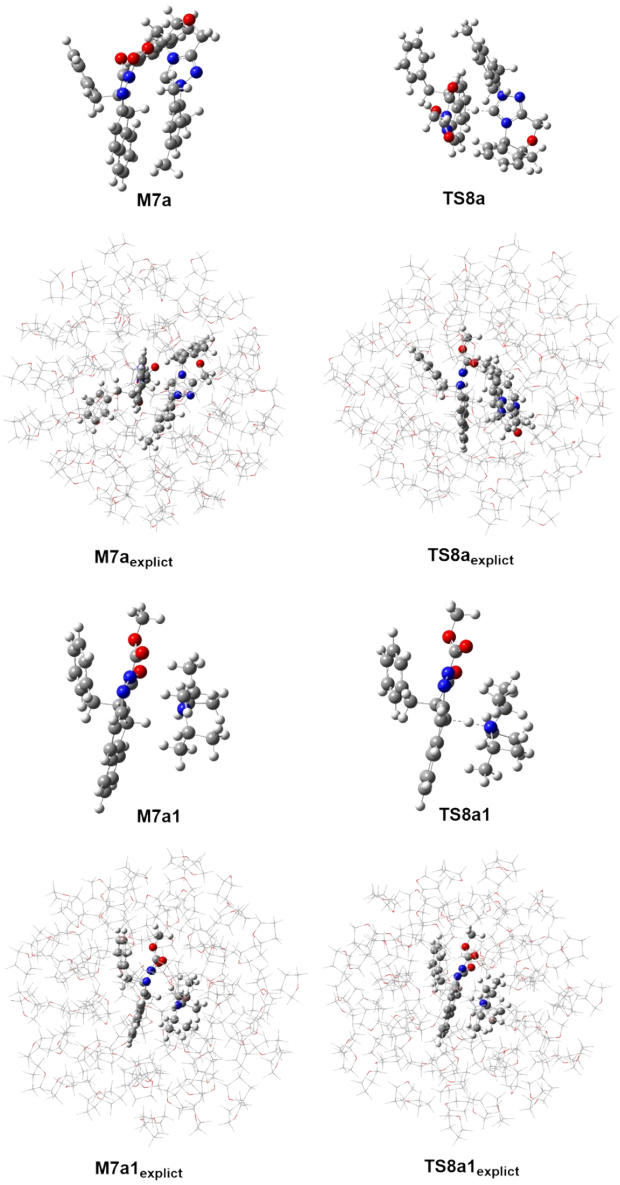


Fig. S9. Optimized geometries of some intermediate and transition state involve in proton transfer process

Table S4 Test the influence of explicit solvent in proton transfer process

Method	kcal/mol
M06-2X($\Delta\Delta G_{tot}^{\ddagger}$[**TS8a-M7a**]^{a})	9.0
M06-2X($\Delta\Delta G_{50\%}^{\ddagger}$[**TS8a-M7a**])	10.4
M06-2X($\Delta\Delta G^{\ddagger}$[**TS8a$_{explicit}$-M7a$_{explicit}$**]^{b})	10.6
B3LYP($\Delta\Delta G_{tot}^{\ddagger}$[**TS8a$_{B3LYP}$-M7a$_{B3LYP}$**]^{a})	8.0
B3LYP($\Delta\Delta G_{50\%}^{\ddagger}$[**TS8a$_{B3LYP}$-M7a$_{B3LYP}$**])	9.6

B3LYP($\Delta\Delta G^{\ddagger}$[**TS8a$_{explicit}$-M7a$_{explicit}$**]^{b})	8.8
M06-2X($\Delta\Delta G_{tot}^{\ddagger}$[**TS8a1-M7a1**])	12.2
M06-2X($\Delta\Delta G_{50\%}^{\ddagger}$[**TS8a1-M7a1**])	12.4
M06-2X($\Delta\Delta G^{\ddagger}$[**TS8a1$_{explicit}$-M7a1$_{explicit}$**])	11.8

[a] The transition state **TS8a/TS8a1** and intermediate **M7a/M7a1** obtained from the IRC calculations were calculated at the level of M06-2X/6-31G(d,p)/IEFPCM$_{THF}$ or B3LYP/6-31G(d,p)/IEFPCM$_{THF}$. [b] The transition state **TS8a$_{explicit}$/TS8a1$_{explicit}$** was first located in the sphere with a radius of 15Å of the explicit solvents at the ONIOM(M06-2X/6-31G(d,p):UFF) or ONIOM(B3LYP/6-31G(d,p):UFF) level. Then IRC calculation was performed to locate the corresponding intermediate **M7a$_{explicit}$/M7a1$_{explicit}$**.

Considering the reviewer's concern and valuable suggestions, we have additionally optimized the proton transfer transition states with explicit solvents to test the reliability of the proton transfer models with using implicit solvent in the main text. In the famous work of Singleton and Plata, they investigated the mechanism of alcohol-mediated Morita-Baylis-Hillman (MBH) reactions using the most popular DFT methods, *i.e.*, B3LYP and M06-2X. They found that the calculated results by using the two methods are remarkably different, and the proton-shuttle step with using implicit solvent even cannot be predicted correctly by using M06-2X method, so they think that the computations aid in interpreting observations but fail utterly as a replacement for experiment. Subsequently, Winter thought that only the proper modeling can lead to the correct results,[10] and the modeling proton transfer barrier with considering explicit solvent should be more reliable in this kind of system. Therefore, to test the reliability of the calculated proton transfer energy barriers with using implicit solvent, we have additionally constructed the explicit solvent models and computed the energy barriers of the favorable proton transfer processes as shown in Figure. S9, in which 100 THF solvents in a sphere shape were added by using the packmol software, and both the B3LYP and M06-2X methods were tested in the revised manuscript.

As summarized in Table S4, the calculated results indicate that the free energy barriers $\Delta\Delta G_{tot}^{\ddagger}$(with the normal Gibbs free energy correction), $\Delta\Delta G_{50\%}^{\ddagger}$(with 50% of the Gibbs free energy correction), and $\Delta\Delta G_{explicit}^{\ddagger}$(calculated in the explicit solvents without implicit model) are close and the free energy barriers obtained by the different DFT methods are not significantly different, which is remarkably different from Singleton's work. As mentioned above, we believe that the computational errors in this system are not very significant and the calculated results using M06-2X method are consistent with the experiment.

Part 10: AIM analysis for transition state TS8a and TS8a1

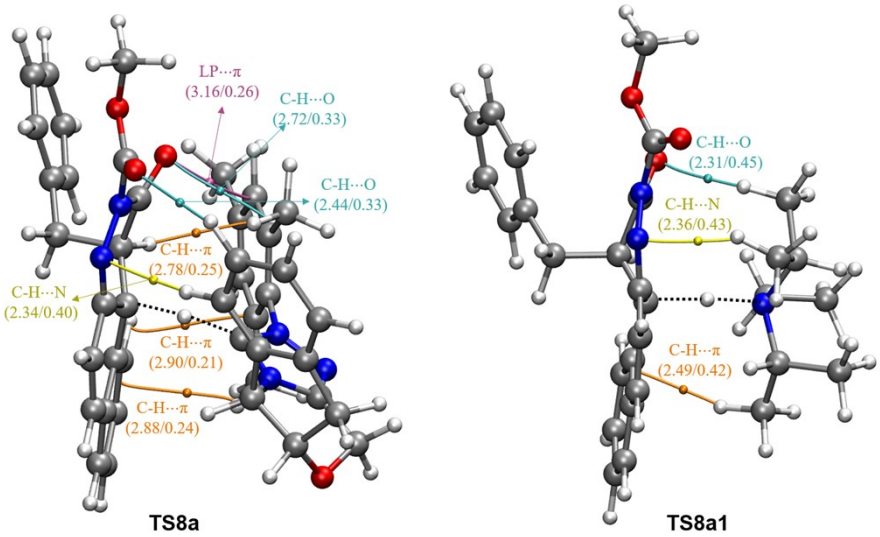


Fig. S10 Different types of weak interactions and their corresponding distances and Laplacian of electron densities (∇^2_ρ)

Part 11: Chemical transformation and equilibrium between NHC and DIPEA

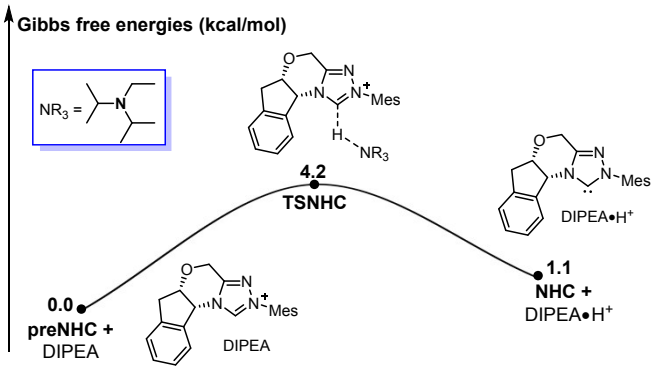
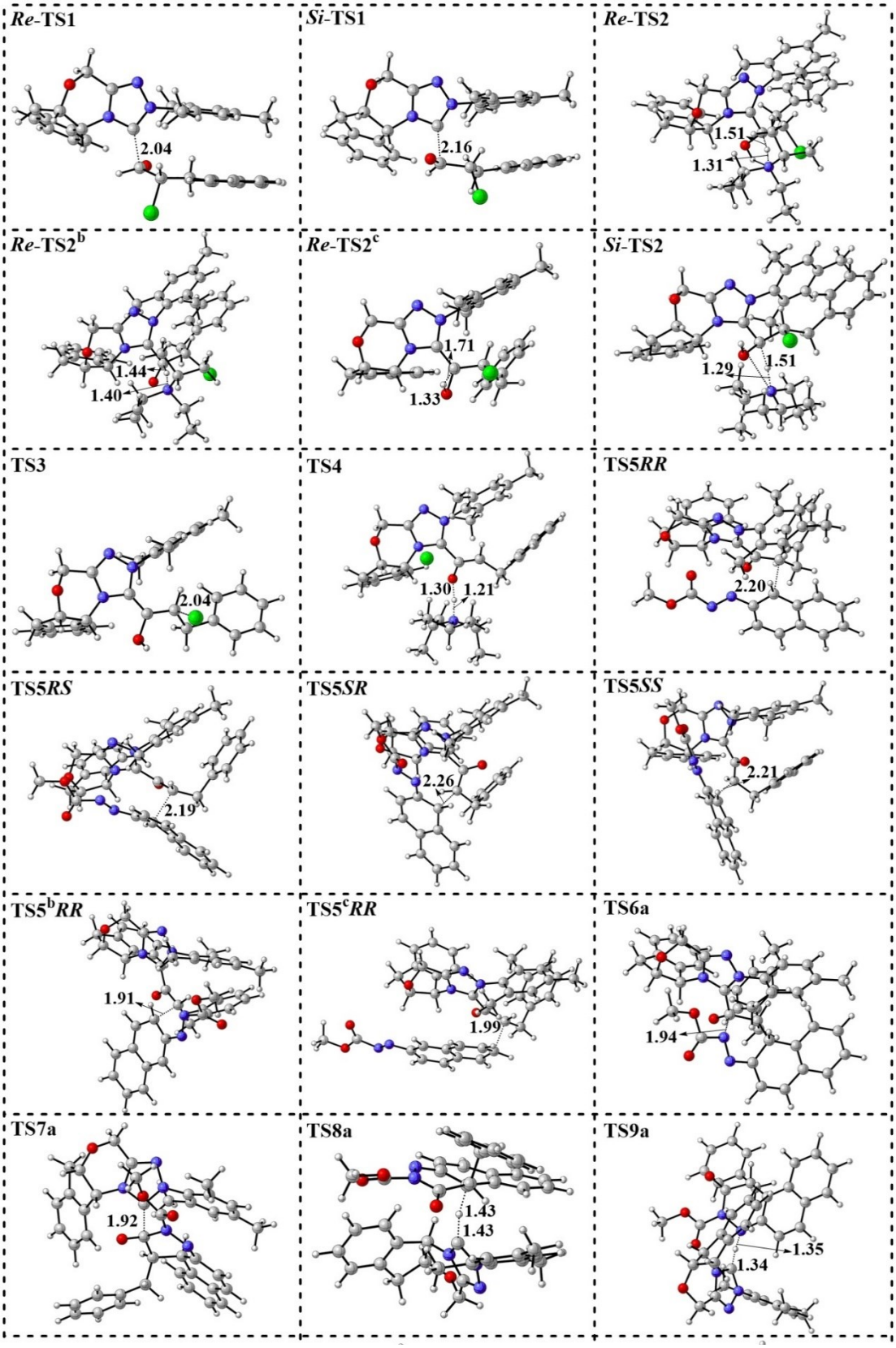


Fig. S11 The Gibbs free energy profile of equilibrium between NHC and DIPEA

Part 12: Optimized geometries of transition state



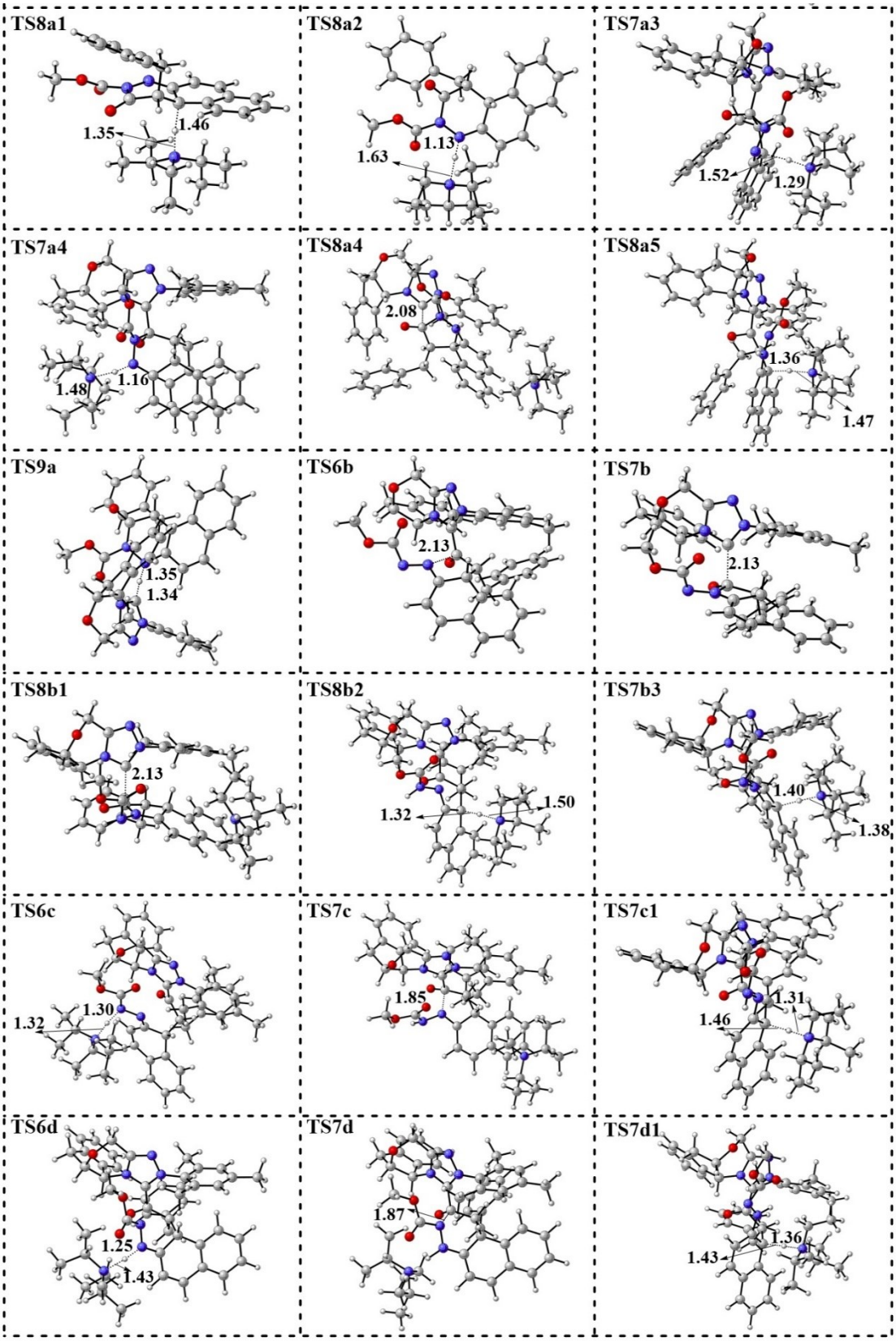


Fig. S12. Optimized geometries of some stationary points (unit: Å)

Part 13: Absolute single-point energies and Gibbs free energy (GFE) of the structures optimized at the L1 level

Table S3. The single-point and GFE (=*E*+GFEC) energies of the stationary points involved in Arylation of Azonaphthalenes with α-Chloroaldehydes (unit: a.u.)

SP	GFEC (M06-2X/6-31G(d, p)/ IEF-PCM$_{THF}$)	*E* (M06-2X/6-311++G (2df, 2pd)/IEF-PCM$_{THF}$)	GFE
NHC	0.333141	-1052.233232	-1051.900091
R1	0.121119	-883.757442	-883.636323
***Re*-TS1**	0.483224	-1935.998222	-1935.514998
***Si*-TS1**	0.483063	-1936.000324	-1935.517261
***Re*-M1**	0.484977	-1936.009343	-1935.524366
***Si*-M1**	0.485851	-1936.012326	-1935.526475
DIPEA·H+	0.245604	-371.425219	-371.179615
***Re*-TS2**	0.749623	-2307.441607	-2306.691984
DIPEA	0.229228	-370.973448	-370.744220
***Re*-TS2^{b}**	0.737865	-2306.957076	-2306.219211
***Re*-TS2^{c}**	0.479703	-1935.940872	-1935.461169
***Si*-TS2**	0.752239	-2307.419331	-2306.667092
M2	0.480104	-1936.024006	-1935.543902
TS3	0.480057	-1936.023665	-1935.543608
M3	0.481522	-1936.063354	-1935.581832
TS4	0.736478	-2307.056026	-2306.319548
DIPEA·H^{+}·Cl^{-}	0.240828	-831.828449	-831.587621
M4	0.469285	-1475.206977	-1474.737692
R2	0.160521	-723.170922	-723.010401

TS5RR	0.660695	-2198.376236	-2197.715541
TS5^{b}R	0.659139	-2198.358117	-2197.698978
TS5^{c}R	0.659378	-2198.359892	-2197.700514
TS5SS	0.660159	-2198.369564	-2197.709405
M5RR	0.665909	-2198.420919	-2197.755010
M5SS	0.663593	-2198.397431	-2197.733838
TS6a	0.666894	-2198.412103	-2197.745209
M6a	0.665757	-2198.417098	-2197.751341
TS7a	0.666388	-2198.407375	-2197.740987
M7a	0.661723	-2198.423623	-2197.761900
TS8a	0.657034	-2198.402679	-2197.745645
M8a	0.657531	-2198.438706	-2197.781175
TS9a	0.654820	-2198.430622	-2197.775802
P+NHC	0.660176	-2198.446329	-2197.786153
TS8a1	0.553364	-1517.136526	-1516.583162
M8a1	0.553625	-1517.163197	-1516.609572
TS8a2	0.568298	-1517.579902	-1517.011604
M8a2	0.567120	-1517.582109	-1517.014989
TS7a3	0.918427	-2569.357701	-2568.439274
M7a3	0.923525	-2569.377186	-2568.453661
TS7a4	0.930258	-2569.845689	-2568.915431
M7a4	0.934834	-2569.860546	-2568.925712
TS8a4	0.929442	-2569.821561	-2568.892119
TS8a5	0.934894	-2569.823094	-2568.888200
M8a5	0.666703	-2198.435681	-2197.768978
TS6b	0.665150	-2198.401461	-2197.736311
M6b	0.665935	-2198.405987	-2197.740052
TS7b	0.663619	-2198.393257	-2197.729638
M7b	0.661563	-2198.400773	-2197.73921

M7b1	0.932835	-2569.860067	-2568.927232
TS8b	0.661933	-2198.3995	-2197.73753
M8b	0.66265	-2198.4604	-2197.7977
TS8b1	0.931809	-2569.831789	-2568.899980
M8b1	0.566176	-1517.588880	-1517.022704
TS8b2	0.931850	-2569.822632	-2568.890782
M8b2	0.938821	-2569.885118	-2568.946297
TS7b3	0.923280	-2569.351270	-2568.427990
M7b3	0.923027	-2569.396574	-2568.473547
TS8b4	0.552407	-1517.1284	-1516.57602
M8b4	0.559306	-1517.1775	-1516.61818
TS6c	0.927627	-2569.853799	-2568.926172
M6c	0.926424	-2569.860672	-2568.934248
TS7c	0.928533	-2569.844347	-2568.915814
TS7c1	0.930616	-2569.826733	-2568.896117
M7c1	0.938094	-2569.885255	-2568.947161
TS6d	0.929994	-2569.856088	-2568.926094
M6d	0.929960	-2569.863582	-2568.933622
TS7d	0.933505	-2569.848998	-2568.915493
TS7d1	0.934040	-2569.810344	-2568.876304
M7d1	0.668803	-2198.418122	-2197.749319

Part 14: List of the Cartesian coordinates of all the SPs involved in the reaction

NHC

Zero-point correction= 0.383955
Thermal correction to Energy= 0.404766
Thermal correction to Enthalpy= 0.405710
Thermal correction to Gibbs Free Energy= 0.333141
Sum of electronic and zero-point Energies= -1051.532314
Sum of electronic and thermal Energies= -1051.511503
Sum of electronic and thermal Enthalpies= -1051.510559
Sum of electronic and thermal Free Energies= -1051.583128
Cartesian coordinates

C	-4.174862	0.271356	-0.053582
C	-2.928892	0.621845	-0.563469
C	-2.464896	1.932010	-0.518619
C	-3.285638	2.907733	0.041056
C	-4.542864	2.565809	0.547577
C	-4.995395	1.248429	0.505892
C	-4.428770	-1.206900	-0.210035
H	-1.478800	2.175481	-0.906548
H	-2.947942	3.937894	0.088396
H	-5.171478	3.335131	0.984804
H	-5.969002	0.987865	0.910673
H	-5.207069	-1.393760	-0.957022
C	-0.637566	-1.202583	0.669749
C	-1.786596	-1.886053	1.334783
C	-3.078960	-1.807465	-0.676577
C	-2.196252	-0.581467	-1.114675
C	0.297411	-0.134081	-1.088961
H	-1.437247	-2.600425	2.080305
H	-2.104480	-0.534305	-2.202453
N	0.602997	-1.067151	1.019224
N	1.144636	-0.405861	-0.070108
N	-0.851680	-0.675203	-0.574975
C	2.530795	-0.054331	-0.032883
C	2.881591	1.293704	0.079025
C	3.487179	-1.072991	-0.096670
C	4.239891	1.611012	0.118173
C	4.831465	-0.708357	-0.048667
C	5.225963	0.626792	0.055311

H	4.532700	2.654502	0.208061
H	5.589556	-1.486754	-0.099636
O	-2.470715	-2.611412	0.325128
H	-2.448840	-1.156625	1.822937
H	-3.216049	-2.488688	-1.517000
H	-4.750786	-1.689227	0.718353
C	1.830016	2.369345	0.150100
H	1.051030	2.112586	0.874503
H	1.338046	2.493214	-0.818975
H	2.276270	3.322549	0.439547
C	6.687634	0.994333	0.072938
H	6.845081	1.968173	0.541844
H	7.085913	1.048092	-0.945556
H	7.275052	0.249885	0.615883
C	3.069630	-2.514105	-0.220736
H	2.320790	-2.634470	-1.009455
H	2.616786	-2.872065	0.708129
H	3.929204	-3.144454	-0.455178

Vibrational frequencies

20.8727	25.7520	47.5396
51.9503	69.9972	75.0281
109.4748	146.3448	163.5937
172.7080	175.9568	192.9268
214.6252	221.1277	238.8420
278.6327	280.5231	291.7092
320.3217	337.3690	375.0687
401.3870	427.7610	443.7078
473.6928	489.4160	504.2932
509.2339	524.1112	529.8507
566.5237	587.4765	598.7502
606.6218	614.6026	625.6787
688.4667	711.3842	722.8581
744.0081	762.0960	767.5646
802.1783	836.5240	854.4910
877.8954	881.1580	886.1471
911.4828	916.1132	955.4925
964.5856	977.0716	987.5097
992.5648	1021.1303	1023.4566
1036.6507	1041.6342	1049.7348
1052.9186	1060.6353	1061.9734
1065.7914	1066.3775	1069.4172
1082.1947	1116.0355	1145.6915
1172.2868	1190.1299	1197.6951
1212.3488	1226.2694	1240.4244

1257.2665	1273.3142	1278.9938
1287.1257	1288.6474	1306.1946
1321.4695	1338.4174	1340.5364
1351.8096	1372.1110	1381.6016
1399.3958	1416.4167	1417.7785
1419.2312	1430.7259	1444.3970
1467.3574	1478.2031	1481.6039
1486.2606	1490.9795	1495.6863
1498.7024	1500.9014	1502.4026
1516.1902	1524.3588	1538.9752
1568.4778	1684.5969	1686.2900
1699.0220	1701.2676	1707.9526
3062.6034	3068.2969	3068.7319
3077.5471	3086.4172	3130.7302
3135.5230	3138.0223	3140.1805
3147.4901	3150.6589	3163.1108
3167.1839	3171.1406	3182.3258
3186.6818	3188.5679	3195.2616
3198.6300	3211.5191	3225.7661

R1

Zero-point correction= 0.158977
Thermal correction to Energy= 0.169118
Thermal correction to Enthalpy= 0.170062
Thermal correction to Gibbs Free Energy= 0.121119
Sum of electronic and zero-point Energies= -883.427417
Sum of electronic and thermal Energies= -883.417276
Sum of electronic and thermal Enthalpies= -883.416332
Sum of electronic and thermal Free Energies= -883.465275
Cartesian coordinates

C	-3.036747	0.492234	0.176862
O	-3.383661	1.301043	-0.645407
H	-3.762099	-0.040280	0.819296
C	-1.575842	0.137155	0.411598
C	-0.652510	0.694072	-0.663210
H	-1.288010	0.495418	1.405929
H	-0.941645	0.269847	-1.629351
H	-0.854422	1.769593	-0.712252
Cl	-1.491255	-1.664561	0.510796
C	0.806313	0.441177	-0.376012
C	1.494914	-0.584871	-1.025536
C	1.484623	1.216425	0.568239
C	2.835238	-0.832943	-0.738256
H	0.974684	-1.192802	-1.760909

C	2.823240	0.970290	0.859497
H	0.960739	2.024284	1.074055
C	3.502264	-0.056579	0.205629
H	3.357681	-1.633346	-1.252452
H	3.338038	1.582889	1.592840
H	4.546690	-0.248168	0.429705

Vibrational frequencies

29.5796	54.9863	73.5701
99.0736	196.2678	217.6023
332.9095	347.9638	378.9649
416.5815	504.7319	549.0959
630.5503	637.2614	708.0616
720.8768	779.0000	853.9988
876.2947	882.5389	939.1372
970.4090	1002.7947	1018.2518
1028.0565	1051.5795	1069.6478
1098.1434	1127.3835	1181.0698
1191.6884	1207.1679	1242.4257
1271.4394	1295.5985	1354.6573
1361.9191	1390.3616	1418.5482
1476.2976	1509.4382	1556.3884
1681.0673	1702.2997	1875.9234
3056.6223	3085.3024	3113.1674
3140.4147	3195.0463	3200.7634
3214.7471	3224.6863	3240.5605

***Re*-TS1**

Zero-point correction= 0.545956
Thermal correction to Energy= 0.576781
Thermal correction to Enthalpy= 0.577725
Thermal correction to Gibbs Free Energy= 0.483224
Sum of electronic and zero-point Energies= -1934.969788
Sum of electronic and thermal Energies= -1934.938964
Sum of electronic and thermal Enthalpies= -1934.938020
Sum of electronic and thermal Free Energies= -1935.032520
Cartesian coordinates

C	-5.365483	0.479527	0.031503
C	-4.017844	0.648096	0.337157
C	-3.572427	0.767928	1.651233
C	-4.522302	0.720970	2.669777
C	-5.878144	0.557072	2.372861
C	-6.309796	0.434768	1.053953
C	-5.582345	0.370573	-1.456111
H	-2.513025	0.886997	1.880933

H	-4.206052	0.810188	3.703988
H	-6.602716	0.519109	3.180229
H	-7.363374	0.299387	0.828263
H	-6.092664	1.257745	-1.844399
C	-2.250267	-1.608499	-1.070531
C	-3.568794	-2.019375	-1.636952
C	-4.166910	0.254316	-2.070142
C	-3.174156	0.666908	-0.918735
C	-0.793784	-0.065689	-0.398396
H	-3.489462	-2.979403	-2.146289
H	-2.751367	1.654965	-1.116025
N	-1.163841	-2.279556	-0.837577
N	-0.286737	-1.305116	-0.417048
N	-2.062309	-0.273410	-0.828738
C	1.038033	-1.664914	-0.004161
C	1.221143	-2.059808	1.325280
C	2.084843	-1.563878	-0.921071
C	2.520958	-2.348972	1.732982
C	3.369818	-1.858944	-0.462702
C	3.605107	-2.245703	0.854984
H	2.695816	-2.645466	2.764758
H	4.209372	-1.747625	-1.145466
O	-3.910750	-1.038030	-2.600991
H	-4.327621	-2.094463	-0.845582
H	-4.043592	0.922354	-2.922909
H	-6.183861	-0.498075	-1.741773
C	0.054154	-2.101601	2.274655
H	-0.739758	-2.752384	1.896067
H	-0.359012	-1.093203	2.392957
H	0.368571	-2.470120	3.252536
C	5.002374	-2.535332	1.337473
H	5.095818	-3.576043	1.662627
H	5.256209	-1.900504	2.191912
H	5.736576	-2.350906	0.550651
C	1.841126	-1.158735	-2.350836
H	1.218497	-0.261361	-2.418857
H	1.317532	-1.952540	-2.893464
H	2.788031	-0.957949	-2.855132
C	-0.213875	1.544057	0.719560
O	-0.252667	1.205555	1.914342
H	-1.028385	2.154580	0.281361
C	1.142520	1.864395	0.049289
C	2.325051	1.391256	0.868017
H	1.154061	1.476860	-0.967957

H	2.394126	2.007810	1.770032
H	2.084043	0.383505	1.225792
Cl	1.218215	3.677093	-0.157140
C	3.659736	1.335980	0.158544
C	4.780710	0.949229	0.902674
C	3.821899	1.563160	-1.208348
C	6.017948	0.764119	0.297583
H	4.667132	0.767532	1.969427
C	5.062114	1.378118	-1.821653
H	2.982588	1.884807	-1.817827
C	6.162147	0.970464	-1.074930
H	6.869931	0.453455	0.895017
H	5.163536	1.555768	-2.888004
H	7.125620	0.823847	-1.552492

Vibrational frequencies

-156.0223	16.3967	25.4650
27.4445	43.4687	50.0394
60.3472	62.6118	70.3720
73.9856	93.8668	109.9425
110.0840	120.3990	154.4480
168.2028	171.9906	180.0904
189.4500	195.0999	200.6400
206.9999	215.8600	218.9236
242.3591	247.1376	265.7328
276.7389	282.7746	294.0007
316.7167	319.4619	341.7085
371.9041	400.7190	418.9061
429.7132	448.5632	453.2200
474.5806	478.2376	489.1437
497.4991	508.1606	516.0889
524.6009	539.4406	548.3463
577.8910	588.6111	599.3645
608.9952	614.7425	624.6702
629.9462	667.4263	701.2279
711.9091	719.2659	723.0220
725.8353	747.5554	755.9277
760.3429	773.5283	806.1403
836.6671	848.2697	857.0029
879.5916	881.1416	881.6573
885.9493	911.7286	914.3060
923.2456	954.9789	960.5838
962.0372	973.4500	980.3042
1001.5587	1003.2132	1008.4708
1017.1843	1025.5576	1029.1664

1034.1390	1037.4105	1042.5123
1052.5586	1054.5670	1060.2898
1064.3268	1068.8080	1070.9853
1071.8094	1073.3816	1082.9803
1101.6335	1121.3755	1128.3355
1151.4369	1153.4767	1178.8690
1180.0645	1198.4065	1201.7563
1208.9926	1211.5603	1216.7124
1223.9712	1238.9086	1247.8780
1269.0383	1275.8268	1278.9782
1281.1048	1286.7029	1295.9016
1309.4323	1321.5808	1331.4977
1338.2050	1343.7269	1346.1808
1361.3699	1366.4761	1371.8092
1380.6137	1382.2908	1407.5713
1413.8069	1416.3741	1418.6588
1427.4021	1430.6466	1458.1187
1466.6247	1470.4833	1479.7459
1484.9846	1490.4867	1491.6004
1493.4726	1501.8013	1504.1074
1504.9210	1511.4317	1515.7242
1525.2428	1547.8821	1557.0239
1568.1216	1650.1255	1676.8912
1683.9277	1686.3690	1694.5447
1699.8564	1699.9163	1701.0975
2984.4864	3062.7621	3067.9630
3068.3189	3072.8778	3087.3632
3093.6084	3131.8995	3135.9118
3136.7567	3137.1252	3139.5551
3140.7206	3155.9610	3166.5431
3167.9457	3168.4586	3169.3436
3180.7037	3181.0233	3186.2517
3187.1269	3189.2632	3201.0272
3203.7055	3211.4859	3217.9633
3221.5927	3222.6910	3235.4663

***Si*-TS1**

Zero-point correction= 0.545625
Thermal correction to Energy= 0.576496
Thermal correction to Enthalpy= 0.577441
Thermal correction to Gibbs Free Energy= 0.483063
Sum of electronic and zero-point Energies= -1934.971154
Sum of electronic and thermal Energies= -1934.940282
Sum of electronic and thermal Enthalpies= -1934.939338

Sum of electronic and thermal Free Energies= -1935.033715

Cartesian coordinates

C	-5.144212	-0.685044	-0.416376
C	-3.787058	-0.895668	-0.190864
C	-3.086008	-1.892462	-0.862409
C	-3.774621	-2.696646	-1.766633
C	-5.139568	-2.496426	-1.991017
C	-5.832428	-1.490972	-1.320228
C	-5.665396	0.461796	0.410607
H	-2.020109	-2.030021	-0.693136
H	-3.249890	-3.480760	-2.302309
H	-5.663777	-3.127864	-2.701227
H	-6.890440	-1.332574	-1.506569
H	-6.352261	0.107636	1.185557
C	-2.169308	1.876434	-0.528563
C	-3.533195	2.453244	-0.714959
C	-4.414997	1.109485	1.054416
C	-3.234189	0.095304	0.808927
C	-0.757920	0.418384	0.393680
H	-3.475429	3.494562	-1.030939
H	-2.929922	-0.370325	1.750648
N	-1.000258	2.276931	-0.926467
N	-0.151180	1.354251	-0.349778
N	-2.060495	0.777827	0.279208
C	1.266418	1.525041	-0.480591
C	1.901419	1.068324	-1.635711
C	1.947591	2.159640	0.563616
C	3.278328	1.263427	-1.733116
C	3.324065	2.325125	0.423782
C	4.000880	1.890559	-0.718880
H	3.800652	0.897757	-2.613619
H	3.879673	2.809287	1.223455
O	-4.161155	2.415035	0.554837
H	-4.099479	1.882734	-1.465089
H	-4.550809	1.257764	2.125730
H	-6.207055	1.205543	-0.182498
C	1.119500	0.388353	-2.726602
H	0.426759	1.088283	-3.204206
H	0.517240	-0.435326	-2.327678
H	1.791895	-0.014847	-3.485807
C	5.485287	2.105537	-0.857018
H	5.696207	3.098470	-1.268052
H	5.925389	1.362337	-1.525967
H	5.984776	2.035958	0.112710

C	1.204072	2.644968	1.782095
H	0.725290	1.821525	2.325954
H	0.409091	3.340698	1.494620
H	1.882427	3.159293	2.464716
C	-0.368851	-0.921789	2.047856
O	-0.766446	-0.313702	3.038241
H	-0.992756	-1.703425	1.563045
C	1.128377	-1.118319	1.757895
C	1.390284	-1.868387	0.464852
H	1.645320	-0.158635	1.795100
H	1.116473	-2.921119	0.607393
H	0.689240	-1.466092	-0.277107
Cl	1.785458	-2.067012	3.168882
C	2.787771	-1.773345	-0.109166
C	2.991782	-2.221348	-1.420056
C	3.873938	-1.247569	0.589687
C	4.243033	-2.143636	-2.019453
H	2.150661	-2.629052	-1.977115
C	5.132908	-1.173502	-0.006808
H	3.750723	-0.887299	1.606123
C	5.323066	-1.616426	-1.310804
H	4.376468	-2.492603	-3.038931
H	5.966022	-0.758498	0.552961
H	6.303351	-1.552416	-1.773094

Vibrational frequencies

-80.4907	18.5565	21.5870
33.4643	43.2811	49.8491
56.6037	66.1142	70.7889
84.6392	94.4594	105.1774
115.0358	129.5423	140.8929
151.0117	162.9828	167.3275
179.8650	197.1868	204.1216
209.4260	220.8882	225.5324
249.2912	261.0223	276.9690
283.1108	295.6763	300.6329
318.9160	324.3505	350.9465
370.5827	387.2518	400.4291
419.9786	431.5427	448.4916
473.8596	476.5342	488.4683
495.5059	498.9353	511.4402
529.3273	533.7580	574.9315
587.6394	589.3368	596.8374
601.8136	607.3006	614.1097
626.2320	631.1363	666.5192

708.2703	715.7538	717.6605
722.2851	744.7254	752.1820
756.7543	769.5473	804.4406
826.7846	835.6690	858.7842
871.9334	876.6909	881.4673
885.6527	910.8875	915.3271
917.5069	958.9844	963.0176
967.9844	979.6840	987.3644
995.2422	1004.6924	1016.9294
1020.5033	1023.7670	1029.1325
1036.4646	1041.5753	1048.8552
1056.3872	1057.1256	1062.3575
1064.0463	1065.3431	1069.1830
1070.1935	1073.8397	1078.7485
1098.3582	1104.9359	1121.7797
1130.9289	1149.1873	1176.5187
1178.3239	1195.5871	1201.1085
1210.4499	1214.1017	1219.4045
1230.9396	1238.2392	1246.3477
1267.2324	1279.3285	1279.7014
1281.8583	1297.0372	1301.8216
1310.0311	1314.2386	1330.7879
1343.2110	1347.4576	1347.9853
1355.8963	1370.3839	1371.9803
1382.7584	1402.4639	1412.8434
1416.8087	1421.4734	1421.8520
1426.2698	1436.2673	1461.4703
1464.5429	1466.1201	1481.4853
1487.0260	1489.7828	1490.8161
1495.5091	1498.1443	1503.0165
1505.2268	1507.7651	1517.2299
1522.0734	1544.5094	1559.0830
1567.6625	1678.3373	1684.8683
1686.4740	1690.9274	1698.4532
1701.9712	1702.7748	1725.7383
2957.0368	3059.3031	3062.5827
3062.9720	3064.9533	3068.3911
3084.5514	3106.5000	3124.5483
3128.4984	3129.3250	3132.4038
3140.4989	3164.1746	3164.6426
3166.2026	3172.3225	3177.6918
3178.8679	3183.5515	3191.2290
3195.0022	3196.5184	3202.7291
3203.9380	3205.2496	3216.8208

3217.9629 3222.7084 3238.6930

***Re*-M1**

Zero-point correction= 0.547625
Thermal correction to Energy= 0.578449
Thermal correction to Enthalpy= 0.579393
Thermal correction to Gibbs Free Energy= 0.484977
Sum of electronic and zero-point Energies= -1934.978103
Sum of electronic and thermal Energies= -1934.947279
Sum of electronic and thermal Enthalpies= -1934.946335
Sum of electronic and thermal Free Energies= -1935.040751
Cartesian coordinates

C	-5.373704	-0.334075	-0.258144
C	-4.034016	-0.490322	-0.600767
C	-3.562758	-0.236747	-1.887160
C	-4.486947	0.182110	-2.842381
C	-5.836251	0.339471	-2.511851
C	-6.290161	0.083061	-1.220180
C	-5.618250	-0.671910	1.190037
H	-2.501053	-0.351953	-2.123363
H	-4.155882	0.390978	-3.854622
H	-6.538627	0.670219	-3.270598
H	-7.338190	0.212389	-0.967054
H	-6.205007	-1.590632	1.286521
C	-2.208640	1.132220	1.464646
C	-3.508048	1.383725	2.155621
C	-4.213902	-0.866212	1.811700
C	-3.220760	-0.944124	0.590126
C	-0.815315	-0.121014	0.321117
H	-3.382573	2.118563	2.950165
H	-2.836784	-1.958936	0.472655
N	-1.102667	1.811882	1.441857
N	-0.248763	1.020825	0.719587
N	-2.070980	-0.059617	0.805660
C	1.078068	1.489863	0.424201
C	1.246721	2.246489	-0.743749
C	2.119699	1.192875	1.302084
C	2.536787	2.670117	-1.042506
C	3.396888	1.639080	0.951115
C	3.622996	2.366131	-0.212545
H	2.703837	3.243460	-1.951436
H	4.236794	1.377511	1.590808
O	-3.885394	0.152813	2.743910
H	-4.262198	1.747272	1.444113

H	-4.155102	-1.787187	2.391294
H	-6.158208	0.112330	1.730284
C	0.075858	2.538175	-1.640480
H	-0.708087	3.076168	-1.097306
H	-0.336145	1.585850	-1.996968
H	0.387273	3.147493	-2.490518
C	5.009310	2.820138	-0.585987
H	5.087111	3.910960	-0.540273
H	5.253285	2.515317	-1.608084
H	5.757180	2.390927	0.083671
C	1.915281	0.445338	2.593616
H	0.949867	-0.062855	2.640021
H	1.963140	1.137125	3.440094
H	2.706767	-0.297526	2.725463
C	-0.299754	-1.155157	-0.721285
O	-0.350062	-0.590052	-1.917159
H	-0.989761	-2.017513	-0.563612
C	1.116492	-1.689897	-0.261959
C	2.228748	-1.233257	-1.185401
H	1.326766	-1.411190	0.773668
H	2.168816	-1.807077	-2.116395
H	1.990779	-0.204079	-1.473460
Cl	1.076116	-3.517037	-0.205794
C	3.632218	-1.271317	-0.620344
C	4.646866	-0.628587	-1.340374
C	3.964208	-1.855415	0.603466
C	5.943275	-0.549028	-0.846140
H	4.401539	-0.159288	-2.290986
C	5.262829	-1.771391	1.108753
H	3.211758	-2.383920	1.181284
C	6.255848	-1.113873	0.390806
H	6.709008	-0.034188	-1.418978
H	5.493892	-2.226702	2.067153
H	7.264832	-1.046403	0.785017

Vibrational frequencies

18.1109	22.0456	26.1575
40.6661	49.8280	53.6026
69.3108	77.3133	80.5293
94.2177	104.7595	121.8036
127.6941	133.2959	158.1750
166.0145	182.1700	189.5972
194.0323	213.0802	216.4361
222.8460	242.7899	253.2487
258.2391	270.1661	272.8372

283.5489 294.4904 320.6816
324.4698 333.7702 383.0671
399.4810 418.3832 421.8404
443.0957 449.2662 467.3700
479.2730 488.8930 496.9177
505.5222 516.9540 528.7573
530.7127 546.0826 577.9902
588.0952 594.9591 601.1757
613.7958 625.2079 630.6277
640.6689 689.4627 711.9249
717.6026 722.0302 735.6006
742.8579 753.7327 764.6575
780.2174 810.0307 811.1480
837.3539 843.1358 861.4026
873.6546 881.0348 886.0928
891.7146 913.2180 924.3521
927.2815 941.7912 961.6334
967.1322 972.0941 978.9488
998.3144 1006.9577 1016.2741
1019.3574 1025.4807 1040.0182
1045.9348 1048.4362 1053.8609
1054.5682 1058.3832 1061.2537
1067.5550 1070.9199 1071.0777
1071.7747 1076.4820 1105.5487
1119.7401 1125.3611 1132.9992
1153.3294 1176.4578 1180.5769
1199.2145 1201.5924 1202.5575
1209.5637 1215.6869 1230.2927
1232.2524 1246.8913 1249.3566
1263.4160 1280.3504 1281.2813
1287.1273 1295.9653 1304.7742
1322.2834 1326.3504 1331.8490
1340.1189 1344.8486 1352.2582
1355.7126 1357.7021 1365.8294
1373.3597 1378.6836 1382.9631
1405.1998 1414.2897 1416.4449
1420.2206 1427.6054 1466.9129
1468.7643 1471.1438 1483.1616
1486.2414 1493.4994 1497.4616
1498.6275 1503.4575 1503.9922
1513.8830 1515.1767 1516.2958
1523.4092 1542.2531 1548.0541
1554.3307 1580.8976 1674.9941
1685.0680 1688.0646 1693.7541

1697.7956	1697.9755	1699.8391
2868.8338	3049.9432	3069.3603
3069.6996	3073.1685	3089.1297
3092.4518	3122.5657	3129.6118
3135.3983	3139.0816	3142.2908
3143.3985	3145.6755	3150.0898
3164.2996	3165.1728	3167.7690
3168.2559	3179.8594	3185.2872
3188.0750	3196.6403	3198.4055
3199.7835	3207.7452	3210.6015
3214.1571	3223.3453	3223.7589

***Si*-M1**

Zero-point correction= 0.547350
Thermal correction to Energy= 0.578189
Thermal correction to Enthalpy= 0.579133
Thermal correction to Gibbs Free Energy= 0.485851
Sum of electronic and zero-point Energies= -1934.979406
Sum of electronic and thermal Energies= -1934.948567
Sum of electronic and thermal Enthalpies= -1934.947622
Sum of electronic and thermal Free Energies= -1935.040905
Cartesian coordinates

C	5.220678	0.632172	-0.265688
C	3.868523	0.879658	-0.043439
C	3.248584	2.015787	-0.554527
C	4.012115	2.917445	-1.291375
C	5.371367	2.678515	-1.509763
C	5.983868	1.536033	-1.000164
C	5.654110	-0.660236	0.375449
H	2.189148	2.196144	-0.389423
H	3.549476	3.809666	-1.699839
H	5.954069	3.388187	-2.088177
H	7.038196	1.348808	-1.180085
H	6.305685	-0.470850	1.234394
C	2.068891	-1.694447	-0.840591
C	3.412450	-2.248115	-1.181569
C	4.348044	-1.348666	0.835335
C	3.240621	-0.227720	0.773329
C	0.744510	-0.468353	0.413583
H	3.315545	-3.195470	-1.710606
H	2.938130	0.071016	1.782034
N	0.869684	-2.042915	-1.198974
N	0.054450	-1.262394	-0.412418
N	2.032518	-0.746383	0.138490

C	-1.369885	-1.437446	-0.509638
C	-2.032326	-0.920776	-1.623814
C	-2.013042	-2.156538	0.505050
C	-3.414867	-1.095448	-1.681598
C	-3.395675	-2.289394	0.405157
C	-4.110069	-1.761801	-0.674549
H	-3.961609	-0.671696	-2.520076
H	-3.927994	-2.821782	1.189486
O	4.044966	-2.501097	0.060421
H	3.984905	-1.542897	-1.799481
H	4.427133	-1.727222	1.854164
H	6.201770	-1.317695	-0.306872
C	-1.289480	-0.218115	-2.727931
H	-0.749792	-0.940887	-3.347910
H	-0.545800	0.485610	-2.340028
H	-1.985745	0.333083	-3.362434
C	-5.604641	-1.927124	-0.755376
H	-5.864089	-2.903679	-1.177420
H	-6.047564	-1.154502	-1.387802
H	-6.059972	-1.863857	0.236179
C	-1.232289	-2.758407	1.644603
H	-0.661689	-2.005438	2.205496
H	-0.509656	-3.487078	1.260583
H	-1.905492	-3.276264	2.329852
C	0.415088	0.403059	1.670447
O	0.789941	-0.316120	2.710141
H	1.011554	1.339021	1.477027
C	-1.059013	0.884013	1.628955
C	-1.366800	1.784089	0.441198
H	-1.731688	0.028095	1.675546
H	-1.008469	2.795996	0.664779
H	-0.757071	1.441928	-0.407022
Cl	-1.369704	1.781660	3.172347
C	-2.809271	1.826551	-0.017835
C	-3.087840	2.337369	-1.290782
C	-3.868560	1.345771	0.752035
C	-4.384363	2.349663	-1.791918
H	-2.269648	2.714312	-1.901020
C	-5.171055	1.357177	0.252987
H	-3.688296	0.954073	1.748532
C	-5.434116	1.851240	-1.020132
H	-4.575655	2.743430	-2.785582
H	-5.981464	0.971983	0.864734
H	-6.448124	1.853581	-1.407738

Vibrational frequencies

24.6192	28.1650	39.8222
44.3636	50.6457	65.8865
75.1541	86.7054	94.4779
96.9065	109.9737	123.8157
131.6738	136.1348	139.6323
146.6998	165.5036	176.6139
189.1586	201.0902	209.4418
218.7903	229.0524	244.5456
261.7248	269.0722	284.4044
288.3779	307.2464	325.8424
330.0712	349.2739	376.1614
387.3953	407.8518	421.7513
428.3295	434.3607	445.3933
474.9462	489.3760	496.8361
507.4802	511.2338	528.8485
540.4953	571.4275	584.6634
587.7564	593.9839	605.3918
609.3980	622.2723	629.7256
634.6277	658.3901	713.2563
715.9534	721.4100	722.9133
742.8260	756.9661	760.6643
769.4124	801.7149	821.9830
831.4723	836.5594	858.4001
875.8932	876.3847	877.6869
890.3231	912.3197	919.3357
923.1509	956.7159	965.8577
977.5218	983.2350	985.1734
999.4343	1016.0401	1019.1503
1021.5908	1022.4511	1037.9720
1039.6472	1045.3223	1048.1360
1052.5394	1058.3915	1061.6278
1069.2631	1071.4130	1072.2091
1081.8339	1090.6415	1098.4230
1112.6446	1121.9392	1129.0957
1147.6116	1175.4771	1178.1956
1193.6956	1204.8639	1210.1115
1213.3543	1220.8384	1232.9129
1238.3795	1245.9545	1252.1671
1265.2988	1281.2799	1282.7548
1284.9801	1298.0060	1308.2625
1318.9892	1324.7400	1339.4643
1341.6543	1346.4685	1347.7743
1356.8185	1368.7817	1371.5121

1375.3708	1383.9520	1398.6496
1415.5604	1419.3427	1421.4438
1422.5609	1441.7776	1463.7459
1467.0584	1469.9833	1474.6434
1484.1954	1490.2442	1494.6701
1496.4573	1497.3018	1506.0185
1509.9833	1517.9630	1522.3353
1523.6090	1538.8183	1544.6342
1556.6302	1570.1320	1677.8204
1685.0106	1685.7041	1691.8386
1695.6576	1702.5376	1703.6366
2758.3200	3034.6945	3061.3622
3065.5390	3066.1635	3075.1588
3087.1134	3099.2934	3116.0757
3126.8638	3132.4961	3133.5351
3139.3056	3160.6885	3161.2248
3163.6746	3166.3726	3179.9752
3180.1380	3188.7215	3195.2651
3195.5818	3199.2613	3207.0580
3207.4481	3210.7036	3217.9333
3218.4440	3223.6131	3227.4126

DIPEA $\cdot H^+$

Zero-point correction= 0.280963
Thermal correction to Energy= 0.292350
Thermal correction to Enthalpy= 0.293294
Thermal correction to Gibbs Free Energy= 0.245604
Sum of electronic and zero-point Energies= -371.037857
Sum of electronic and thermal Energies= -371.026469
Sum of electronic and thermal Enthalpies= -371.025525
Sum of electronic and thermal Free Energies= -371.073215
Cartesian coordinates

N	-0.018077	0.007329	-0.496351
C	-1.284910	-0.441283	0.228315
C	-1.351326	-1.957426	0.361831
C	-2.495210	0.088455	-0.533384
H	-1.229495	0.010672	1.220322
H	-0.601907	-2.359119	1.044948
H	-2.332269	-2.210087	0.768750
H	-1.258407	-2.451721	-0.610319
H	-2.506589	1.175434	-0.624704
H	-2.543500	-0.350797	-1.535850
H	-3.398156	-0.207026	0.003260
C	1.259477	-0.716327	-0.069074

C	1.652521	-0.394583	1.362084
C	2.382522	-0.443730	-1.062115
H	0.996950	-1.770982	-0.150602
H	0.831776	-0.541402	2.068563
H	2.460440	-1.071746	1.647336
H	2.031989	0.625745	1.453362
H	2.048703	-0.555531	-2.097802
H	2.829254	0.544367	-0.934831
H	3.167995	-1.181791	-0.887820
C	0.118221	1.522661	-0.554601
C	-0.254103	2.266690	0.718496
H	-0.508641	1.852630	-1.383624
H	1.151624	1.723765	-0.831850
H	-0.003341	3.317121	0.556816
H	-1.321878	2.215263	0.936465
H	0.299900	1.924702	1.592699
H	-0.151064	-0.287545	-1.469974

Vibrational frequencies

87.0802	109.6649	166.9281
206.3638	214.0314	235.5365
258.6259	279.4142	299.2394
317.6927	324.9045	356.1373
384.2112	431.8201	449.0306
468.4059	500.3623	611.1488
737.8881	800.0363	865.6538
889.5815	939.8739	944.1952
952.2811	962.0799	972.7849
984.9831	1060.6242	1076.1235
1112.8906	1142.0344	1166.8634
1182.2423	1204.1262	1217.2675
1219.0958	1329.0780	1337.1105
1350.6045	1374.7213	1385.6266
1412.5452	1420.1574	1432.1793
1437.0502	1437.9461	1443.2935
1456.9619	1464.9006	1488.8741
1490.9749	1495.3833	1500.1274
1503.4135	1509.7983	1512.3534
1522.4524	1527.3932	1534.1715
1540.5516	3078.4517	3079.6297
3082.3226	3083.9362	3099.6951
3139.0018	3153.9282	3157.7501
3163.3521	3164.8391	3166.1335
3171.3494	3172.8792	3175.4887
3182.4264	3186.4056	3186.8686

3196.2641 3210.9643 3437.7282

***Re*-TS2**

Zero-point correction= 0.824385
Thermal correction to Energy= 0.867824
Thermal correction to Enthalpy= 0.868768
Thermal correction to Gibbs Free Energy= 0.749623
Sum of electronic and zero-point Energies= -2306.034849
Sum of electronic and thermal Energies= -2305.991411
Sum of electronic and thermal Enthalpies= -2305.990467
Sum of electronic and thermal Free Energies= -2306.109612
Cartesian coordinates

C	3.568913	-3.447448	-0.477063
C	2.529912	-2.576947	-0.793722
C	1.447789	-2.982828	-1.569705
C	1.407784	-4.303273	-2.009320
C	2.440507	-5.187585	-1.684263
C	3.529355	-4.766122	-0.924735
C	4.641056	-2.758478	0.327085
H	0.666481	-2.275517	-1.838820
H	0.573698	-4.646349	-2.612383
H	2.395135	-6.214276	-2.032636
H	4.332558	-5.455422	-0.682856
H	5.558894	-2.650277	-0.258509
C	1.500056	-1.324747	1.917212
C	2.710403	-1.951982	2.527530
C	4.063478	-1.365915	0.677902
C	2.762619	-1.208358	-0.196354
C	0.450664	-0.184937	0.348938
H	2.667373	-1.870466	3.613171
H	2.885466	-0.452939	-0.967163
N	0.334835	-1.091984	2.422115
N	-0.341717	-0.408109	1.431015
N	1.623414	-0.809170	0.650321
C	-1.787902	-0.453582	1.538904
C	-2.433386	-1.609886	1.092850
C	-2.469732	0.573517	2.207111
C	-3.819942	-1.681364	1.255226
C	-3.848006	0.454704	2.339451
C	-4.543175	-0.661352	1.861567
H	-4.339961	-2.562709	0.887648
H	-4.394527	1.249581	2.840836
O	3.819857	-1.205087	2.065454
H	2.784492	-3.012206	2.250428

H	4.769213	-0.569682	0.435159
H	4.909737	-3.295958	1.242076
C	-1.709454	-2.784405	0.487033
H	-1.753126	-3.640004	1.166993
H	-0.656059	-2.587224	0.276717
H	-2.193926	-3.084374	-0.447892
C	-6.034585	-0.763804	2.038999
H	-6.281632	-1.033106	3.071026
H	-6.457555	-1.520509	1.375296
H	-6.518280	0.191574	1.819868
C	-1.737861	1.753989	2.780916
H	-0.910895	1.430516	3.420055
H	-2.413914	2.370468	3.374964
H	-1.316979	2.385078	1.993666
C	0.262697	0.715919	-0.779179
O	0.912319	0.163946	-1.924289
H	1.128084	1.903705	-0.444310
C	-1.189904	1.026428	-1.085490
C	-1.913275	-0.105889	-1.813064
H	-1.713230	1.313337	-0.172533
H	-1.612333	-0.100548	-2.865773
H	-1.527888	-1.049287	-1.407218
Cl	-1.261740	2.515155	-2.147067
C	-3.421938	-0.118424	-1.695263
C	-4.099563	-1.273900	-2.101970
C	-4.163462	0.936038	-1.163602
C	-5.478065	-1.382431	-1.963560
H	-3.532474	-2.101789	-2.522773
C	-5.548160	0.832843	-1.028730
H	-3.674447	1.852319	-0.846023
C	-6.209326	-0.325527	-1.421514
H	-5.982824	-2.291109	-2.276613
H	-6.107223	1.662794	-0.606967
H	-7.285628	-0.406860	-1.306865
N	2.017190	2.859267	-0.292863
C	1.675995	3.498141	1.026060
C	1.689831	2.462955	2.151185
C	0.324099	4.206086	0.948090
H	2.441916	4.251055	1.238154
H	2.651025	1.958933	2.268840
H	1.467911	2.969216	3.093685
H	0.919249	1.703529	2.002135
H	0.378426	5.142990	0.390156
H	-0.431651	3.573671	0.469425

H	-0.015131	4.443909	1.958691
C	3.372940	2.187390	-0.259385
C	4.480388	2.978613	0.444722
C	3.837222	1.775734	-1.654470
H	3.201566	1.279232	0.328490
H	4.273514	3.161634	1.499779
H	5.397198	2.385511	0.393378
H	4.679181	3.935610	-0.039911
H	3.059510	1.249833	-2.211508
H	4.167437	2.637660	-2.239872
H	4.694826	1.104713	-1.554330
C	1.827983	3.794690	-1.442386
C	2.700702	5.043951	-1.460280
H	0.777353	4.076372	-1.437677
H	1.976582	3.217244	-2.356794
H	2.330503	5.707379	-2.245441
H	2.656679	5.594068	-0.516523
H	3.745126	4.821758	-1.684281
H	0.886725	0.837535	-2.618610

Vibrational frequencies

-1320.8506	19.2913	22.8733
28.8210	35.6227	42.1254
49.6361	54.1092	58.1099
59.8480	72.8203	80.9769
82.4328	89.3647	103.3922
112.5816	116.8335	124.7887
127.1823	133.4459	141.2655
149.0099	151.4455	160.5841
162.5870	172.3079	174.3544
198.9187	200.4466	203.1117
211.3475	217.2840	234.2526
241.9011	245.2550	250.3431
258.4315	267.7057	273.6833
282.3397	288.4736	294.9621
307.4170	312.0735	318.4931
324.7482	343.6974	357.3158
363.2921	368.7723	378.1083
387.0342	399.7625	408.3813
414.7860	420.9548	425.9267
443.7728	449.8430	450.2608
458.9839	463.0332	477.1652
481.7595	489.1481	496.5267
501.5694	512.0288	526.4963
528.5668	548.8172	552.7738

577.8202	589.8434	597.1971
611.0200	614.7577	624.4780
629.9057	645.5135	665.4974
681.8596	705.3811	713.7029
716.7932	735.0496	745.0306
753.1533	758.3845	764.2640
778.2829	799.8163	807.4235
823.4457	839.3500	848.6229
862.8491	865.9727	868.6161
876.2995	879.3250	885.5460
902.4960	913.1127	918.7645
921.9916	935.0200	951.5561
957.4228	961.0699	964.3291
969.5751	975.0203	976.8934
980.1220	981.7981	987.7747
991.6145	993.5238	1015.9537
1021.0363	1028.4104	1029.6614
1043.4534	1043.7915	1047.7436
1051.0403	1056.5330	1057.5812
1062.7253	1064.4992	1065.8060
1067.7050	1075.0519	1081.4763
1083.3512	1106.1831	1116.8837
1121.2332	1137.9780	1141.3871
1147.2016	1151.7923	1172.1442
1174.9489	1175.3073	1188.8009
1194.0673	1200.0749	1201.9509
1203.4280	1209.5517	1211.1001
1215.6479	1220.3022	1225.2593
1227.6377	1235.2851	1243.3860
1258.2266	1265.4429	1279.6595
1284.2980	1288.7979	1299.1557
1307.9783	1315.4778	1331.5962
1334.2758	1342.0478	1346.5161
1353.6418	1362.6784	1363.6588
1372.3515	1374.2860	1376.0337
1378.5085	1380.9753	1383.0290
1391.6732	1409.4791	1412.3531
1414.6444	1415.5939	1419.5265
1421.4208	1429.8385	1431.0429
1432.2275	1437.3063	1443.1142
1448.2051	1463.6396	1472.0338
1478.1383	1480.1285	1485.0890
1486.7659	1492.8874	1493.2340
1494.9166	1495.6627	1497.5201

1499.4844	1502.4689	1502.8118
1506.2754	1507.4251	1513.7210
1514.0450	1515.6705	1517.8480
1524.0613	1531.7412	1533.3900
1539.1616	1543.8521	1547.4473
1553.7515	1555.2144	1599.9070
1614.0600	1677.4207	1682.2335
1682.4214	1694.7194	1697.3586
1698.2757	1717.5965	3069.6571
3069.8296	3073.4074	3078.1167
3080.1023	3082.4317	3083.9688
3086.9461	3090.3633	3096.9891
3098.8992	3111.0608	3113.6793
3128.0154	3128.4727	3133.4477
3138.1946	3144.5031	3145.9819
3150.3011	3152.8628	3157.9705
3159.2743	3164.9380	3168.3513
3169.5753	3170.9051	3171.0101
3172.1242	3176.7441	3177.0428
3179.4171	3182.5863	3191.7452
3194.5229	3195.9447	3196.0125
3197.9657	3199.5835	3205.4557
3207.8927	3211.5084	3212.1623
3212.1788	3219.1669	3227.0411
3231.7431	3236.2700	3829.1504

DIPEA

Zero-point correction= 0.265112
Thermal correction to Energy= 0.276611
Thermal correction to Enthalpy= 0.277555
Thermal correction to Gibbs Free Energy= 0.229228
Sum of electronic and zero-point Energies= -370.597445
Sum of electronic and thermal Energies= -370.585946
Sum of electronic and thermal Enthalpies= -370.585002
Sum of electronic and thermal Free Energies= -370.633329
Cartesian coordinates

N	-0.069505	0.045338	-0.512746
C	-1.298972	-0.317666	0.208563
C	-1.640181	-1.794638	-0.006753
C	-2.483078	0.532910	-0.256562
H	-1.188739	-0.156110	1.296767
H	-0.918237	-2.470715	0.456601
H	-2.618754	-2.012613	0.428643
H	-1.680024	-2.013397	-1.079097

H	-2.389319	1.581602	0.034812
H	-2.578710	0.481283	-1.346420
H	-3.404532	0.149958	0.189218
C	1.080757	-0.826045	-0.205727
C	1.422301	-1.000393	1.283108
C	2.329934	-0.412334	-0.981172
H	0.805935	-1.817500	-0.585231
H	0.560465	-1.334375	1.867349
H	2.206813	-1.755910	1.391212
H	1.791380	-0.071738	1.725672
H	2.096624	-0.238898	-2.035352
H	2.786043	0.494429	-0.570399
H	3.073891	-1.210913	-0.918990
C	0.198694	1.483164	-0.551661
C	0.410599	2.208460	0.783350
H	-0.634277	1.957219	-1.078129
H	1.069016	1.648343	-1.190986
H	0.421285	3.290420	0.620710
H	-0.392253	1.985952	1.493544
H	1.359614	1.934852	1.250430

Vibrational frequencies

59.0444	106.2954	119.9493
193.0706	207.0723	222.9424
260.7045	275.9470	290.7320
316.6038	354.2074	358.5786
427.6134	443.6874	447.9492
477.7025	496.7245	602.0818
715.6842	780.3266	860.6843
895.2779	921.1038	932.6317
950.4979	964.1725	975.6935
1013.1488	1070.9394	1107.9394
1136.0450	1145.9487	1162.0962
1188.6115	1207.6540	1249.7030
1277.1562	1365.8311	1370.5982
1376.1872	1385.0987	1392.1984
1405.8816	1411.3976	1416.2121
1420.1933	1426.1631	1434.4479
1488.7926	1494.7880	1497.1067
1499.1632	1502.2515	1506.2679
1510.0807	1516.1972	1519.1808
1522.8968	1543.9332	2987.9179
3062.6627	3063.2894	3064.8424
3068.4347	3074.3165	3075.6197
3103.3718	3132.1228	3139.5593

3142.9776	3146.9515	3147.5018
3150.6274	3152.7528	3155.4802
3155.9756	3158.4741	3166.6555

***Re*-TS2[b]**

Zero-point correction= 0.810713
Thermal correction to Energy= 0.853451
Thermal correction to Enthalpy= 0.854395
Thermal correction to Gibbs Free Energy= 0.737865
Sum of electronic and zero-point Energies= -2305.557207
Sum of electronic and thermal Energies= -2305.514469
Sum of electronic and thermal Enthalpies= -2305.513525
Sum of electronic and thermal Free Energies= -2305.630055
Cartesian coordinates

C	2.822791	-3.839188	-0.429149
C	2.088635	-2.729484	-0.836591
C	1.012155	-2.835452	-1.712112
C	0.647840	-4.107026	-2.149278
C	1.360257	-5.233458	-1.724356
C	2.456747	-5.108465	-0.872915
C	3.986863	-3.441306	0.443804
H	0.523966	-1.919864	-2.050257
H	-0.187242	-4.227120	-2.832773
H	1.063096	-6.217598	-2.073339
H	3.018293	-5.986580	-0.567259
H	4.939741	-3.714913	-0.018373
C	1.536746	-1.135040	1.989866
C	2.692552	-1.828023	2.632834
C	3.880620	-1.898283	0.588091
C	2.615993	-1.454500	-0.231167
C	0.491876	-0.120618	0.313648
H	2.796372	-1.503926	3.668737
H	2.839712	-0.727898	-1.007208
N	0.438229	-0.731450	2.528308
N	-0.261012	-0.123834	1.477955
N	1.628243	-0.827927	0.656594
C	-1.696750	-0.218085	1.595337
C	-2.354556	-1.376877	1.174472
C	-2.386987	0.828826	2.227371
C	-3.743590	-1.438099	1.334931
C	-3.764316	0.719329	2.372150
C	-4.463806	-0.405365	1.920713
H	-4.267860	-2.326270	0.988379
H	-4.308783	1.530172	2.851069

O	3.866664	-1.457827	1.938164
H	2.538991	-2.915569	2.621960
H	4.760314	-1.413130	0.160514
H	3.969461	-3.927102	1.425262
C	-1.639228	-2.567139	0.589883
H	-1.863492	-3.460987	1.179206
H	-0.555495	-2.446584	0.560241
H	-1.983448	-2.762130	-0.432131
C	-5.956203	-0.498768	2.101610
H	-6.209371	-0.709787	3.145917
H	-6.377617	-1.291206	1.479335
H	-6.440438	0.441861	1.825186
C	-1.644342	2.031745	2.739533
H	-0.854402	1.735423	3.436685
H	-2.323525	2.717776	3.248955
H	-1.161167	2.573197	1.920996
C	0.381910	0.648928	-0.904889
O	1.049131	0.276273	-1.989193
H	1.256159	1.681383	-0.406983
C	-1.059016	1.115917	-1.121794
C	-1.861830	0.059405	-1.874364
H	-1.541842	1.383704	-0.181103
H	-1.592864	0.110110	-2.934577
H	-1.493989	-0.914351	-1.529186
Cl	-1.126379	2.671121	-2.097250
C	-3.363219	0.087500	-1.692319
C	-4.096346	-1.043401	-2.073358
C	-4.052189	1.161693	-1.127783
C	-5.472769	-1.106106	-1.888885
H	-3.571342	-1.889936	-2.511827
C	-5.433797	1.105309	-0.945593
H	-3.515495	2.054316	-0.820943
C	-6.149219	-0.026739	-1.320894
H	-6.018443	-1.997070	-2.184762
H	-5.948978	1.950521	-0.498058
H	-7.223358	-0.071269	-1.169386
N	2.309378	2.596397	-0.331489
C	2.076518	3.346317	0.942739
C	2.002093	2.384468	2.128608
C	0.795322	4.175554	0.862417
H	2.917589	4.033107	1.096181
H	2.869702	1.724989	2.208298
H	1.940031	2.964742	3.053138
H	1.103793	1.765668	2.064126

H	0.913445	5.067730	0.243424
H	-0.026059	3.582526	0.445539
H	0.512971	4.500023	1.867134
C	3.608190	1.822979	-0.308825
C	4.791678	2.555387	0.336272
C	3.994872	1.325367	-1.700555
H	3.398159	0.947906	0.313862
H	4.633238	2.779961	1.392842
H	5.664013	1.899001	0.270955
H	5.036033	3.485681	-0.181260
H	3.126048	0.886805	-2.199330
H	4.408019	2.131343	-2.314605
H	4.777733	0.568283	-1.591627
C	2.141493	3.450569	-1.537906
C	3.109614	4.619216	-1.689458
H	1.120950	3.824340	-1.508165
H	2.176623	2.782389	-2.398209
H	2.769079	5.248974	-2.515642
H	3.143756	5.243288	-0.791261
H	4.126530	4.296608	-1.920299

Vibrational frequencies

-1452.8410	17.8616	22.4922
37.9952	42.3604	50.4239
54.0709	58.3321	64.8314
73.6656	76.6703	85.7793
97.7145	111.1590	116.3110
118.2986	119.2816	134.3416
138.1406	139.7568	151.0152
153.6653	157.9275	164.2933
170.2895	179.8020	186.9038
190.1116	206.8017	210.8673
218.6165	226.9169	233.2473
242.5045	246.3270	252.4936
256.9655	260.8937	272.9420
279.1431	287.9026	294.6266
296.5497	310.4782	312.8048
324.6478	349.7592	363.6487
364.2184	372.4826	390.0885
402.0932	405.1584	417.3229
424.2074	427.5987	443.4974
446.2294	455.0708	458.5918
466.2444	479.0957	483.0972
490.7424	498.2615	502.2567
513.5296	527.4794	529.5529

547.3014 557.9097 573.8010
586.7327 596.2468 609.6391
615.1226 622.1419 629.5865
636.4070 652.4585 671.3281
682.0454 703.5398 714.5821
727.4172 739.6332 748.3501
757.4561 763.8892 779.1579
790.2998 796.5747 811.5937
833.6093 849.6317 861.0953
871.2420 874.3485 875.0873
878.4482 888.3199 906.9252
909.3118 914.2668 923.9256
936.6468 953.8898 959.9488
961.7414 965.3932 966.3835
970.1937 973.0614 980.8413
984.1352 992.2348 996.0741
1005.4099 1015.9863 1018.8291
1027.5768 1034.7142 1037.0689
1040.0520 1043.5828 1048.5565
1054.6585 1062.4110 1063.1294
1064.7152 1067.3683 1070.1259
1080.5035 1083.2443 1084.0155
1106.4879 1115.3569 1119.9576
1135.1858 1143.2803 1147.0963
1156.1198 1170.7382 1172.0501
1175.0011 1176.9948 1196.5592
1198.4966 1201.7616 1205.1322
1210.4306 1213.8345 1218.4897
1222.5894 1230.7962 1235.8220
1237.7538 1249.2072 1266.7852
1278.3071 1282.4669 1283.7343
1299.5258 1312.9951 1319.3649
1326.5766 1338.5375 1339.6456
1341.9968 1353.6673 1359.3101
1365.4875 1367.5170 1370.9004
1372.3276 1374.3858 1377.0305
1382.1223 1384.4615 1402.9964
1406.4584 1410.4816 1412.3622
1415.8016 1417.8615 1419.8046
1424.7364 1426.0855 1430.1420
1435.4910 1438.1977 1458.0111
1466.2472 1466.9743 1475.3488
1480.9711 1481.8043 1484.7183
1487.1000 1489.0107 1493.1194

1496.5459	1496.9075	1499.8892
1503.5402	1504.7321	1505.8829
1506.7507	1508.4128	1514.0739
1514.3198	1517.5900	1518.8674
1524.8272	1528.8757	1536.3936
1541.7323	1546.7290	1549.2501
1555.7062	1562.1599	1674.3997
1680.0239	1680.7418	1697.9318
1699.6733	1700.3494	1726.9787
3057.2978	3066.7725	3067.2662
3067.8873	3068.2305	3072.9683
3077.6145	3080.8120	3086.0091
3086.3449	3087.1300	3087.4400
3122.6761	3124.9838	3126.4501
3133.5109	3135.2003	3140.3690
3143.9806	3146.5968	3149.9927
3151.3222	3156.1823	3156.5903
3157.5438	3159.4149	3160.9861
3161.8507	3164.9558	3165.9045
3168.6398	3170.9308	3173.6556
3178.1747	3178.7047	3185.0710
3186.3193	3186.6314	3196.3461
3199.0243	3199.3762	3208.4874
3208.7972	3210.4917	3219.8063
3222.8527	3224.9726	3225.6284

***Re*-TS2[c]**

Zero-point correction= 0.542586
Thermal correction to Energy= 0.573824
Thermal correction to Enthalpy= 0.574768
Thermal correction to Gibbs Free Energy= 0.479703
Sum of electronic and zero-point Energies= -1934.915608
Sum of electronic and thermal Energies= -1934.884369
Sum of electronic and thermal Enthalpies= -1934.883425
Sum of electronic and thermal Free Energies= -1934.978490
Cartesian coordinates

C	-4.645216	0.275699	0.250655
C	-3.321083	0.417267	-0.150119
C	-2.596006	1.575548	0.101647
C	-3.226947	2.609447	0.789456
C	-4.557425	2.477984	1.198766
C	-5.277254	1.315221	0.929550
C	-5.192025	-1.069625	-0.156873
H	-1.567262	1.655918	-0.243198

H	-2.683154	3.521007	1.015714
H	-5.035212	3.291201	1.735975
H	-6.309575	1.219513	1.252828
H	-5.918368	-0.965284	-0.969180
C	-1.603597	-2.003538	0.954749
C	-2.933562	-2.500390	1.415072
C	-3.963657	-1.883141	-0.637237
C	-2.814384	-0.827595	-0.836451
C	-0.257942	-0.979713	-0.470523
H	-2.808796	-3.355314	2.079419
H	-2.601024	-0.644319	-1.887831
N	-0.425600	-2.199845	1.446978
N	0.415086	-1.553267	0.562966
N	-1.568615	-1.284154	-0.211432
C	1.767184	-1.306969	0.962692
C	2.030430	-0.128500	1.663938
C	2.756521	-2.232625	0.619377
C	3.359653	0.133147	1.999773
C	4.066926	-1.928843	0.978075
C	4.385416	-0.749314	1.659903
H	3.595714	1.051362	2.532204
H	4.860871	-2.624112	0.715960
O	-3.629496	-2.931757	0.261288
H	-3.478950	-1.709048	1.948144
H	-4.164244	-2.392967	-1.579780
H	-5.695231	-1.599212	0.658215
C	0.915402	0.822942	2.005192
H	0.084673	0.296003	2.485151
H	0.528381	1.309318	1.100403
H	1.269891	1.607611	2.674921
C	5.816568	-0.452655	2.026317
H	5.914890	0.539550	2.470833
H	6.462021	-0.500020	1.144829
H	6.192914	-1.186330	2.745420
C	2.395378	-3.488514	-0.126922
H	3.285583	-4.084684	-0.332878
H	1.913776	-3.248017	-1.080313
H	1.693132	-4.094942	0.452810
C	0.217152	-0.344243	-1.656281
O	-0.753892	0.439762	-2.406917
H	-0.317667	-0.808464	-2.590107
C	1.670258	-0.009112	-1.870253
C	1.890591	1.415017	-2.371131
H	2.294017	-0.197980	-1.000084

H	2.921794	1.502655	-2.722987
H	1.210533	1.595270	-3.204919
Cl	2.402681	-1.160240	-3.143105
C	1.646237	2.405091	-1.257855
C	0.422559	3.068312	-1.140756
C	2.649978	2.666362	-0.319415
C	0.212401	3.986512	-0.111946
H	-0.361081	2.842392	-1.858726
C	2.439650	3.577312	0.711975
H	3.605195	2.151771	-0.401487
C	1.219083	4.243155	0.816235
H	-0.736309	4.511055	-0.044906
H	3.229254	3.770711	1.432145
H	1.055933	4.960827	1.614007

Vibrational frequencies

-1762.9397	19.4647	28.3219
38.7022	40.2359	44.0570
62.8433	70.0991	70.5803
75.8658	85.6068	94.0566
101.1440	115.1663	116.1643
133.6887	155.5433	158.6000
180.2976	186.1605	195.3719
210.1985	222.7564	233.3536
249.7879	254.7825	271.3904
280.3342	289.0166	309.9696
316.2135	332.8391	358.6363
374.6986	389.8083	399.8100
409.7958	422.5176	437.9372
448.8935	472.1551	491.2799
495.1670	508.8528	521.4929
530.2603	531.4771	553.7689
567.9494	586.2123	589.9613
598.4440	611.9786	617.0879
630.5961	634.0569	661.9387
674.4677	705.8760	716.9139
726.5804	734.4818	755.6864
770.8123	773.3379	782.2039
807.3026	835.5056	850.4528
857.7164	873.1527	877.0635
884.2755	891.2739	912.3285
916.2393	922.7304	938.9896
951.2665	955.4769	961.4661
979.3814	982.3627	987.0741
1002.0302	1016.6624	1018.4024

1026.0907	1027.2069	1031.5012
1038.4796	1050.9609	1053.3672
1059.9032	1063.4717	1064.7834
1066.9889	1067.9281	1073.4550
1076.4647	1091.5415	1118.3096
1121.2477	1151.7426	1162.2300
1173.2497	1177.5131	1183.2865
1196.2826	1200.2125	1208.1490
1210.4418	1217.9490	1225.9745
1241.9658	1245.1902	1248.5937
1259.1101	1278.9905	1280.4681
1303.4820	1312.3713	1325.9519
1339.1901	1341.3917	1347.2128
1355.7915	1356.0470	1366.4889
1374.3689	1379.6044	1385.3567
1403.8350	1413.5768	1418.6887
1422.5169	1429.1940	1451.2185
1467.3358	1474.4590	1474.6312
1482.8397	1486.0744	1492.9843
1494.2007	1498.5511	1499.3775
1502.9445	1508.7151	1518.1477
1524.3281	1541.8373	1555.8440
1558.1640	1586.1707	1676.9334
1684.4633	1686.8842	1695.3318
1699.2169	1701.7087	1720.2225
2677.9910	3060.9266	3062.6678
3067.1395	3076.9457	3088.3385
3098.8964	3130.5560	3136.0849
3137.6810	3146.6551	3154.3961
3169.6521	3170.0688	3171.1740
3171.3544	3178.2845	3184.4431
3186.1757	3187.2463	3194.6506
3197.9577	3198.4742	3203.1652
3209.0865	3215.6195	3216.3940
3216.7898	3226.1277	3233.0076

***Si*-TS2**

Zero-point correction= 0.825604
Thermal correction to Energy= 0.868614
Thermal correction to Enthalpy= 0.869558
Thermal correction to Gibbs Free Energy= 0.752239
Sum of electronic and zero-point Energies= -2306.011507
Sum of electronic and thermal Energies= -2305.968498
Sum of electronic and thermal Enthalpies= -2305.967553

Sum of electronic and thermal Free Energies= -2306.084873

Cartesian coordinates

C	-5.367924	-1.176649	-0.348804
C	-4.132436	-0.847780	0.212555
C	-3.961822	-0.793782	1.589336
C	-5.071146	-1.009452	2.408118
C	-6.318975	-1.286101	1.849982
C	-6.473433	-1.383738	0.466617
C	-5.241545	-1.332602	-1.845866
H	-2.984120	-0.621811	2.028914
H	-4.956988	-0.975733	3.486352
H	-7.170941	-1.457789	2.499660
H	-7.434668	-1.647342	0.036244
H	-5.570783	-0.429135	-2.372265
C	-1.751590	-2.577590	-0.277066
C	-2.934902	-3.399751	-0.690038
C	-3.730135	-1.531192	-2.045131
C	-3.106337	-0.686559	-0.899119
C	-0.543290	-0.725511	-0.362025
H	-2.616765	-4.431679	-0.839536
H	-2.983481	0.349856	-1.208264
N	-0.582188	-2.940121	0.137909
N	0.161074	-1.785230	0.107813
N	-1.795475	-1.233390	-0.544628
C	1.482260	-1.880761	0.675601
C	1.675930	-1.372186	1.966205
C	2.463588	-2.600347	-0.007641
C	2.929116	-1.538027	2.543733
C	3.700290	-2.755928	0.623424
C	3.953298	-2.228308	1.885553
H	3.108283	-1.132557	3.536537
H	4.490988	-3.284758	0.097811
O	-3.358144	-2.906257	-1.953648
H	-3.730946	-3.373408	0.060921
H	-3.380523	-1.199234	-3.025211
H	-5.801048	-2.180806	-2.246470
C	0.560820	-0.666293	2.686638
H	-0.343512	-1.284084	2.718741
H	0.302141	0.265694	2.173649
H	0.850043	-0.421393	3.709324
C	5.294086	-2.405368	2.545951
H	5.243877	-3.178737	3.319222
H	5.614788	-1.476894	3.025605
H	6.054841	-2.695979	1.818513

C	2.214101	-3.216440	-1.357706
H	1.532544	-2.619519	-1.970522
H	1.759070	-4.205439	-1.246117
H	3.155584	-3.330608	-1.898919
C	-0.086102	0.619172	-0.793912
O	-1.010117	1.063143	-1.780726
H	-0.221740	1.920146	-0.035933
C	1.387678	0.503309	-1.312613
C	2.446882	1.019504	-0.344803
H	1.615710	-0.535133	-1.564691
H	2.481804	2.111891	-0.402376
H	2.110843	0.780795	0.670873
Cl	1.570471	1.354234	-2.907130
C	3.844180	0.458653	-0.522286
C	4.769779	0.672589	0.504451
C	4.246602	-0.280536	-1.636717
C	6.055252	0.148062	0.432278
H	4.469129	1.243856	1.380190
C	5.531264	-0.818180	-1.707257
H	3.562509	-0.456731	-2.461220
C	6.437983	-0.611506	-0.672723
H	6.756309	0.321354	1.242972
H	5.819986	-1.399390	-2.577550
H	7.437543	-1.030634	-0.728936
H	-0.861588	0.591910	-2.615997
N	-0.497179	3.090256	0.419551
C	-0.260454	4.237528	-0.538711
C	-1.014132	4.069367	-1.856675
C	1.213864	4.483916	-0.844592
H	-0.642602	5.127277	-0.028132
H	-2.074023	3.845795	-1.727989
H	-0.936674	5.010195	-2.407288
H	-0.568411	3.271804	-2.451478
H	1.817939	4.702258	0.038042
H	1.649366	3.645386	-1.391788
H	1.271690	5.357996	-1.497899
C	-1.972754	2.948609	0.737378
C	-2.733839	4.257990	0.958312
C	-2.195606	2.011628	1.916219
H	-2.382550	2.460602	-0.153103
H	-2.767406	4.892081	0.071594
H	-3.765056	4.001449	1.213656
H	-2.323607	4.840289	1.785210
H	-1.646069	1.074743	1.791167

H	-1.906376	2.465702	2.868304
H	-3.259005	1.771182	1.970882
C	0.390850	3.177296	1.616598
C	0.297262	4.435269	2.472049
H	1.409768	3.057044	1.247755
H	0.189352	2.300006	2.232015
H	1.107214	4.408958	3.204904
H	0.412294	5.350418	1.886073
H	-0.642227	4.492583	3.024371

Vibrational frequencies

-1253.0146	21.7457	27.5662
39.9301	40.4774	46.8132
54.5018	54.8010	63.4445
68.5291	81.5171	85.1393
89.4351	95.5496	101.8265
105.7163	111.4148	118.2972
125.0849	131.8674	141.0744
145.9444	150.6855	157.7649
166.8844	178.3962	181.3561
184.0708	207.3774	214.5838
222.1501	237.2954	241.2253
247.1310	255.6803	259.7437
265.9618	272.6382	276.7895
284.5220	284.6176	310.1591
311.2941	320.6242	324.9918
329.4481	348.7392	351.0708
362.7112	373.9484	385.1209
396.0076	401.1041	417.5492
421.1244	429.9674	433.5896
445.6908	451.3385	453.2846
463.9309	482.2261	485.8659
488.0884	496.5490	501.3661
505.3928	508.0643	521.3150
534.8763	552.9449	554.2653
581.1453	589.7278	593.9957
612.2930	614.2701	623.4618
630.5454	648.2592	659.5578
683.2079	716.2893	724.2190
733.4053	745.8777	754.4734
757.4274	765.7649	766.4238
774.0220	791.1735	807.8654
819.6063	836.0779	846.4920
852.5761	871.2545	882.7767
884.1613	896.3731	898.8110

906.7967 918.9769 925.6164
935.7087 942.2225 952.8502
954.2922 963.3540 964.6620
967.4494 975.5086 979.2628
980.5825 986.1536 989.0668
991.0928 1005.6037 1011.5035
1016.2448 1024.1209 1029.0059
1036.6158 1039.6306 1041.6781
1053.0224 1058.1547 1061.3256
1065.5974 1066.8452 1071.8915
1076.6671 1081.2839 1088.8939
1094.2895 1107.2790 1110.2011
1117.2158 1128.0486 1141.5246
1143.3135 1146.4777 1163.5100
1171.8373 1177.8999 1178.7068
1184.9852 1195.0436 1201.0052
1214.8818 1217.8208 1218.6489
1221.5566 1222.5513 1225.8197
1230.9259 1238.7131 1249.4982
1262.2322 1269.5247 1288.6626
1290.7945 1302.8929 1304.3788
1315.2812 1323.9016 1335.0836
1343.6554 1344.9685 1347.2043
1352.8576 1358.9596 1368.6850
1371.5760 1374.1842 1376.1151
1377.1477 1383.0325 1385.7772
1400.4310 1402.8159 1411.6209
1414.2315 1417.1345 1417.7941
1418.7554 1428.7112 1430.1386
1433.6009 1440.2740 1443.1007
1446.2716 1465.7373 1472.7747
1473.0994 1483.2573 1484.5744
1487.0818 1488.2242 1489.4919
1492.1394 1495.6696 1501.2017
1502.9121 1503.1855 1505.0640
1505.8262 1507.3018 1511.3105
1514.6421 1516.4248 1518.0823
1522.3031 1523.7525 1525.1827
1527.8276 1534.2667 1544.2749
1554.5646 1556.8296 1602.1257
1665.9491 1675.1243 1682.4941
1684.8017 1696.7965 1700.6836
1703.6683 1709.9376 3068.5784
3072.7866 3074.9651 3075.3011

3081.1472	3081.2775	3086.6432
3090.7768	3093.5694	3095.7871
3108.8575	3109.6492	3111.2679
3134.6706	3136.3228	3140.7127
3142.5031	3143.4495	3147.3269
3147.4166	3149.4882	3158.1651
3160.3257	3163.6458	3163.8778
3165.4057	3166.8655	3169.2378
3171.5862	3175.9763	3179.6092
3185.5877	3186.4482	3188.4191
3190.1884	3193.8164	3195.0005
3199.7097	3202.3187	3203.2378
3206.4758	3210.7468	3216.1189
3219.7230	3219.9761	3226.4299
3235.1886	3238.3501	3775.9921

M2

Zero-point correction= 0.545745
Thermal correction to Energy= 0.577941
Thermal correction to Enthalpy= 0.578885
Thermal correction to Gibbs Free Energy= 0.480104
Sum of electronic and zero-point Energies= -1934.994889
Sum of electronic and thermal Energies= -1934.962694
Sum of electronic and thermal Enthalpies= -1934.961749
Sum of electronic and thermal Free Energies= -1935.060530
Cartesian coordinates

C	5.034641	-1.097262	0.477612
C	3.662239	-1.166817	0.253302
C	2.818825	-1.844726	1.130220
C	3.377072	-2.450691	2.253250
C	4.753504	-2.381542	2.485161
C	5.591249	-1.708546	1.598811
C	5.730361	-0.326875	-0.615267
H	1.751259	-1.900194	0.935500
H	2.740133	-2.983372	2.952041
H	5.173981	-2.857275	3.365494
H	6.660446	-1.657100	1.782518
H	6.355504	-0.988154	-1.223409
C	2.539983	1.785960	-0.202124
C	3.981523	2.171374	-0.183865
C	4.597206	0.284461	-1.476767
C	3.270217	-0.422404	-1.003598
C	0.844797	0.406010	-0.635448
H	4.085846	3.255986	-0.155652

H	2.907409	-1.102429	-1.771253
N	1.508925	2.455076	0.177089
N	0.438464	1.617257	-0.109835
N	2.221066	0.564755	-0.748922
C	-0.855567	1.951908	0.383072
C	-1.217386	1.524882	1.665033
C	-1.731344	2.656011	-0.448707
C	-2.510603	1.806311	2.103964
C	-3.016327	2.909759	0.027203
C	-3.425118	2.481835	1.292822
H	-2.816601	1.476999	3.094616
H	-3.718507	3.444302	-0.608006
O	4.554003	1.699887	-1.388201
H	4.484753	1.742567	0.695227
H	4.755810	0.088508	-2.537409
H	6.381598	0.467079	-0.235075
C	-0.244585	0.736041	2.499621
H	0.720828	1.246152	2.569142
H	-0.059494	-0.243185	2.040850
H	-0.633520	0.576813	3.506672
C	-4.840161	2.711394	1.755242
H	-4.914453	2.670055	2.844146
H	-5.501175	1.940657	1.344600
H	-5.215725	3.680022	1.416899
C	-1.289117	3.082893	-1.822101
H	-1.058364	2.207037	-2.437453
H	-0.382615	3.692349	-1.767536
H	-2.071860	3.657339	-2.320107
C	0.110073	-0.719775	-0.925884
O	0.793295	-1.833240	-1.420348
H	0.568045	-1.920323	-2.359440
C	-1.333191	-0.841778	-0.867428
C	-1.853888	-2.179524	-0.344698
H	-1.829460	-0.010087	-0.377020
H	-1.563513	-2.981766	-1.026846
H	-1.327179	-2.355698	0.602572
Cl	-2.067971	-0.683679	-2.674292
C	-3.342096	-2.171778	-0.100264
C	-4.222709	-2.884305	-0.913948
C	-3.863185	-1.414058	0.953276
C	-5.596371	-2.842371	-0.681691
H	-3.828154	-3.471273	-1.739125
C	-5.233981	-1.366662	1.187582
H	-3.184390	-0.852089	1.592446

C	-6.105719	-2.083289	0.368657
H	-6.268515	-3.403585	-1.323310
H	-5.620981	-0.776791	2.013318
H	-7.175218	-2.051423	0.550407

Vibrational frequencies

20.3262	22.8239	25.7016
29.0003	37.6621	50.1758
51.7566	56.6223	60.1947
71.5924	90.9648	103.4841
109.0723	117.0453	134.9388
138.3801	142.1796	174.2068
187.2508	192.5628	204.2742
208.7938	217.1141	226.2779
241.1256	250.1977	270.4236
279.7579	284.0071	299.1475
313.4812	360.4259	362.7352
368.4678	387.6499	400.7952
418.6928	424.8393	431.4083
444.1454	449.2568	484.3407
491.3760	504.6364	523.0982
524.9678	532.6055	538.7552
558.7086	581.8983	585.5692
589.3002	597.6014	609.6608
618.3240	630.9918	647.4677
659.3390	691.4465	715.4849
718.0740	737.2325	753.5970
767.0669	774.4172	780.8932
810.6862	835.7995	858.3899
868.5236	873.3922	879.3203
880.7248	889.9564	910.2752
913.0782	915.0623	950.7740
956.2551	964.8570	976.8306
987.0191	993.8702	998.6386
1017.9942	1018.6069	1021.5262
1027.0909	1038.1960	1042.0129
1049.2344	1055.3831	1061.0981
1062.2432	1065.7664	1067.8263
1069.0175	1070.4032	1079.0036
1096.0870	1117.4347	1121.3218
1152.4906	1159.4075	1174.5841
1178.5980	1182.9005	1195.7947
1201.4246	1202.4613	1214.6660
1219.5759	1237.1755	1243.1125
1248.4208	1257.3266	1268.8735

1279.1342	1280.6945	1297.6354
1304.2258	1314.6504	1319.4659
1330.2550	1338.2047	1342.6930
1352.2144	1355.1989	1361.5614
1372.5774	1381.4952	1386.4419
1413.9593	1417.9468	1422.1642
1425.0554	1429.6815	1450.2183
1466.7252	1473.8169	1483.3285
1487.0880	1488.2167	1491.3418
1493.3181	1494.3556	1496.9581
1498.5274	1506.3256	1517.9575
1523.7996	1543.1753	1553.6174
1562.8329	1678.1336	1680.4310
1681.7998	1683.8921	1700.2626
1702.3513	1702.6806	1745.7056
3059.1348	3060.8567	3062.3053
3068.3716	3071.3023	3085.8614
3128.8455	3129.6912	3139.8016
3140.4262	3140.5109	3152.1296
3168.0257	3171.4018	3172.7555
3178.3476	3183.4068	3185.9750
3187.4615	3190.3426	3192.8373
3197.6008	3200.0758	3205.7794
3210.1132	3215.8134	3222.9390
3223.4512	3242.1383	3778.4053

TS3

Zero-point correction= 0.545081
Thermal correction to Energy= 0.576781
Thermal correction to Enthalpy= 0.577725
Thermal correction to Gibbs Free Energy= 0.480057
Sum of electronic and zero-point Energies= -1934.995469
Sum of electronic and thermal Energies= -1934.963769
Sum of electronic and thermal Enthalpies= -1934.962825
Sum of electronic and thermal Free Energies= -1935.060493
Cartesian coordinates

C	5.067934	-1.060008	0.459153
C	3.693375	-1.157286	0.260689
C	2.877009	-1.835343	1.162790
C	3.465430	-2.413733	2.284752
C	4.844401	-2.317060	2.490985
C	5.654602	-1.643724	1.579869
C	5.731150	-0.294934	-0.657224
H	1.807050	-1.911962	0.988745

H	2.850433	-2.946087	3.003074
H	5.288232	-2.771974	3.370815
H	6.725724	-1.570583	1.743806
H	6.364051	-0.952380	-1.261263
C	2.528085	1.782983	-0.231810
C	3.963219	2.190093	-0.263837
C	4.573362	0.274069	-1.515267
C	3.265619	-0.439016	-0.999316
C	0.843678	0.376336	-0.589654
H	4.050451	3.276492	-0.271736
H	2.888804	-1.133183	-1.746721
N	1.494295	2.448399	0.151271
N	0.434706	1.585196	-0.078314
N	2.211163	0.541271	-0.729168
C	-0.862415	1.928609	0.404484
C	-1.229774	1.507454	1.686722
C	-1.730247	2.632122	-0.435547
C	-2.525098	1.791924	2.116705
C	-3.016246	2.891894	0.034531
C	-3.433221	2.467839	1.298628
H	-2.837091	1.466219	3.106580
H	-3.713264	3.427090	-0.605706
O	4.509294	1.690370	-1.468555
H	4.495916	1.796363	0.614177
H	4.715746	0.048745	-2.572318
H	6.368537	0.520939	-0.300462
C	-0.263769	0.720277	2.530689
H	0.704461	1.225148	2.599555
H	-0.084420	-0.264603	2.081714
H	-0.656857	0.573191	3.537890
C	-4.850005	2.702658	1.752723
H	-4.930319	2.664007	2.841290
H	-5.510731	1.932772	1.340073
H	-5.220819	3.671550	1.410027
C	-1.284215	3.047254	-1.811178
H	-1.111264	2.163094	-2.434283
H	-0.347968	3.610461	-1.765916
H	-2.044375	3.663748	-2.293756
C	0.108139	-0.769331	-0.841959
O	0.797978	-1.880972	-1.329946
H	0.560174	-1.979730	-2.265286
C	-1.317778	-0.878542	-0.795836
C	-1.884415	-2.226747	-0.369939
H	-1.832167	-0.049494	-0.322506

H	-1.623015	-2.993147	-1.102868
H	-1.366745	-2.486129	0.563480
Cl	-2.051632	-0.640185	-2.685068
C	-3.372171	-2.181792	-0.125404
C	-4.271456	-2.846126	-0.958764
C	-3.872581	-1.441788	0.950481
C	-5.643333	-2.775232	-0.723465
H	-3.892719	-3.416284	-1.802831
C	-5.241591	-1.364684	1.187417
H	-3.179197	-0.917661	1.606158
C	-6.132188	-2.034296	0.349257
H	-6.330644	-3.297994	-1.381331
H	-5.612109	-0.788729	2.030381
H	-7.200445	-1.979215	0.532804

Vibrational frequencies

-137.4024	20.4472	21.0143
29.3947	34.3378	39.2389
47.5280	54.3402	60.1665
60.8143	78.3576	92.4727
102.4655	108.3523	111.1098
120.1996	141.7252	146.7783
180.3985	188.1548	192.6876
203.9926	208.6383	216.7715
228.8981	242.1664	260.7363
279.4701	284.0798	300.2693
314.4225	353.5140	362.7541
368.5524	388.0137	400.6270
416.2141	419.6199	437.3979
446.7038	450.5101	485.0374
491.3205	505.1305	514.7810
524.5457	533.2464	536.3957
557.9937	580.2855	584.2507
589.2483	597.8245	609.5981
620.0310	631.0688	648.0566
669.2862	695.3734	714.6165
716.2682	737.4803	754.7898
765.2409	773.3750	780.7557
811.9527	835.1617	859.5873
867.7995	869.5856	879.0689
879.8008	889.2752	901.0458
912.0581	913.3743	946.9091
956.9361	965.7971	978.8896
986.0130	994.6058	997.5000
1018.3619	1018.4534	1019.4388

1027.6910	1039.1749	1042.7105
1049.2788	1055.9199	1060.8233
1062.9440	1066.7554	1067.5502
1068.9359	1069.5466	1082.2668
1100.0705	1114.5252	1121.6828
1133.7328	1152.9983	1173.6650
1178.2656	1182.4146	1197.5726
1201.1964	1202.3948	1216.1400
1223.0504	1230.2194	1242.8761
1244.2877	1258.5389	1271.3417
1278.6988	1281.9152	1299.1645
1307.1817	1314.0243	1324.4892
1332.8963	1339.3466	1343.4448
1351.7664	1356.5945	1361.2994
1372.3781	1382.1592	1387.0590
1414.5973	1417.6409	1421.3155
1429.0536	1436.5938	1458.5333
1466.8068	1467.7846	1483.9734
1485.1341	1488.9006	1491.0386
1493.0862	1494.4480	1498.0772
1500.6072	1506.2789	1517.9097
1523.7983	1542.4587	1553.2444
1563.3701	1651.3528	1679.9271
1682.0417	1682.9834	1699.3688
1702.0563	1702.1187	1737.9662
3058.1061	3061.5073	3064.6730
3064.8083	3068.9174	3086.6604
3129.7163	3130.2147	3137.7343
3140.4144	3141.9929	3152.5038
3166.4187	3168.3642	3172.3842
3177.9195	3179.1261	3186.7689
3191.1711	3192.5832	3198.3476
3199.0604	3200.6550	3206.6639
3207.9004	3215.4215	3220.6135
3223.4046	3256.0251	3768.4741

M3

Zero-point correction= 0.546409
Thermal correction to Energy= 0.578164
Thermal correction to Enthalpy= 0.579109
Thermal correction to Gibbs Free Energy= 0.481522
Sum of electronic and zero-point Energies= -1935.032927
Sum of electronic and thermal Energies= -1935.001171
Sum of electronic and thermal Enthalpies= -1935.000227

Sum of electronic and thermal Free Energies= -1935.097813

Cartesian coordinates

C	5.213020	0.127745	-0.669344
C	3.846564	0.266740	-0.894476
C	3.253727	-0.167464	-2.076423
C	4.062293	-0.756149	-3.044843
C	5.435348	-0.899430	-2.826436
C	6.020064	-0.458101	-1.641819
C	5.606966	0.681551	0.675571
H	2.184745	-0.053057	-2.241757
H	3.625430	-1.105694	-3.974265
H	6.052711	-1.362298	-3.589555
H	7.086709	-0.575296	-1.476344
H	6.192112	1.599428	0.563248
C	2.249395	-1.021474	1.532364
C	3.609277	-1.187693	2.126878
C	4.275533	0.984641	1.403256
C	3.163317	0.912614	0.289718
C	0.750857	0.057395	0.366715
H	3.558786	-1.800194	3.026516
H	2.752493	1.896478	0.062598
N	1.156739	-1.709779	1.683944
N	0.228968	-1.027498	0.952769
N	2.041669	0.077294	0.745707
C	-1.131257	-1.495486	0.883981
C	-1.380663	-2.634674	0.109883
C	-2.129760	-0.763268	1.527094
C	-2.706820	-3.033565	-0.021338
C	-3.442686	-1.207185	1.358292
C	-3.748973	-2.328177	0.589492
H	-2.935403	-3.909873	-0.622851
H	-4.245537	-0.649608	1.832620
O	4.039118	0.107437	2.494473
H	4.291046	-1.661221	1.406929
H	4.277364	1.976448	1.854157
H	6.209172	-0.012561	1.270118
C	-0.260148	-3.372502	-0.574825
H	0.398351	-3.853304	0.154052
H	0.359290	-2.693716	-1.172192
H	-0.660274	-4.139744	-1.238734
C	-5.172639	-2.793099	0.433994
H	-5.359961	-3.675448	1.054437
H	-5.381788	-3.068108	-0.603186
H	-5.874628	-2.010915	0.729326

C	-1.825820	0.469791	2.332393
H	-1.728350	1.354666	1.689938
H	-0.896744	0.363168	2.899688
H	-2.635725	0.666561	3.037111
C	0.069671	1.057936	-0.473776
O	0.600562	2.298339	-0.375191
H	-0.042378	2.927230	0.096538
C	-0.965291	0.690231	-1.242262
C	-1.873768	1.629296	-1.975840
H	-1.241122	-0.359550	-1.274290
H	-1.621739	2.664107	-1.730750
H	-1.761607	1.489852	-3.057510
Cl	-1.250236	4.081366	1.001606
C	-3.295672	1.297455	-1.558359
C	-3.884319	1.941144	-0.467222
C	-3.996074	0.277334	-2.207186
C	-5.162962	1.578728	-0.046824
H	-3.330953	2.723638	0.048659
C	-5.271244	-0.087421	-1.784553
H	-3.538547	-0.232206	-3.052353
C	-5.859391	0.565304	-0.702689
H	-5.615954	2.089805	0.797474
H	-5.807502	-0.877616	-2.301572
H	-6.856315	0.286197	-0.375017

Vibrational frequencies

12.9838	21.2408	25.5820
34.6675	46.8104	55.3617
65.3649	70.7517	76.2105
80.5761	89.9494	99.4028
104.0405	117.5049	125.3861
144.4252	155.7780	173.3617
186.1887	191.4646	198.5318
208.2055	217.5859	224.7063
244.2961	254.5449	274.3093
282.9389	296.8685	321.5220
330.6999	345.3799	355.8998
367.3340	391.5326	403.6220
421.1878	432.0010	436.5649
445.9777	486.2511	499.5548
502.2094	515.9371	526.4332
528.5209	538.5332	570.0956
584.9621	588.8454	596.1218
608.0050	616.7687	627.3375
630.8701	652.6425	692.5329

704.5790 720.8934 727.4651
738.1722 746.2376 768.5604
771.7432 777.9787 789.5711
809.6916 831.2415 839.2209
863.3096 876.0164 887.8257
889.3188 891.1565 906.8319
916.4051 925.3358 955.0757
956.5292 966.5043 968.8295
982.5271 988.7201 1014.7811
1016.5908 1024.0178 1026.6074
1032.0743 1037.7621 1041.3587
1043.4697 1051.5025 1051.7726
1058.4812 1064.1962 1064.5409
1069.9382 1070.9791 1071.5468
1094.2603 1117.9105 1121.1111
1140.8903 1153.9419 1176.1799
1178.0025 1182.4010 1198.3835
1210.7350 1213.3853 1219.6778
1226.4361 1235.4522 1239.9099
1249.0811 1268.9119 1281.6803
1288.7289 1309.2936 1310.9660
1313.2974 1326.3579 1338.0206
1339.7154 1344.1027 1356.5248
1360.0623 1369.1505 1371.6366
1380.4153 1386.5731 1420.2344
1421.2410 1423.0784 1431.0082
1434.1259 1462.6265 1467.7937
1477.4636 1479.9850 1484.6928
1489.1488 1493.5862 1496.3774
1497.8426 1500.1780 1510.6369
1514.9346 1523.7430 1529.2627
1544.9466 1545.9645 1553.8284
1594.4011 1677.9509 1682.9981
1686.9630 1692.8852 1696.4022
1698.9544 1700.7160 1751.6379
2884.6045 3057.4092 3065.4416
3069.3103 3074.8846 3076.4661
3089.6239 3130.2366 3134.6575
3134.8022 3142.3545 3157.2415
3164.4789 3168.6167 3168.7806
3173.7694 3186.8840 3190.4102
3192.2487 3196.7343 3197.4149
3203.9078 3206.9017 3207.1675
3216.9017 3217.4723 3219.9326

3229.3522 3229.3975 3233.7288

TS4

Zero-point correction= 0.812147
Thermal correction to Energy= 0.855819
Thermal correction to Enthalpy= 0.856763
Thermal correction to Gibbs Free Energy= 0.736478
Sum of electronic and zero-point Energies= -2305.651868
Sum of electronic and thermal Energies= -2305.608196
Sum of electronic and thermal Enthalpies= -2305.607252
Sum of electronic and thermal Free Energies= -2305.727538
Cartesian coordinates

C	4.373798	-1.779427	-0.968964
C	3.105407	-1.211386	-1.074088
C	2.659335	-0.631350	-2.256179
C	3.518221	-0.630717	-3.354674
C	4.792974	-1.194220	-3.257643
C	5.230686	-1.770695	-2.065474
C	4.600941	-2.329571	0.417833
H	1.668043	-0.188488	-2.302278
H	3.194552	-0.189378	-4.292046
H	5.447739	-1.189199	-4.123243
H	6.219585	-2.214247	-1.997318
H	5.260129	-1.668239	0.991763
C	0.713771	-3.101478	-0.099804
C	1.867129	-4.047617	-0.058556
C	3.198722	-2.368248	1.063772
C	2.366381	-1.328622	0.239983
C	-0.169131	-1.119573	0.142879
H	1.513624	-5.066094	0.100091
H	2.317006	-0.380527	0.772130
N	-0.569437	-3.307997	-0.161436
N	-1.107702	-2.058985	-0.029769
N	0.995300	-1.780036	0.063114
C	-2.530546	-1.883347	-0.152257
C	-3.028948	-1.280373	-1.308644
C	-3.338303	-2.309418	0.905805
C	-4.407489	-1.085922	-1.380439
C	-4.708832	-2.089706	0.782408
C	-5.257368	-1.475488	-0.345930
H	-4.822859	-0.598161	-2.258116
H	-5.362865	-2.398232	1.594573
O	2.656368	-3.685203	1.057934
H	2.433664	-4.003639	-0.998580

H	3.196599	-2.075149	2.113460
H	5.048820	-3.326901	0.426801
C	-2.116779	-0.822475	-2.414567
H	-2.693199	-0.598544	-3.313924
H	-1.371045	-1.585140	-2.660588
H	-1.581777	0.087970	-2.120883
C	-6.744638	-1.260242	-0.448005
H	-7.259926	-2.204438	-0.651851
H	-6.984794	-0.560040	-1.250905
H	-7.146574	-0.862044	0.487640
C	-2.742175	-2.959124	2.125386
H	-2.370755	-3.960435	1.885737
H	-3.493989	-3.051362	2.911044
H	-1.889596	-2.388161	2.511787
C	-0.335764	0.353344	0.215109
O	0.631345	1.014475	-0.401450
C	-1.457875	0.838821	0.784427
C	-1.918644	2.259251	0.632729
H	-2.127701	0.153624	1.293053
H	-2.004382	2.762784	1.604256
H	-1.189297	2.807128	0.030300
C	-3.263274	2.268616	-0.067661
C	-3.340995	2.428760	-1.453355
C	-4.440926	2.049461	0.651161
C	-4.570272	2.383777	-2.107131
H	-2.427894	2.594674	-2.020755
C	-5.671048	1.999216	0.001178
H	-4.390359	1.915686	1.729230
C	-5.739813	2.170059	-1.380297
H	-4.614866	2.517435	-3.183924
H	-6.578621	1.828882	0.572777
H	-6.699530	2.136804	-1.887273
N	1.988571	2.873683	0.532823
C	2.236660	2.838881	2.017973
C	2.832988	1.505163	2.463756
C	0.940589	3.059611	2.795791
H	2.939157	3.647768	2.245962
H	3.723907	1.206633	1.906629
H	3.125423	1.598900	3.512604
H	2.079657	0.709156	2.419429
H	0.536602	4.068841	2.696777
H	0.185849	2.327370	2.483573
H	1.141831	2.889230	3.855586
C	3.212924	2.540897	-0.291752

C	4.495590	3.244719	0.145891
C	2.943017	2.742069	-1.779382
H	3.342919	1.462994	-0.146501
H	4.769727	3.021855	1.178792
H	5.308344	2.890510	-0.493541
H	4.431917	4.328239	0.032735
H	2.000179	2.272745	-2.071683
H	2.927134	3.800667	-2.055644
H	3.746367	2.258325	-2.340237
C	1.258195	4.101862	0.099716
C	1.979854	5.431574	0.275428
H	0.326542	4.114169	0.663866
H	0.977305	3.951044	-0.944120
H	1.263251	6.237565	0.100705
H	2.377972	5.556389	1.285812
H	2.795722	5.557310	-0.438326
H	1.250293	1.975230	0.210019
Cl	0.632069	-1.418519	3.227709

Vibrational frequencies

-126.6383	21.4902	29.7011
31.8227	33.1716	41.1055
44.8202	47.4307	59.8548
67.2358	68.4840	76.3804
85.5702	87.8471	93.6279
97.9892	100.5216	108.1113
114.6910	120.0138	126.0229
133.5133	136.4385	156.1152
161.5230	166.3859	174.3397
178.4685	183.3154	197.3535
211.6528	215.4596	219.6538
226.3646	231.7910	244.0541
246.2035	250.1145	277.1248
282.5467	285.0392	291.3607
303.5873	323.5816	329.0927
340.7082	343.4106	347.2248
356.3964	362.9822	368.1276
376.5261	389.8163	401.8886
408.8777	410.7526	416.3814
427.0454	442.0648	446.1534
448.9791	479.3689	486.2471
493.2965	497.5059	509.0673
512.7990	527.5233	529.8156
532.7179	550.4985	577.8431
588.4890	590.4599	599.3177

612.9773 617.6869 630.9277
654.5668 665.6868 696.1140
713.1134 718.1726 731.7069
742.5080 749.1534 759.2055
772.4263 775.0715 791.8150
794.8446 802.4499 811.1151
833.7783 841.0738 852.7437
867.5358 872.6324 875.6167
877.0835 885.1420 902.4677
906.4831 914.4669 920.6493
936.3635 941.4149 948.6987
959.0657 962.7188 964.2700
968.9096 971.7093 980.4327
985.2049 991.5628 995.5560
996.1028 1016.0698 1016.8887
1018.7386 1024.3281 1039.6254
1043.2172 1046.1467 1051.5980
1054.4520 1057.4323 1063.7593
1064.2439 1064.9916 1067.9214
1074.9464 1087.2346 1092.9236
1105.1221 1114.2166 1115.6771
1138.7821 1144.1908 1147.8008
1150.8207 1170.2090 1175.4354
1178.0000 1185.7900 1188.6474
1200.6841 1203.3926 1205.5773
1206.6353 1218.3500 1220.6813
1227.5222 1234.7784 1237.3737
1243.9447 1247.6138 1269.0273
1275.6341 1283.3817 1288.8341
1304.8536 1313.6161 1324.5192
1335.1992 1344.9397 1351.5160
1353.4002 1356.8781 1360.9323
1367.8525 1373.1809 1379.7445
1380.8486 1386.1165 1388.1427
1396.1377 1415.8111 1417.3024
1423.4661 1424.3762 1427.2303
1428.1393 1433.9822 1434.5684
1440.5844 1446.4285 1455.8378
1469.2067 1472.3766 1475.3575
1488.6825 1489.5649 1491.9463
1493.2189 1496.9861 1497.7630
1499.6928 1502.4713 1503.1076
1504.5592 1504.9324 1505.9550
1507.0677 1509.2542 1514.2986

1518.0796	1521.9930	1525.0740
1526.3626	1535.4497	1540.7063
1547.1139	1548.0823	1549.5667
1554.2969	1560.3083	1592.2914
1677.0237	1682.1699	1688.8460
1694.6575	1697.4770	1698.2692
1698.8945	1704.5341	1745.8831
3057.3607	3059.7213	3061.4411
3064.1811	3068.2862	3069.2321
3071.0439	3077.3628	3078.8537
3085.0785	3089.9808	3102.9785
3108.6972	3127.2964	3128.7093
3133.0267	3135.1602	3138.7251
3141.1538	3145.6876	3157.0836
3161.3675	3163.8233	3164.9517
3165.7408	3167.2651	3167.8209
3168.0453	3169.0790	3170.2932
3171.0614	3180.4038	3181.8639
3185.8104	3186.5041	3189.5612
3189.7547	3192.7831	3198.2034
3198.6284	3201.9562	3207.4066
3209.0382	3212.5943	3216.4664
3218.4116	3222.3490	3232.9349

DIPEA ·H^+·Cl^-

Zero-point correction= 0.280369
Thermal correction to Energy= 0.293914
Thermal correction to Enthalpy= 0.294858
Thermal correction to Gibbs Free Energy= 0.240828
Sum of electronic and zero-point Energies= -831.400356
Sum of electronic and thermal Energies= -831.386811
Sum of electronic and thermal Enthalpies= -831.385866
Sum of electronic and thermal Free Energies= -831.439896
Cartesian coordinates

H	-0.849981	-0.338957	-0.163699
Cl	-2.609050	-1.104224	-0.330571
N	0.146739	0.049389	-0.109656
C	-0.000890	1.432773	0.491168
C	-0.700131	1.329727	1.845060
C	-0.800413	2.335356	-0.445240
H	1.008903	1.833885	0.614255
H	-0.107792	0.805401	2.596414
H	-0.884851	2.338804	2.218260
H	-1.661959	0.820182	1.730715

H	-0.255780	2.590255	-1.356175
H	-1.751363	1.862828	-0.711443
H	-1.017231	3.267828	0.079292
C	0.860326	-0.936962	0.802323
C	2.162440	-0.405268	1.390313
C	1.051528	-2.277024	0.103700
H	0.141896	-1.092713	1.611699
H	2.017883	0.488586	1.999822
H	2.574223	-1.180952	2.040349
H	2.906196	-0.187160	0.622150
H	0.119589	-2.620466	-0.353125
H	1.839111	-2.235833	-0.654137
H	1.351170	-3.010398	0.855358
C	0.582966	0.052462	-1.545157
C	1.954025	0.647615	-1.815829
H	-0.193634	0.594152	-2.084480
H	0.525960	-0.979507	-1.889253
H	2.069831	0.760194	-2.896023
H	2.074858	1.636383	-1.365523
H	2.760561	0.001493	-1.465178

Vibrational frequencies

52.1987	67.8996	76.1124
121.1111	146.5318	169.1765
198.2821	214.5608	247.6907
266.5657	278.7618	293.3445
330.2293	352.3387	360.4472
414.1631	437.4896	450.8625
471.0354	483.1330	632.3466
753.8503	792.8224	860.2855
901.6865	939.7689	953.1383
957.8673	971.8049	976.2639
986.9480	1081.6604	1090.9871
1129.3914	1148.4705	1162.3741
1195.8699	1205.7467	1223.2982
1233.3525	1342.1248	1354.7811
1368.4907	1382.4531	1386.0263
1415.8910	1419.6350	1428.0706
1434.1489	1440.6984	1442.2318
1487.0579	1494.6491	1495.4821
1500.4278	1502.9532	1507.2493
1509.1781	1516.0780	1522.1223
1523.6238	1535.1427	1540.6963
1544.1526	2641.4313	3073.0610
3076.8213	3081.0027	3087.0623

3090.6359	3120.4348	3123.8074
3152.1632	3160.5157	3161.9974
3164.9986	3166.8190	3168.5796
3169.1041	3171.3966	3172.6579
3177.1011	3185.7504	3199.2852

M4

Zero-point correction= 0.532770
Thermal correction to Energy= 0.562707
Thermal correction to Enthalpy= 0.563651
Thermal correction to Gibbs Free Energy= 0.469285
Sum of electronic and zero-point Energies= -1474.226104
Sum of electronic and thermal Energies= -1474.196167
Sum of electronic and thermal Enthalpies= -1474.195223
Sum of electronic and thermal Free Energies= -1474.289590
Cartesian coordinates

C	4.690512	0.328210	-0.149617
C	3.375485	0.290444	-0.604654
C	3.055722	-0.146920	-1.886363
C	4.093329	-0.569637	-2.713582
C	5.416582	-0.543073	-2.263153
C	5.725812	-0.089551	-0.982767
C	4.767165	0.866758	1.256202
H	2.020110	-0.123193	-2.214508
H	3.875273	-0.917745	-3.718096
H	6.213205	-0.877353	-2.920399
H	6.755607	-0.067701	-0.638789
H	5.201197	1.871739	1.264326
C	1.586830	-1.342225	1.449212
C	2.860316	-1.384697	2.227177
C	3.303998	0.912710	1.755138
C	2.415106	0.765466	0.463399
C	0.115951	-0.328967	0.179859
H	2.770183	-2.072627	3.067295
H	1.918041	1.693042	0.181510
N	0.560557	-2.138498	1.444544
N	-0.344681	-1.500911	0.637276
N	1.359859	-0.230257	0.687696
C	-1.566807	-2.173783	0.293827
C	-1.696678	-2.694010	-0.996073
C	-2.546522	-2.307896	1.279129
C	-2.879497	-3.368692	-1.292085
C	-3.709520	-2.993218	0.932638
C	-3.893778	-3.524752	-0.345192

H	-3.008534	-3.787723	-2.286817
H	-4.490219	-3.112958	1.679423
O	3.043927	-0.078371	2.741056
H	3.699508	-1.698864	1.591889
H	3.076028	1.853297	2.256518
H	5.371781	0.249170	1.927590
C	-0.612788	-2.517035	-2.025258
H	0.375186	-2.738725	-1.608974
H	-0.594528	-1.484014	-2.390309
H	-0.783925	-3.177244	-2.876762
C	-5.174702	-4.232112	-0.703881
H	-5.001484	-5.008247	-1.452616
H	-5.898699	-3.525399	-1.121996
H	-5.631230	-4.692362	0.175055
C	-2.349092	-1.722124	2.651868
H	-2.076945	-0.663166	2.589767
H	-1.542535	-2.233682	3.184719
H	-3.264020	-1.808005	3.239463
C	-0.505549	0.696386	-0.723820
O	0.333471	1.325209	-1.460585
C	-1.855484	0.851445	-0.599312
C	-2.577869	1.893599	-1.408490
H	-2.412414	0.267910	0.125348
H	-2.028349	2.031567	-2.347342
H	-3.587433	1.552430	-1.662857
C	-2.666456	3.234184	-0.702939
C	-3.888071	3.807228	-0.351577
C	-1.484964	3.914653	-0.380409
C	-3.936366	5.036493	0.308040
H	-4.811389	3.287221	-0.595352
C	-1.530523	5.141257	0.272356
H	-0.538146	3.456161	-0.659560
C	-2.758401	5.707387	0.620548
H	-4.896217	5.467975	0.576477
H	-0.607714	5.661782	0.511642
H	-2.794118	6.664508	1.131658

Vibrational frequencies

15.1522	21.0189	25.5817
30.2458	35.3341	43.5200
51.6159	68.8070	73.1495
82.1659	95.9344	110.3904
126.4726	147.6630	150.9904
167.5405	174.9694	187.7211
195.7461	212.9548	227.0751

234.8697 238.1823 246.0100
277.2210 280.6309 296.3671
317.5061 321.1071 353.8206
388.6125 395.2045 403.3268
420.6038 427.4764 443.8244
448.9446 488.5849 495.9339
505.7137 515.2742 525.4048
529.4684 532.9921 571.1550
587.3984 594.0708 603.1118
608.9672 623.8646 630.0273
639.9495 680.7975 707.4686
711.2617 721.9870 726.8058
740.6382 750.3272 763.4475
776.8494 778.9898 787.7043
812.2715 834.9180 837.9708
860.3152 879.4457 885.9585
890.6979 892.7509 920.3069
926.6880 947.4058 954.9443
961.1675 963.7402 983.0273
997.9566 1004.0318 1016.8003
1024.0224 1027.2006 1028.8233
1037.4978 1041.3129 1047.4539
1050.8745 1053.0506 1057.3929
1064.5575 1065.2729 1065.9827
1068.9802 1069.4682 1086.5856
1113.0409 1115.6573 1137.4801
1149.3894 1172.0867 1173.0157
1179.7877 1197.2276 1202.5731
1208.9039 1213.2396 1226.5956
1231.3948 1238.2962 1246.3262
1265.0949 1275.7601 1290.0253
1295.8510 1310.8371 1319.5874
1327.1589 1342.6105 1343.9730
1351.8653 1359.2896 1361.4520
1371.1416 1374.9348 1379.5800
1412.7016 1416.5716 1420.7095
1430.1377 1455.6104 1463.5759
1468.1528 1480.9591 1481.5879
1482.6344 1487.2028 1493.2744
1496.6195 1497.5290 1498.1847
1505.5386 1513.9157 1515.4136
1523.7255 1538.3238 1542.0899
1549.0229 1570.6044 1677.8168
1682.3873 1689.3220 1694.9428

1696.6658	1699.9640	1700.7366
1706.0356	3055.4221	3063.1781
3070.7271	3071.8850	3076.2978
3085.0111	3107.7472	3132.3895
3134.0279	3144.7945	3147.3442
3156.6540	3167.8495	3168.3888
3173.4265	3179.8457	3180.8774
3183.5212	3185.8262	3196.3886
3201.4170	3203.5995	3210.0708
3211.4381	3211.6107	3215.7953
3218.3395	3219.2828	3224.7800

R2

Zero-point correction= 0.202291
Thermal correction to Energy= 0.215467
Thermal correction to Enthalpy= 0.216411
Thermal correction to Gibbs Free Energy= 0.160521
Sum of electronic and zero-point Energies= -722.736102
Sum of electronic and thermal Energies= -722.722927
Sum of electronic and thermal Enthalpies= -722.721982
Sum of electronic and thermal Free Energies= -722.777872
Cartesian coordinates

N	1.386345	-0.526108	-0.000181
N	2.282884	0.339247	-0.000275
C	3.593684	-0.287637	-0.000392
O	3.836822	-1.465420	-0.000079
O	4.493698	0.687641	0.000059
C	5.855981	0.247132	0.000503
H	6.056985	-0.351440	-0.889673
H	6.460367	1.150897	0.000842
H	6.056333	-0.351669	0.890672
C	0.067807	-0.013438	-0.000122
C	-0.922133	-0.969135	-0.000055
C	-0.251898	1.374764	-0.000126
C	-2.287333	-0.592623	0.000011
H	-0.639111	-2.017675	-0.000056
C	-1.562338	1.757134	-0.000061
H	0.553440	2.099467	-0.000178
C	-3.329730	-1.555584	0.000080
C	-2.614448	0.793169	0.000009
H	-1.825939	2.810858	-0.000061
C	-4.642545	-1.157112	0.000144
H	-3.068512	-2.609768	0.000080
C	-3.979060	1.173387	0.000077

C	-4.968810	0.220405	0.000142
H	-5.437176	-1.895667	0.000195
H	-4.229060	2.230372	0.000075
H	-6.011151	0.522114	0.000193

Vibrational frequencies

14.1787	50.8042	80.6257
92.9177	170.9895	176.5547
184.9390	229.7914	234.6094
244.4668	337.0154	362.9560
405.5792	409.4206	495.0186
521.7888	528.7663	539.9742
590.1133	631.9064	656.9850
717.9887	773.3018	780.5470
791.5280	802.0795	834.9941
856.3903	905.8975	912.5804
957.0171	981.2343	999.2872
1005.8148	1018.4783	1030.4454
1058.3768	1088.9467	1146.9931
1170.4886	1174.0134	1188.7228
1191.1225	1222.8085	1245.4491
1275.8976	1289.8770	1332.9428
1392.3259	1422.3878	1458.4375
1490.6242	1495.9474	1503.0206
1503.2317	1515.9405	1572.8471
1658.0799	1670.1521	1696.4014
1727.4770	1880.6120	3096.6884
3179.8126	3209.6483	3217.4751
3220.7746	3223.6213	3227.8802
3236.5621	3239.3662	3243.5070

TS5RR(TS5R)

Zero-point correction= 0.736746
Thermal correction to Energy= 0.779938
Thermal correction to Enthalpy= 0.780882
Thermal correction to Gibbs Free Energy= 0.660695
Sum of electronic and zero-point Energies= -2196.969044
Sum of electronic and thermal Energies= -2196.925852
Sum of electronic and thermal Enthalpies= -2196.924908
Sum of electronic and thermal Free Energies= -2197.045095
Cartesian coordinates

C	-4.831353	1.292939	-0.421712
C	-3.439417	1.272188	-0.401193
C	-2.697587	2.447817	-0.311063
C	-3.381589	3.658044	-0.233961

C	-4.778701	3.686364	-0.252188
C	-5.512105	2.506222	-0.349479
C	-5.401631	-0.096023	-0.540926
H	-1.611160	2.430142	-0.314032
H	-2.818575	4.583747	-0.163924
H	-5.297501	4.637752	-0.189238
H	-6.597671	2.530907	-0.362988
H	-5.873462	-0.243235	-1.517339
C	-2.405980	-0.871248	1.822249
C	-3.857871	-1.173796	1.984322
C	-4.197328	-1.055279	-0.373830
C	-2.917019	-0.146227	-0.480127
C	-0.641955	-0.211730	0.713336
H	-4.009907	-1.848864	2.826090
H	-2.377498	-0.337512	-1.405795
N	-1.424422	-0.993166	2.667248
N	-0.334727	-0.572769	1.964450
N	-1.972986	-0.411526	0.616041
C	0.954427	-0.573688	2.596797
C	1.673317	-1.767797	2.622432
C	1.415258	0.625211	3.151986
C	2.948801	-1.722661	3.192335
C	2.688718	0.614885	3.710370
C	3.471402	-0.546373	3.729155
H	3.543166	-2.632319	3.216415
H	3.084352	1.532953	4.137906
O	-4.294923	-1.825393	0.813021
H	-4.415877	-0.242949	2.164943
H	-4.162542	-1.798581	-1.172783
H	-6.158583	-0.316336	0.218568
C	1.082459	-3.044400	2.084789
H	0.530963	-2.885334	1.151241
H	0.374716	-3.460418	2.809659
H	1.867543	-3.783743	1.914491
C	4.850555	-0.515700	4.334319
H	5.467623	0.250107	3.855896
H	5.352445	-1.478839	4.225980
H	4.799867	-0.274337	5.400101
C	0.577122	1.874219	3.091605
H	-0.422178	1.699126	3.501227
H	0.458067	2.213727	2.055063
H	1.048367	2.680202	3.656271
C	0.180746	0.402295	-0.389258
O	-0.423309	0.518358	-1.474745

C	1.547027	0.690145	-0.236255
C	2.110775	1.682508	-1.231987
H	2.000606	0.673172	0.747930
H	3.198090	1.738096	-1.117071
H	1.898464	1.338432	-2.248879
C	1.481399	3.040949	-1.006580
C	0.464790	3.505688	-1.844376
C	1.848875	3.820302	0.097093
C	-0.174048	4.717830	-1.583997
H	0.162271	2.897768	-2.691375
C	1.210365	5.027901	0.362786
H	2.636519	3.465720	0.759514
C	0.192718	5.480312	-0.477637
H	-0.965040	5.062069	-2.243999
H	1.506522	5.618305	1.224635
H	-0.305831	6.422834	-0.273375
N	0.194203	-2.289143	-1.276961
N	-0.708277	-2.868998	-1.980700
C	-1.719034	-3.340011	-1.122518
O	-1.779194	-3.261662	0.090284
O	-2.671467	-3.939226	-1.861053
C	-3.693121	-4.589026	-1.102454
H	-4.143959	-3.899383	-0.386111
H	-4.426760	-4.937005	-1.827702
H	-3.271661	-5.437303	-0.556901
C	1.280286	-1.763443	-1.882460
C	2.255730	-1.259239	-0.974339
C	1.477908	-1.639062	-3.299682
C	3.558756	-0.899698	-1.501416
H	2.219054	-1.630854	0.044172
C	2.647158	-1.157879	-3.789268
H	0.668995	-1.946692	-3.953583
C	4.632690	-0.608585	-0.640736
C	3.734307	-0.801463	-2.902916
H	2.804585	-1.056665	-4.859129
C	5.855889	-0.213285	-1.148241
H	4.476860	-0.689555	0.433710
C	4.986184	-0.386411	-3.397821
C	6.028358	-0.094994	-2.537644
H	6.679646	0.009937	-0.478258
H	5.124310	-0.303186	-4.472446
H	6.986091	0.223896	-2.936550

Vibrational frequencies

-371.6456 21.7338 26.6338

30.1021	37.0198	42.9362
45.0527	53.5426	56.8596
59.7497	65.2205	69.4427
74.1288	77.2703	79.3444
86.7773	89.9669	97.7811
112.7521	119.4860	131.0868
137.8015	144.2259	150.8823
159.3111	161.2500	168.4827
187.4398	195.0527	201.1584
214.7052	217.7192	231.7789
232.7215	233.9254	238.4878
242.0001	253.7724	259.2686
273.7035	283.0642	287.1780
307.7120	324.2920	346.6413
353.6576	358.9992	372.9780
385.8309	397.0603	404.9076
412.1092	413.5726	419.1707
420.4808	441.3094	448.0241
488.4441	499.9069	506.7468
515.8051	518.8624	525.3282
528.5239	529.9582	534.8786
545.8241	556.2704	565.7803
588.7162	593.7821	597.9431
599.6618	609.8809	623.3069
632.2845	636.3156	641.9760
665.1814	692.7849	704.0914
716.6844	718.9606	721.6165
739.0229	746.4251	761.6935
767.7665	775.3456	776.3839
778.5376	787.1049	792.9395
805.1773	810.6075	818.1917
827.0260	836.1873	838.2007
841.9149	868.6984	871.2712
877.9316	888.8533	891.9259
906.5631	911.5040	914.4840
922.9338	929.2296	954.4513
963.9532	967.6096	969.2420
983.1858	985.9533	989.6260
992.2622	1005.6554	1014.1579
1015.6787	1018.0622	1019.0063
1023.6253	1027.6911	1033.8073
1040.8586	1044.5489	1050.5342
1054.5489	1062.7275	1063.8909
1065.1186	1068.1478	1069.1356

1070.2115	1071.0967	1074.7968
1077.4765	1106.4431	1119.2250
1122.6389	1138.1375	1144.8876
1160.4224	1161.7242	1170.6317
1172.8522	1177.3209	1182.5639
1190.8873	1197.7903	1201.4079
1206.2251	1207.7566	1210.7218
1224.0545	1231.3770	1233.1098
1240.8029	1246.1250	1250.5110
1252.7111	1273.0995	1285.0222
1285.9842	1287.5059	1306.1196
1309.6897	1328.9625	1329.6767
1337.3905	1339.3922	1346.4570
1355.6672	1360.7014	1362.7710
1373.3470	1375.2699	1376.0804
1383.4318	1389.5179	1417.9056
1423.8735	1432.0912	1434.8906
1440.4435	1450.9332	1463.9114
1466.1154	1470.8203	1477.7403
1484.1193	1486.0547	1489.9760
1491.6897	1493.1089	1494.8484
1497.1224	1498.0302	1504.5689
1508.9088	1510.4637	1511.8060
1514.7452	1521.2688	1523.6587
1532.4169	1538.6540	1542.1435
1553.5814	1556.9248	1579.3959
1628.7020	1668.9760	1676.4396
1682.2309	1683.6804	1686.0723
1689.7860	1696.0257	1698.0888
1698.2353	1700.1137	1796.4294
3054.7784	3056.9258	3064.5360
3072.4198	3084.4112	3090.4388
3091.5776	3129.6858	3135.0852
3135.8976	3140.9658	3141.6038
3154.3127	3168.5558	3170.6773
3173.7943	3175.8188	3178.2847
3180.2960	3181.6032	3185.7861
3196.6175	3199.4348	3201.6967
3203.3009	3203.6009	3207.2796
3209.7565	3211.2311	3211.6114
3213.8125	3215.2266	3222.9557
3225.4586	3227.6179	3228.2115
3231.3769	3231.6543	3232.1434

TS5^{b}R

Zero-point correction= 0.736439
Thermal correction to Energy= 0.779386
Thermal correction to Enthalpy= 0.780330
Thermal correction to Gibbs Free Energy= 0.659139
Sum of electronic and zero-point Energies= -2196.948103
Sum of electronic and thermal Energies= -2196.905156
Sum of electronic and thermal Enthalpies= -2196.904212
Sum of electronic and thermal Free Energies= -2197.025404
Cartesian coordinates

C	-5.687182	-0.293498	-0.591293
C	-4.395927	-0.167469	-0.084292
C	-4.113138	-0.401372	1.258655
C	-5.160142	-0.777516	2.097164
C	-6.457012	-0.907817	1.595949
C	-6.732494	-0.664037	0.252767
C	-5.735480	0.021890	-2.064269
H	-3.104056	-0.276622	1.639674
H	-4.965469	-0.968071	3.146555
H	-7.261569	-1.202314	2.263357
H	-7.741358	-0.768333	-0.132709
H	-6.256109	0.968457	-2.244426
C	-2.413810	-1.928780	-1.839425
C	-3.625581	-2.155582	-2.679572
C	-4.257489	0.132907	-2.509926
C	-3.422832	0.222817	-1.176791
C	-1.090151	-0.704342	-0.604586
H	-3.433058	-2.927735	-3.423628
H	-3.005893	1.216363	-1.024139
N	-1.357956	-2.667345	-1.653102
N	-0.549788	-1.898424	-0.874074
N	-2.293544	-0.721568	-1.215819
C	0.676533	-2.449584	-0.361101
C	1.748272	-2.595465	-1.244090
C	0.721881	-2.810059	0.985533
C	2.926401	-3.114826	-0.718494
C	1.939151	-3.296323	1.466630
C	3.048659	-3.443400	0.634446
H	3.774724	-3.254368	-1.380760
H	2.012645	-3.563725	2.517892
O	-3.865387	-0.937791	-3.356001
H	-4.480351	-2.458919	-2.058500
H	-4.081030	1.025421	-3.108691
H	-6.246754	-0.743045	-2.654009

C	1.629144	-2.198689	-2.690034
H	1.216408	-1.189159	-2.779614
H	0.968399	-2.882212	-3.231006
H	2.612072	-2.196168	-3.159117
C	4.374352	-3.915095	1.170410
H	5.098630	-3.091789	1.142740
H	4.778499	-4.728570	0.560793
H	4.289013	-4.261244	2.203651
C	-0.473661	-2.656974	1.887800
H	-1.395082	-2.971453	1.385503
H	-0.594889	-1.613163	2.205190
H	-0.348915	-3.254786	2.791191
C	-0.590837	0.416537	0.253745
O	-1.462622	1.205520	0.659244
C	0.813388	0.631977	0.404393
C	1.185429	1.392517	1.668499
H	1.464995	-0.208971	0.175349
H	2.258892	1.599095	1.652194
H	0.648033	2.348761	1.670938
C	0.838577	0.586850	2.897740
C	-0.373793	0.782616	3.568344
C	1.702717	-0.416339	3.351472
C	-0.716884	-0.009880	4.663178
H	-1.050938	1.552644	3.213135
C	1.363789	-1.204473	4.450100
H	2.646699	-0.580803	2.835224
C	0.150768	-1.005146	5.106441
H	-1.660559	0.155284	5.171465
H	2.048682	-1.973284	4.793451
H	-0.113174	-1.618358	5.962932
N	3.654775	1.455962	-0.866025
N	3.454152	0.289777	-1.347393
C	4.645972	-0.467619	-1.307297
O	5.442940	-0.521348	-0.398981
O	4.752243	-1.194851	-2.431288
C	5.916196	-2.018882	-2.500122
H	5.945540	-2.715755	-1.658018
H	5.843596	-2.558249	-3.441221
H	6.818911	-1.404542	-2.479722
C	2.556320	2.267384	-0.778107
C	2.801931	3.556882	-0.310802
C	1.189624	1.799288	-1.053961
C	1.788159	4.510482	-0.219631
H	3.824216	3.809071	-0.044562

C	0.207070	2.854658	-1.125728
H	1.149122	1.037782	-1.834236
C	2.029802	5.840676	0.242839
C	0.464499	4.138086	-0.670984
H	-0.777828	2.634866	-1.527157
C	1.036679	6.773831	0.252757
H	3.030875	6.091204	0.584070
C	-0.544844	5.165236	-0.663020
C	-0.269480	6.423110	-0.216555
H	1.224826	7.782268	0.605959
H	-1.541886	4.907729	-1.011077
H	-1.054194	7.174208	-0.210246

Vibrational frequencies

-408.0189	4.1341	22.9913
25.9708	35.4357	41.1134
47.7212	51.2279	54.2796
63.1945	65.7494	67.5327
75.7354	81.2787	85.8607
93.3713	98.1092	103.5040
114.9299	118.1201	132.1471
139.7533	155.7850	161.5555
167.7983	170.7913	179.8026
186.8353	203.7043	207.5194
215.1516	224.4150	227.3543
237.2694	243.8931	256.3843
263.5372	263.9062	279.6659
287.0053	288.7224	301.0474
314.6818	328.9750	336.6781
341.6247	352.0411	371.1830
391.1987	401.2100	405.3018
405.7041	418.9037	421.9707
442.7951	447.8287	450.6963
472.1862	490.2278	501.4270
511.7386	517.3322	521.1996
523.9972	530.5697	538.6012
544.2908	557.0561	573.9256
589.1588	594.0458	597.4016
603.8794	608.8842	621.1277
622.8214	632.9413	648.4016
673.8343	693.0540	706.9008
717.7955	721.1744	722.2286
739.4102	744.6909	748.4711
759.9497	764.7705	766.7365
774.7029	779.2344	781.3064

793.1798 813.4837 816.3637
835.1380 841.2079 850.0884
863.5640 869.2608 871.5258
875.6543 878.0874 888.9306
903.3414 908.1223 916.5061
926.4920 938.4075 940.3374
959.5330 962.0098 967.1662
981.7777 983.9734 992.1028
992.7862 995.1133 1003.8158
1009.7922 1017.4625 1019.7141
1024.9196 1026.1248 1026.3326
1032.5696 1037.7697 1045.8011
1053.0463 1056.1342 1058.6545
1060.9731 1065.3450 1067.1352
1070.7179 1073.8655 1076.1535
1081.9020 1115.6984 1118.3522
1119.8385 1123.2306 1146.0026
1151.0859 1164.2951 1175.5078
1179.0502 1179.4784 1184.2728
1187.4454 1193.0184 1199.5619
1201.7020 1208.1220 1216.2821
1223.5691 1224.5789 1234.8221
1239.8455 1244.7881 1247.1944
1249.6879 1267.0937 1277.5640
1283.5018 1297.2925 1303.4247
1311.1814 1328.4662 1330.3374
1341.2951 1342.5955 1344.3471
1351.9970 1356.9457 1365.7273
1371.2135 1372.9407 1376.5245
1383.1722 1411.6713 1415.4976
1418.7616 1419.3460 1429.4196
1445.9008 1450.8167 1453.9929
1465.6762 1468.0798 1474.5586
1479.7649 1481.5507 1482.0265
1485.5554 1489.2213 1490.7562
1494.5447 1496.7111 1497.5957
1499.9246 1507.6761 1510.0859
1512.7523 1515.1680 1516.6380
1521.5529 1537.1622 1540.6961
1555.8224 1558.6750 1569.7451
1608.7962 1653.4555 1676.8789
1677.7595 1682.6174 1688.7890
1692.3204 1694.7572 1695.0560
1698.1456 1717.7178 1832.2810

3055.5472	3060.2536	3069.0709
3075.5831	3076.4151	3084.5954
3087.3754	3127.4146	3127.6696
3138.7976	3139.0447	3139.5525
3144.5385	3153.3452	3165.1091
3170.0009	3171.2080	3181.6689
3185.5435	3190.3777	3191.9636
3193.5785	3194.2376	3198.2200
3198.8964	3201.7520	3202.8678
3203.6252	3208.4102	3210.7671
3215.4117	3217.9461	3218.1148
3219.7613	3224.2007	3224.9138
3227.6087	3234.7973	3237.4069

TS5^{c}R

Zero-point correction= 0.736572
Thermal correction to Energy= 0.779672
Thermal correction to Enthalpy= 0.780617
Thermal correction to Gibbs Free Energy= 0.659378
Sum of electronic and zero-point Energies= -2196.949119
Sum of electronic and thermal Energies= -2196.906019
Sum of electronic and thermal Enthalpies= -2196.905075
Sum of electronic and thermal Free Energies= -2197.026313
Cartesian coordinates

C	2.466327	2.954217	-1.026356
C	1.384700	2.326941	-0.411737
C	0.359567	3.065825	0.176501
C	0.437793	4.455278	0.139481
C	1.523408	5.090159	-0.470143
C	2.544027	4.345045	-1.054168
C	3.435145	1.955363	-1.600035
H	-0.471914	2.565876	0.663792
H	-0.350317	5.049212	0.591250
H	1.569332	6.174342	-0.490957
H	3.384072	4.839310	-1.532832
H	4.382259	1.954721	-1.050880
C	0.122198	0.251738	-2.493273
C	1.304402	0.589228	-3.338073
C	2.746352	0.579463	-1.455540
C	1.496337	0.818872	-0.519145
C	-0.894044	-0.147789	-0.598687
H	1.193607	0.154628	-4.331254
H	1.616431	0.327356	0.448293
N	-1.067122	-0.148134	-2.837213

N	-1.693201	-0.379914	-1.650398
N	0.273522	0.269324	-1.136862
C	-3.096055	-0.694516	-1.658238
C	-3.493184	-1.963457	-2.079439
C	-3.991417	0.307309	-1.264882
C	-4.858119	-2.251233	-2.018757
C	-5.340190	-0.032558	-1.227895
C	-5.788484	-1.308430	-1.582624
H	-5.197879	-3.238070	-2.324177
H	-6.059221	0.718422	-0.909198
O	2.419058	-0.004029	-2.707840
H	1.413642	1.678736	-3.432472
H	3.416666	-0.144139	-0.997312
H	3.677530	2.147827	-2.650308
C	-2.506715	-2.965611	-2.616447
H	-1.542872	-2.897843	-2.107429
H	-2.328143	-2.784171	-3.680893
H	-2.892821	-3.980706	-2.505020
C	-7.256230	-1.637877	-1.512452
H	-7.653993	-1.421810	-0.515459
H	-7.439277	-2.691917	-1.735496
H	-7.823639	-1.033246	-2.228259
C	-3.519237	1.687145	-0.892035
H	-2.762591	2.052412	-1.593714
H	-3.088436	1.702784	0.116405
H	-4.358285	2.384448	-0.893872
C	-1.196739	-0.196479	0.873972
O	-0.403149	0.422053	1.607910
C	-2.249418	-1.016924	1.366970
C	-2.823463	-0.585920	2.706792
H	-2.977143	-1.390724	0.653082
H	-3.490390	-1.369120	3.083714
H	-2.002948	-0.465069	3.419704
C	-3.577801	0.715794	2.571110
C	-2.941462	1.937564	2.818740
C	-4.900778	0.726678	2.119692
C	-3.612281	3.141530	2.610589
H	-1.909239	1.933752	3.157313
C	-5.574527	1.928537	1.916154
H	-5.402478	-0.217536	1.918263
C	-4.930091	3.140964	2.157785
H	-3.105008	4.081724	2.805712
H	-6.603861	1.919081	1.569303
H	-5.452924	4.078665	1.998464

N	4.790440	-1.499707	0.331512
N	5.729210	-0.978219	1.014077
C	6.806490	-0.599925	0.177560
O	6.793336	-0.423122	-1.020447
O	7.882957	-0.393112	0.949166
C	9.043356	0.053383	0.250184
H	8.842941	0.999944	-0.256426
H	9.816155	0.181940	1.005434
H	9.353160	-0.686898	-0.490527
C	3.636448	-1.792758	1.011256
C	2.599970	-2.349410	0.245473
C	3.408644	-1.504468	2.396005
C	1.338744	-2.568449	0.781455
H	2.804408	-2.587471	-0.796969
C	2.183739	-1.721082	2.943545
H	4.226810	-1.098584	2.979763
C	0.280426	-3.211101	0.037179
C	1.082228	-2.211728	2.158126
H	1.999290	-1.487800	3.988720
C	-0.959742	-3.331841	0.561809
H	0.518954	-3.630661	-0.938257
C	-0.193143	-2.356676	2.682286
C	-1.292052	-2.694145	1.834864
H	-1.748472	-3.846288	0.019998
H	-0.367631	-2.127623	3.728993
H	-2.184129	-3.075186	2.329804

Vibrational frequencies

-478.1247	12.3378	20.3734
23.6600	26.2609	38.3202
45.4503	46.1913	49.4728
59.4059	68.1648	68.9919
76.1415	77.5851	82.3632
88.1283	99.5654	107.8741
111.5850	117.3858	124.6051
134.4336	160.0568	162.5123
172.6792	184.4046	188.9279
195.4058	200.7811	205.1731
212.4715	220.1019	224.1910
230.6621	243.1343	247.5345
251.2933	259.6684	267.9883
279.8572	283.8641	289.9186
308.5094	327.6235	339.4859
344.8597	346.5067	382.2103
385.7860	402.1440	404.6700

407.6812	410.8221	426.3194
442.6466	446.6244	452.6323
483.2724	490.4797	500.1789
503.0628	508.9216	514.9466
523.3104	524.4398	531.4647
541.2691	548.0207	573.2160
587.5690	590.9771	594.7030
597.5586	609.7979	619.1675
621.1105	630.3677	646.8237
649.7991	687.6161	702.5388
717.4813	720.6590	726.4154
738.6946	748.6119	757.8410
764.9639	774.2135	778.3320
782.4974	789.0777	789.9535
805.7002	813.0077	822.2009
830.4163	834.7811	839.5285
865.4747	876.0138	879.9118
883.6533	885.8305	888.9525
899.8649	917.2569	918.2664
921.9806	941.7624	945.9438
955.7422	965.1797	966.3437
968.2553	982.6756	994.0472
998.9836	1007.5176	1009.4605
1011.9632	1017.2390	1019.9681
1025.6490	1026.7774	1033.9681
1038.9207	1040.2407	1042.2150
1055.6638	1057.8749	1062.3218
1064.4770	1067.0181	1067.9855
1068.4104	1070.5595	1073.9578
1084.5122	1114.4858	1117.7126
1121.2817	1125.1885	1137.2972
1146.4303	1155.0663	1171.9602
1175.2213	1176.7043	1180.2478
1186.6989	1192.8648	1196.7922
1204.4108	1208.0072	1213.5791
1218.0931	1226.1025	1230.8668
1238.3056	1248.4002	1251.5855
1257.1957	1261.4432	1279.5548
1284.5173	1296.0477	1300.7296
1314.1819	1327.2963	1338.0390
1341.4063	1344.5912	1351.7488
1358.7003	1359.8322	1365.4837
1369.7561	1372.0422	1383.3996
1388.6839	1408.4706	1415.0333

1422.2515	1429.5947	1430.9031
1437.8439	1458.1704	1464.0259
1465.1595	1467.4867	1480.1032
1485.3451	1485.7956	1488.2186
1492.1797	1492.9459	1495.4842
1495.9248	1497.0599	1500.1322
1503.0325	1506.0155	1507.7999
1511.3070	1513.7869	1520.7833
1533.1698	1540.3266	1541.4964
1549.8998	1560.9574	1567.2260
1603.1412	1649.7373	1673.8274
1680.1222	1682.0208	1686.1521
1689.6415	1694.7901	1695.4198
1699.1734	1712.5473	1828.4898
3059.4508	3064.9020	3071.4309
3076.3761	3077.6023	3085.9496
3088.4395	3128.4931	3130.9576
3135.5431	3136.1643	3151.1244
3156.9524	3157.0949	3164.8134
3167.5849	3168.4707	3175.7436
3180.2116	3184.2295	3192.0661
3192.1459	3193.5749	3198.5803
3204.7940	3205.1257	3206.5299
3208.3866	3212.9659	3213.0372
3214.0721	3216.5329	3218.0435
3222.8092	3224.5815	3226.9393
3230.9660	3236.2692	3238.4951

TS5RRb

Zero-point correction= 0.736460
Thermal correction to Energy= 0.779894
Thermal correction to Enthalpy= 0.780838
Thermal correction to Gibbs Free Energy= 0.657477
Sum of electronic and zero-point Energies= -2196.962610
Sum of electronic and thermal Energies= -2196.919176
Sum of electronic and thermal Enthalpies= -2196.918232
Sum of electronic and thermal Free Energies= -2197.041593
Cartesian coordinates

C	-4.922149	-1.693077	-2.103101
C	-3.705793	-1.032746	-1.958314
C	-3.364122	0.060021	-2.749546
C	-4.284641	0.497990	-3.696922
C	-5.512286	-0.154339	-3.846489
C	-5.838204	-1.254826	-3.057215

C	-5.033941	-2.855055	-1.149210
H	-2.395006	0.537587	-2.632100
H	-4.047130	1.349134	-4.326344
H	-6.219597	0.201649	-4.588678
H	-6.792443	-1.757893	-3.179776
H	-4.979714	-3.807074	-1.685132
C	-3.339194	-0.212019	1.091451
C	-4.595040	-0.996872	1.280145
C	-3.829173	-2.715081	-0.188061
C	-2.874947	-1.657589	-0.861027
C	-1.361698	0.100994	0.227351
H	-4.982899	-0.858188	2.288892
H	-1.958915	-2.106004	-1.247642
N	-2.832177	0.774814	1.772790
N	-1.606066	0.970788	1.209750
N	-2.480349	-0.637003	0.120357
C	-0.834335	2.127445	1.588324
C	-0.280429	2.157765	2.869858
C	-0.719268	3.174742	0.669691
C	0.438474	3.297594	3.224586
C	-0.003022	4.296156	1.084295
C	0.583674	4.374094	2.347658
H	0.897141	3.342272	4.208962
H	0.107946	5.124823	0.389957
O	-4.226185	-2.356101	1.128790
H	-5.360031	-0.694885	0.552479
H	-3.301883	-3.660715	-0.058404
H	-5.967764	-2.860969	-0.577997
C	-0.448244	0.996544	3.807908
H	-0.377307	0.045562	3.274315
H	-1.429942	1.024291	4.292249
H	0.319891	1.013482	4.583580
C	1.340942	5.609173	2.760497
H	1.844366	6.065666	1.904547
H	2.089459	5.379323	3.521633
H	0.658404	6.356022	3.179165
C	-1.311950	3.102130	-0.711943
H	-2.314017	2.660480	-0.701607
H	-0.677199	2.502729	-1.376248
H	-1.381840	4.101355	-1.144256
C	-0.140735	-0.066360	-0.635293
O	-0.364936	-0.472505	-1.793420
C	1.123724	0.136657	-0.039812
C	2.253964	0.477702	-0.986040

H	1.146316	0.603045	0.942883
H	3.183383	0.553694	-0.414186
H	2.392321	-0.338203	-1.703393
C	1.982629	1.774285	-1.715788
C	1.436208	1.769881	-3.003619
C	2.231562	3.002625	-1.097397
C	1.143510	2.966348	-3.655282
H	1.234917	0.818211	-3.485421
C	1.944281	4.200085	-1.748104
H	2.647480	3.018843	-0.092136
C	1.395528	4.185843	-3.029424
H	0.721758	2.945680	-4.655772
H	2.151988	5.145396	-1.254986
H	1.172593	5.118299	-3.538481
N	3.711804	-2.060727	-0.524205
N	4.993173	-2.005164	-0.439211
C	5.576615	-2.194689	-1.701968
O	5.040537	-2.326043	-2.782854
O	6.916125	-2.190839	-1.546363
C	7.654867	-2.355489	-2.752147
H	7.438441	-1.544427	-3.451426
H	8.705056	-2.338105	-2.465666
H	7.407451	-3.306106	-3.230141
C	3.019489	-1.863163	0.623909
C	1.599198	-1.859965	0.501991
C	3.615639	-1.595700	1.906718
C	0.835856	-2.119900	1.721438
H	1.200784	-2.241576	-0.437163
C	2.863135	-1.607219	3.034645
H	4.685498	-1.423249	1.941907
C	-0.508361	-2.525097	1.672280
C	1.461596	-1.960290	2.980197
H	3.310954	-1.425437	4.007250
C	-1.240443	-2.735370	2.828841
H	-0.959588	-2.704643	0.699645
C	0.711595	-2.200566	4.148464
C	-0.619453	-2.571753	4.077749
H	-2.282512	-3.032685	2.763046
H	1.195594	-2.084065	5.114292
H	-1.183340	-2.743832	4.988785

Vibrational frequencies

-412.2797	4.3510	26.2430
28.3096	31.9579	32.8188
43.5317	51.6023	53.7915

54.8727	58.5908	62.7878
71.4697	74.1846	76.5651
85.9579	93.2359	96.9968
102.3824	112.4260	114.1232
117.8804	125.5689	137.0984
162.8998	167.1859	171.8388
187.6037	191.1916	198.1631
217.6562	219.6722	222.4711
226.3672	232.0116	243.0359
243.9232	249.2545	261.4710
279.7181	281.7482	290.5424
308.3476	329.1317	338.8494
342.7667	355.0899	371.5468
387.9171	401.4976	406.4312
407.8587	412.8708	421.2618
423.6475	446.1977	450.7753
489.7042	499.5469	511.8973
517.3390	518.9276	523.5797
525.2410	532.5985	535.4303
539.9409	550.2589	582.2033
591.6719	595.2968	598.0035
599.8034	610.5497	619.0177
631.1955	635.3233	646.7155
655.1604	690.5270	708.6379
721.0193	722.4475	724.5907
742.8105	750.5322	764.0308
776.7895	778.8251	783.5413
788.4263	793.5334	797.8765
806.0897	810.8756	820.9134
835.4346	840.5729	842.9475
862.4375	877.1991	883.5841
889.6777	892.3106	904.9659
915.6408	921.2597	923.2176
929.3275	937.0114	953.8074
957.2873	968.2106	970.8605
983.8029	998.1217	999.3021
1001.7523	1011.0458	1018.2246
1021.4532	1021.9177	1026.0133
1028.7676	1032.1022	1033.4756
1040.2861	1041.7936	1050.0447
1054.3481	1058.3540	1060.5517
1062.5927	1065.1817	1067.9645
1068.8787	1069.7934	1071.2511
1084.0164	1114.4630	1119.0555

1121.6179	1137.8087	1142.3755
1148.8049	1160.2401	1171.3696
1174.0822	1180.8499	1185.2576
1186.7835	1191.4233	1199.7955
1201.0154	1207.6304	1212.1035
1214.7994	1224.7278	1226.6805
1237.9338	1246.4912	1253.2634
1255.6050	1262.6778	1278.2298
1281.0070	1286.2096	1304.0287
1312.6303	1328.2702	1336.9057
1342.0677	1347.5158	1347.9272
1352.2300	1357.0949	1359.4117
1368.9925	1370.9663	1373.1077
1378.4075	1379.2152	1414.7012
1415.9343	1417.8959	1424.7775
1428.7866	1448.2708	1466.2034
1466.9322	1468.5313	1474.7550
1482.0274	1483.7671	1484.7057
1487.5271	1488.4451	1491.8302
1494.4979	1494.7225	1496.3803
1500.5156	1503.8643	1508.4471
1511.5795	1518.3870	1521.6479
1527.2278	1539.4144	1542.2027
1548.4546	1551.9823	1579.0746
1629.2689	1668.9973	1674.3841
1679.1062	1684.1869	1687.8873
1693.6494	1695.0367	1695.6050
1696.6419	1698.4821	1818.5098
3062.6129	3070.3208	3071.0620
3082.6103	3082.9969	3085.1342
3089.8779	3133.5189	3133.6041
3137.1582	3141.7478	3146.3808
3153.7738	3159.2131	3160.5604
3162.5124	3168.1221	3173.8262
3179.9947	3184.2315	3186.9994
3188.0177	3194.3007	3196.4314
3201.0137	3202.9462	3203.2219
3206.5923	3209.6615	3211.8096
3212.9829	3216.8032	3218.4364
3222.3171	3224.4733	3227.7099
3230.2314	3234.7816	3239.0280

TS5RRc

Zero-point correction= 0.737594

Thermal correction to Energy= 0.780424
Thermal correction to Enthalpy= 0.781368
Thermal correction to Gibbs Free Energy= 0.661494
Sum of electronic and zero-point Energies= -2196.966792
Sum of electronic and thermal Energies= -2196.923962
Sum of electronic and thermal Enthalpies= -2196.923018
Sum of electronic and thermal Free Energies= -2197.042892
Cartesian coordinates

C	5.316167	-0.225476	-1.238306
C	4.117922	0.307463	-0.769923
C	3.905652	1.681915	-0.711821
C	4.925526	2.525520	-1.144933
C	6.130791	1.998511	-1.617216
C	6.336291	0.621540	-1.664078
C	5.303940	-1.731590	-1.186380
H	2.970422	2.072994	-0.322061
H	4.784989	3.600973	-1.112655
H	6.914803	2.670125	-1.952311
H	7.273469	0.215893	-2.033193
H	5.965081	-2.099329	-0.395189
C	1.666271	-0.980401	-2.318087
C	2.751323	-1.770612	-2.971709
C	3.838197	-2.116047	-0.878780
C	3.159047	-0.791786	-0.369059
C	0.707310	-0.043654	-0.589542
H	2.354038	-2.325561	-3.821115
H	2.982760	-0.816935	0.705810
N	0.473320	-0.670400	-2.732997
N	-0.109990	-0.076442	-1.653256
N	1.854181	-0.606745	-1.019998
C	-1.459750	0.410766	-1.758352
C	-2.480083	-0.521349	-1.982519
C	-1.686310	1.785141	-1.641269
C	-3.785720	-0.039750	-1.959971
C	-3.016059	2.208121	-1.615966
C	-4.074730	1.307586	-1.736624
H	-4.598615	-0.747004	-2.110127
H	-3.220970	3.268583	-1.493010
O	3.186845	-2.700928	-1.997876
H	3.566106	-1.118554	-3.313957
H	3.773978	-2.879921	-0.103691
H	5.625607	-2.202359	-2.120550
C	-2.202809	-1.965586	-2.302796
H	-1.349176	-2.348793	-1.741735

H	-1.965265	-2.070027	-3.366429
H	-3.074181	-2.576794	-2.064617
C	-5.508409	1.753603	-1.630018
H	-5.584726	2.834620	-1.497887
H	-5.981940	1.263576	-0.773066
H	-6.074684	1.474177	-2.523571
C	-0.552450	2.770717	-1.549504
H	0.253752	2.509119	-2.242199
H	-0.133724	2.813130	-0.538201
H	-0.908010	3.773400	-1.793348
C	0.563082	0.589082	0.775803
O	1.652823	0.886455	1.318841
C	-0.703664	0.722691	1.357323
C	-0.829748	1.709751	2.495219
H	-1.592165	0.530131	0.766564
H	-1.747843	1.513599	3.059520
H	0.024950	1.586093	3.167715
C	-0.853522	3.122979	1.957797
C	0.322008	3.875652	1.871471
C	-2.040052	3.665031	1.454547
C	0.311009	5.141085	1.287747
H	1.247920	3.449924	2.248040
C	-2.053322	4.930229	0.874023
H	-2.956391	3.081296	1.507924
C	-0.875769	5.671796	0.785923
H	1.230961	5.714780	1.227430
H	-2.983759	5.338406	0.489809
H	-0.884655	6.658331	0.333234
N	-2.861457	-1.754800	1.347593
N	-3.483641	-2.463111	0.483542
C	-4.796941	-1.984808	0.301806
O	-5.362669	-1.063554	0.849752
O	-5.376122	-2.733424	-0.659253
C	-6.717322	-2.365394	-0.970160
H	-6.755184	-1.346428	-1.366769
H	-7.058061	-3.075874	-1.721003
H	-7.346171	-2.416853	-0.079203
C	-1.546851	-2.040515	1.538779
C	-0.874522	-1.186403	2.450731
C	-0.784740	-2.984166	0.777552
C	0.468023	-1.523411	2.868674
H	-1.496030	-0.624293	3.141316
C	0.544826	-3.157012	1.018352
H	-1.300019	-3.561832	0.018893

C	1.075589	-0.907696	3.978131
C	1.192751	-2.484960	2.119468
H	1.125583	-3.865131	0.432375
C	2.367605	-1.231982	4.347992
H	0.505094	-0.186018	4.556307
C	2.506747	-2.803419	2.516713
C	3.087016	-2.183523	3.608791
H	2.823689	-0.756059	5.209300
H	3.050876	-3.570862	1.972060
H	4.097667	-2.446247	3.904706

Vibrational frequencies

-321.9988	14.8180	18.7423
23.5918	37.8211	43.3346
44.4234	52.9614	57.1208
60.9646	66.2001	71.4246
72.5629	79.7991	84.8301
91.9736	96.6987	102.1828
107.9295	119.2974	129.3963
150.3962	160.4204	166.0109
176.1935	177.8023	182.7768
191.6934	204.8090	219.0818
219.7308	223.3527	226.7206
236.9596	243.3492	250.9847
257.8180	261.0424	272.4327
284.8966	287.2889	299.5192
307.6955	335.7720	341.9495
345.2032	352.0706	375.6780
385.0420	398.5208	407.6785
410.1887	411.2021	418.2245
423.5709	441.8142	450.6623
490.9792	500.9348	510.4376
513.3153	518.4099	521.3360
524.9206	530.4695	531.9062
545.1709	553.4835	574.5263
589.8282	591.5741	598.8566
604.8587	610.4231	621.5056
630.3914	634.0186	652.7171
657.6952	679.7236	710.1152
721.5980	723.5221	724.5791
740.7063	749.7723	759.9861
771.7508	775.4672	780.7739
784.4718	786.8297	792.8309
802.0084	813.7006	824.4105
833.0232	837.2841	838.8048

862.4233	877.2667	878.9905
881.8763	892.7423	896.0222
906.0771	921.1350	923.6667
938.2173	942.0151	959.5135
961.0884	965.7652	969.1514
983.6955	985.9990	999.1316
1002.7997	1014.7488	1017.1225
1019.2220	1021.6528	1025.3978
1025.8070	1028.6549	1035.8174
1039.0595	1047.9016	1051.5344
1054.3551	1056.4628	1057.4341
1062.1175	1067.2546	1068.1525
1070.6978	1074.7147	1076.1602
1082.0311	1104.3283	1117.4072
1119.6700	1137.4589	1142.9100
1149.3052	1163.8654	1173.9999
1177.1089	1179.6786	1181.2476
1188.1151	1192.7114	1198.4383
1205.6746	1210.1132	1211.7718
1218.7393	1224.8579	1228.5294
1237.8970	1247.8529	1248.5246
1258.9640	1268.2702	1278.7386
1283.7981	1288.8202	1298.6880
1312.8536	1328.9180	1337.9986
1339.5903	1343.4714	1352.0399
1353.1763	1359.6023	1363.7236
1370.4871	1372.8186	1374.9026
1379.4019	1385.9609	1416.9339
1417.4525	1418.5654	1428.5506
1442.0584	1456.4809	1461.8959
1464.7310	1473.1464	1479.0464
1480.9289	1484.2653	1488.2322
1489.9967	1490.1721	1493.6669
1495.3763	1497.5926	1500.3118
1506.8151	1509.7851	1513.6525
1516.9903	1518.4006	1520.1038
1521.9463	1534.1427	1540.5170
1552.6805	1559.2381	1560.9639
1630.5500	1661.4751	1672.8410
1674.6985	1681.4428	1682.3252
1691.9800	1695.9282	1697.4876
1701.5525	1702.4064	1825.0218
3065.7816	3066.0489	3071.7560
3075.8668	3077.6641	3078.0368

3084.3226	3131.3945	3133.2704
3136.8454	3137.2247	3158.7530
3159.2111	3166.2217	3166.4829
3171.4783	3178.5173	3188.1724
3191.2668	3192.5129	3194.6477
3196.5311	3196.6137	3198.0136
3201.5768	3201.8959	3205.2210
3206.0422	3210.3975	3215.1186
3218.5621	3220.0394	3223.4930
3227.8623	3229.1500	3229.7253
3231.6211	3241.0639	3245.7442

TS5RS

Zero-point correction= 0.736800
Thermal correction to Energy= 0.779880
Thermal correction to Enthalpy= 0.780824
Thermal correction to Gibbs Free Energy= 0.660426
Sum of electronic and zero-point Energies= -2196.966725
Sum of electronic and thermal Energies= -2196.923646
Sum of electronic and thermal Enthalpies= -2196.922702
Sum of electronic and thermal Free Energies= -2197.043099
Cartesian coordinates

C	3.493816	-2.385459	-2.458594
C	2.537836	-1.443635	-2.088996
C	2.113125	-0.449203	-2.965597
C	2.658462	-0.423961	-4.246227
C	3.613677	-1.369797	-4.628716
C	4.042084	-2.352240	-3.738681
C	3.801736	-3.327645	-1.323014
H	1.390421	0.294009	-2.639965
H	2.343760	0.338749	-4.950939
H	4.028552	-1.336267	-5.631097
H	4.787482	-3.082127	-4.040142
H	4.801405	-3.137379	-0.920207
C	-0.023234	-2.935038	-0.986169
C	0.826695	-4.152386	-1.148665
C	2.729716	-3.035435	-0.246528
C	2.073151	-1.670785	-0.667809
C	-0.342842	-0.859604	-0.395112
H	0.229490	-5.053179	-1.009532
H	2.353179	-0.851973	-0.006958
N	-1.314888	-2.777610	-1.026242
N	-1.498305	-1.471121	-0.673513
N	0.608882	-1.781175	-0.625600

C	-2.803916	-0.878519	-0.796975
C	-3.798783	-1.284228	0.093245
C	-3.016115	0.049042	-1.823667
C	-5.056162	-0.696680	-0.045393
C	-4.293630	0.594924	-1.922293
C	-5.318621	0.244176	-1.041393
H	-5.846456	-0.983601	0.643311
H	-4.488316	1.321556	-2.707147
O	1.791855	-4.095392	-0.114866
H	1.289605	-4.176391	-2.144646
H	3.168209	-2.940174	0.747360
H	3.766175	-4.383259	-1.610223
C	-3.514997	-2.309203	1.154718
H	-2.549510	-2.125004	1.635415
H	-3.478335	-3.314159	0.722508
H	-4.287414	-2.289766	1.925000
C	-6.677199	0.881532	-1.173715
H	-7.094953	0.704802	-2.168929
H	-6.609336	1.965175	-1.036843
H	-7.375809	0.486938	-0.433761
C	-1.924722	0.465966	-2.773010
H	-1.277680	1.225657	-2.315959
H	-2.358498	0.908880	-3.671222
H	-1.302212	-0.382898	-3.074214
C	-0.075880	0.562296	0.005621
O	1.036988	1.011462	-0.335123
C	-1.001672	1.221035	0.834014
C	-0.915635	2.733532	0.845376
H	-1.977245	0.767425	0.984540
H	-1.591834	3.131201	1.610305
H	0.107200	3.024202	1.110540
C	-1.277748	3.293827	-0.511453
C	-0.278459	3.657908	-1.419717
C	-2.614824	3.390549	-0.908047
C	-0.610477	4.106158	-2.697003
H	0.760739	3.571696	-1.116465
C	-2.948896	3.842250	-2.182055
H	-3.400102	3.098083	-0.213698
C	-1.946305	4.199008	-3.082535
H	0.176248	4.385413	-3.391333
H	-3.993325	3.917418	-2.471671
H	-2.205321	4.550486	-4.076353
N	2.002214	1.838057	2.397515
N	3.262100	1.729106	2.197020

C	3.838827	2.995684	1.994821
O	3.296285	4.075617	1.889650
O	5.173396	2.835661	1.902876
C	5.901006	4.037555	1.671227
H	5.737425	4.750572	2.482415
H	6.950012	3.749932	1.625328
H	5.591449	4.499198	0.730731
C	1.308175	0.681092	2.561235
C	-0.095046	0.815544	2.744895
C	1.877031	-0.634504	2.480720
C	-0.829803	-0.330405	3.266876
H	-0.444248	1.798579	3.047574
C	1.126681	-1.737806	2.741775
H	2.930179	-0.714002	2.229828
C	-2.112304	-0.183763	3.823753
C	-0.229627	-1.610690	3.229960
H	1.557695	-2.734263	2.679814
C	-2.779210	-1.271009	4.359586
H	-2.565910	0.804425	3.843793
C	-0.935324	-2.710729	3.756950
C	-2.185412	-2.542380	4.324878
H	-3.761439	-1.142674	4.802645
H	-0.470746	-3.692851	3.732978
H	-2.709792	-3.395837	4.742955

Vibrational frequencies

-356.0013	18.7057	24.6775
27.0885	29.8474	37.5406
47.8208	52.8893	53.9925
59.6154	66.8433	71.5167
72.8671	76.4403	84.3355
90.6923	93.9706	98.9158
108.8908	119.1990	122.5115
127.9961	157.0025	160.2744
172.8318	178.9089	184.5174
194.1869	197.2928	206.2601
210.8309	216.0832	220.7324
228.0056	238.9312	246.5614
250.7632	256.7224	264.4251
272.2014	285.6067	290.5301
307.4195	332.3734	336.3163
344.4605	351.5315	374.6490
377.1834	402.7372	406.3987
409.9940	412.7207	415.5565
426.0437	446.3865	450.6914

493.8333 503.1560 510.8274
513.6424 518.6237 522.9154
524.5042 531.5539 535.5511
537.9334 547.8093 579.5457
589.7050 591.8948 599.0744
600.4617 611.5149 621.8153
629.8881 635.2212 648.0246
665.3146 683.7817 709.4802
722.7028 723.0831 723.8652
742.9584 749.1349 763.9974
771.0534 774.0366 779.7565
780.8801 788.6173 790.2115
803.8620 810.9775 822.7261
835.5071 837.3014 842.4150
864.4327 869.7049 877.6149
880.8943 890.2581 893.1840
898.1147 911.3934 916.9435
927.9696 941.1812 962.2331
964.0053 970.7763 972.8646
977.8932 985.4649 993.2373
1000.5645 1015.1504 1017.9640
1021.5204 1023.2083 1024.6010
1026.4602 1029.6145 1040.0027
1040.5954 1047.4681 1051.7273
1054.8636 1056.6333 1057.0224
1063.5053 1065.0196 1065.3980
1068.7975 1069.9966 1072.3398
1082.0021 1109.8686 1115.7702
1119.5425 1137.5578 1141.7575
1152.0078 1160.6363 1170.6143
1173.9602 1176.9333 1185.6267
1186.8892 1191.1701 1198.3771
1200.9509 1207.2170 1210.8801
1221.7191 1229.2114 1231.7465
1239.5015 1247.1320 1254.9532
1256.4373 1266.3964 1279.2047
1281.7291 1285.4590 1307.3619
1310.0012 1326.8286 1338.4432
1342.6687 1345.1275 1346.3093
1352.6635 1356.8436 1360.6805
1366.3569 1373.2713 1374.3508
1379.4444 1381.9217 1417.5497
1420.9007 1425.6028 1430.6420
1438.5343 1453.2228 1467.7729

1468.8148	1478.5757	1481.3529
1483.1003	1484.4412	1486.2159
1489.4994	1490.9174	1492.9129
1493.0695	1496.8811	1501.2379
1502.0249	1505.4755	1511.6801
1514.3533	1517.0239	1523.2244
1528.5840	1538.2088	1541.2242
1549.0350	1551.1343	1575.8159
1629.9537	1672.0972	1674.9859
1676.2841	1683.2611	1686.9482
1692.8639	1696.2741	1696.5000
1696.8224	1699.8505	1819.9777
3060.6325	3071.5512	3072.9026
3074.5798	3081.9074	3083.9919
3091.6822	3132.3819	3136.4521
3136.9144	3142.5346	3145.6636
3162.2525	3163.9384	3164.9548
3172.5657	3173.3832	3176.7116
3185.7243	3186.0707	3188.1063
3191.2952	3193.9543	3194.1377
3194.3566	3198.9614	3200.9146
3201.8929	3203.7960	3204.8297
3207.6455	3211.3812	3213.1909
3215.0042	3219.8054	3220.1046
3224.0219	3224.3326	3237.7726

TS5RSb

Zero-point correction= 0.736744
Thermal correction to Energy= 0.779643
Thermal correction to Enthalpy= 0.780587
Thermal correction to Gibbs Free Energy= 0.660633
Sum of electronic and zero-point Energies= -2196.962885
Sum of electronic and thermal Energies= -2196.919986
Sum of electronic and thermal Enthalpies= -2196.919042
Sum of electronic and thermal Free Energies= -2197.038996
Cartesian coordinates

C	-5.755378	-0.196111	-0.705736
C	-4.482642	-0.289852	-0.149062
C	-4.216894	-1.129520	0.929092
C	-5.261999	-1.893754	1.441248
C	-6.542200	-1.808209	0.886664
C	-6.799288	-0.957594	-0.185997
C	-5.786103	0.793515	-1.842153
H	-3.221651	-1.168848	1.363531

H	-5.082139	-2.558644	2.279672
H	-7.345214	-2.411617	1.297798
H	-7.795408	-0.892790	-0.613254
H	-6.335509	1.696172	-1.557124
C	-2.360315	-0.924958	-2.422930
C	-3.550721	-0.790017	-3.313774
C	-4.304986	1.136680	-2.126096
C	-3.510033	0.614559	-0.872210
C	-1.131644	-0.354645	-0.708051
H	-3.307764	-1.119041	-4.323639
H	-3.159418	1.426091	-0.235594
N	-1.260598	-1.607710	-2.563212
N	-0.511510	-1.251452	-1.482837
N	-2.323561	-0.144025	-1.302725
C	0.767226	-1.866691	-1.247417
C	1.860351	-1.436108	-2.002238
C	0.857703	-2.808960	-0.216992
C	3.102517	-1.981176	-1.681487
C	2.124447	-3.320900	0.060506
C	3.253697	-2.908890	-0.650000
H	3.973590	-1.639076	-2.236122
H	2.229397	-4.042998	0.866081
O	-3.851367	0.591514	-3.357167
H	-4.391951	-1.385150	-2.932698
H	-4.151366	2.210492	-2.237661
H	-6.258495	0.401679	-2.748254
C	1.743958	-0.409899	-3.096495
H	0.854648	0.215706	-2.982442
H	1.672609	-0.898796	-4.073486
H	2.630816	0.227343	-3.077271
C	4.626758	-3.419990	-0.299578
H	5.127034	-3.835421	-1.183407
H	4.580814	-4.196366	0.470678
H	5.252228	-2.598603	0.075497
C	-0.335344	-3.200006	0.611895
H	-0.527975	-2.446042	1.387217
H	-0.147918	-4.146853	1.121311
H	-1.238682	-3.304469	0.003210
C	-0.715217	0.268842	0.596969
O	-1.657550	0.731592	1.279129
C	0.653320	0.379916	0.886350
C	1.016855	0.630408	2.329632
H	1.362327	-0.200487	0.308217
H	2.069754	0.917401	2.399315

H	0.407001	1.446301	2.728502
C	0.764407	-0.647618	3.104352
C	-0.457687	-0.865314	3.749670
C	1.712315	-1.675704	3.096323
C	-0.725767	-2.085334	4.368170
H	-1.203063	-0.075546	3.743252
C	1.446925	-2.894516	3.713954
H	2.661177	-1.519716	2.585782
C	0.224338	-3.104400	4.351805
H	-1.679456	-2.239280	4.864269
H	2.195523	-3.681732	3.699797
H	0.016210	-4.054303	4.834124
N	3.380917	1.494385	-0.718980
N	4.628664	1.438692	-0.420532
C	5.330645	0.690350	-1.374348
O	5.021116	0.446918	-2.524391
O	6.494234	0.283880	-0.832942
C	7.337995	-0.448095	-1.718079
H	7.599855	0.155804	-2.588808
H	8.229825	-0.696419	-1.143463
H	6.840418	-1.360770	-2.057016
C	2.595961	2.269711	0.067405
C	1.203332	2.185758	-0.207423
C	3.054892	3.108174	1.142440
C	0.323327	3.191195	0.349511
H	0.935941	1.738404	-1.160512
C	2.195284	3.942825	1.781377
H	4.107208	3.074606	1.402069
C	-0.994569	3.347448	-0.113962
C	0.809555	4.038222	1.376622
H	2.541715	4.592394	2.579898
C	-1.825773	4.313553	0.422055
H	-1.340724	2.709629	-0.925520
C	-0.061035	4.999088	1.927440
C	-1.356228	5.133407	1.459276
H	-2.837374	4.433066	0.047548
H	0.305791	5.648957	2.717056
H	-2.010529	5.886118	1.890050

Vibrational frequencies

-357.6369	17.6265	23.0437
24.7471	28.8281	38.2366
43.6491	50.3695	53.4388
57.4058	69.8600	75.8578
77.8012	80.6147	96.1169

97.1177	103.0438	106.1369
111.5745	122.5627	130.3805
135.8200	155.9760	159.9929
173.5546	178.9907	184.9042
195.9748	197.6235	209.3460
216.3384	219.8302	226.7991
235.5861	242.6150	246.4237
251.7151	255.0681	260.8707
281.8814	287.8226	291.3829
310.1509	333.3464	344.6813
345.5827	351.6938	376.8729
383.2082	402.4952	408.8168
410.6381	412.0298	417.6968
422.9281	442.1763	451.4750
489.4486	499.5942	511.2898
513.3894	519.3792	522.0198
527.8531	531.2364	533.4959
544.8804	550.3542	575.1790
589.5145	593.5603	598.4103
602.6899	609.5606	622.3279
626.7408	630.2931	648.9292
655.8785	682.4359	708.5070
721.9819	722.9778	725.7747
741.3792	751.4174	765.1871
771.8762	774.1567	778.7580
781.9403	786.6123	792.2537
793.4283	813.1660	829.8476
832.6875	837.1945	839.7567
861.7569	877.2368	878.7591
880.2972	890.0857	897.3046
906.1352	920.3048	923.0402
940.7958	950.4648	956.3278
957.5873	968.7933	972.5258
973.6556	983.6296	994.7394
1002.9512	1007.9502	1016.6696
1017.7596	1020.8317	1022.8866
1024.7150	1025.6891	1028.3747
1042.4942	1053.5794	1055.1151
1056.7181	1057.2050	1058.9566
1065.3390	1066.0349	1067.2447
1071.1299	1075.3627	1077.3455
1084.2323	1110.2488	1114.8656
1119.0582	1136.3767	1143.0395
1149.6262	1160.9967	1167.9424

1172.4560	1174.6485	1176.1909
1189.0208	1190.9237	1197.3687
1200.4745	1204.6432	1210.2264
1216.5821	1222.2148	1230.1764
1234.3046	1236.4801	1247.7615
1254.1341	1267.1326	1277.3023
1289.0134	1291.1700	1299.7356
1313.0338	1319.6031	1330.4870
1344.4015	1346.6799	1349.1837
1350.7610	1353.4284	1355.7877
1370.5099	1372.3002	1374.3718
1379.3492	1379.9334	1420.0492
1421.6058	1422.2084	1431.6760
1435.2346	1452.5860	1466.6471
1469.1399	1470.5445	1476.2767
1480.7112	1487.0708	1489.8953
1492.1562	1493.9750	1498.5701
1499.3969	1500.0014	1502.4873
1503.6866	1506.6171	1509.3528
1513.3235	1515.6179	1516.9656
1523.2528	1536.9419	1539.6329
1546.5980	1554.1139	1570.5977
1630.9334	1662.9011	1671.4519
1681.3015	1681.9819	1686.4001
1689.6001	1693.5493	1693.7667
1699.4172	1700.0486	1803.3627
3036.4901	3063.1883	3069.5454
3078.8260	3085.5464	3086.3746
3087.7066	3104.5113	3132.1361
3132.3982	3137.2995	3138.2644
3146.9105	3160.2518	3164.4951
3168.2067	3177.2954	3179.2680
3180.0945	3183.1596	3188.5626
3195.5114	3196.2824	3199.9489
3201.4641	3202.0240	3202.2462
3203.5230	3203.8460	3206.2036
3209.5436	3210.2455	3212.9846
3217.6366	3223.1068	3224.5603
3225.5886	3236.3740	3245.8437

TS5RSc

Zero-point correction= 0.736831
Thermal correction to Energy= 0.779834
Thermal correction to Enthalpy= 0.780779

Thermal correction to Gibbs Free Energy= 0.661432
Sum of electronic and zero-point Energies= -2196.967158
Sum of electronic and thermal Energies= -2196.924155
Sum of electronic and thermal Enthalpies= -2196.923211
Sum of electronic and thermal Free Energies= -2197.042557
Cartesian coordinates

C	4.742235	-1.553652	-1.789321
C	3.366090	-1.644253	-1.591639
C	2.672423	-2.829287	-1.810653
C	3.393684	-3.946118	-2.228151
C	4.773973	-3.865048	-2.427957
C	5.457409	-2.669076	-2.214914
C	5.235132	-0.157397	-1.502009
H	1.595817	-2.866037	-1.672591
H	2.879604	-4.885627	-2.402242
H	5.321020	-4.745105	-2.750962
H	6.530456	-2.611340	-2.370396
H	5.420061	0.384985	-2.435772
C	2.419868	-0.662985	1.283144
C	3.898848	-0.586149	1.450727
C	4.084715	0.507742	-0.720556
C	2.814328	-0.313107	-1.125305
C	0.590565	-0.537456	0.107848
H	4.147270	-0.378139	2.491965
H	2.245772	0.197577	-1.904810
N	1.459921	-0.850164	2.145169
N	0.326523	-0.775334	1.394120
N	1.926436	-0.481397	0.025011
C	-0.945008	-1.169123	1.943590
C	-1.599424	-0.314297	2.829687
C	-1.451871	-2.411770	1.546145
C	-2.855727	-0.720087	3.282911
C	-2.700494	-2.772367	2.041885
C	-3.422072	-1.933525	2.893166
H	-3.404105	-0.065104	3.955991
H	-3.128829	-3.723101	1.737441
O	4.346608	0.507832	0.680714
H	4.364591	-1.532741	1.144494
H	3.949736	1.563389	-0.957973
H	6.155944	-0.125804	-0.913982
C	-0.978597	0.972935	3.300980
H	-0.210852	1.347688	2.618763
H	-0.501376	0.820927	4.274716
H	-1.744859	1.742150	3.420826

C	-4.779138	-2.346235	3.399455
H	-4.705075	-2.771826	4.405396
H	-5.225627	-3.098371	2.744925
H	-5.454768	-1.488646	3.452119
C	-0.683986	-3.330703	0.630622
H	-0.724036	-2.988502	-0.409079
H	-1.115274	-4.332775	0.662331
H	0.368657	-3.400890	0.925794
C	-0.366063	-0.475805	-1.056203
O	0.027005	-1.057247	-2.089137
C	-1.530531	0.290462	-0.870997
C	-2.690547	0.044007	-1.802606
H	-1.786676	0.575279	0.146972
H	-3.337331	0.925330	-1.838720
H	-2.306335	-0.132284	-2.812811
C	-3.499860	-1.147005	-1.334523
C	-3.133555	-2.447608	-1.695669
C	-4.609392	-0.967675	-0.504932
C	-3.866680	-3.542464	-1.244553
H	-2.266006	-2.590037	-2.336375
C	-5.347281	-2.060035	-0.055447
H	-4.899086	0.040281	-0.216481
C	-4.980730	-3.351519	-0.427767
H	-3.573628	-4.546124	-1.538518
H	-6.212761	-1.901360	0.581579
H	-5.558300	-4.204360	-0.083588
N	1.189176	2.466882	0.187183
N	1.574366	2.671066	1.402123
C	2.961673	2.770494	1.507720
O	3.719219	3.273931	0.701285
O	3.352341	2.335176	2.721101
C	4.737238	2.528029	3.002021
H	4.988108	3.591082	2.976231
H	4.896865	2.127042	4.002151
H	5.346344	1.997314	2.267898
C	-0.120187	2.679703	-0.072982
C	-0.603573	2.221800	-1.334545
C	-1.047864	3.312606	0.825707
C	-1.784287	2.863043	-1.879846
H	0.135485	1.856121	-2.044631
C	-2.287130	3.669531	0.398867
H	-0.709767	3.544782	1.829292
C	-2.090478	2.802371	-3.249831
C	-2.665713	3.521897	-0.988868

H	-2.980300	4.169957	1.069009
C	-3.254369	3.370748	-3.736083
H	-1.401597	2.295703	-3.920813
C	-3.856942	4.069884	-1.500439
C	-4.147521	3.994646	-2.851708
H	-3.482192	3.324775	-4.795689
H	-4.540533	4.570544	-0.820132
H	-5.067724	4.427444	-3.231086

Vibrational frequencies

-361.5310	21.9032	23.1858
29.6735	34.4021	39.4916
48.3747	57.4523	59.5019
64.1844	72.6277	75.2644
77.7057	84.0864	92.9994
95.4257	101.7825	104.8495
118.2345	125.7244	129.1505
136.4010	144.4885	160.3741
165.7152	169.6513	181.0866
185.6811	189.2550	203.7311
209.5192	212.9638	217.3319
221.8265	241.7985	247.2589
248.2467	255.8782	272.2375
279.5381	287.3549	290.8363
304.3635	334.4759	337.2074
342.2246	345.2809	378.3240
383.0296	392.9888	401.6924
410.6353	415.3474	418.1364
422.3855	440.5406	445.3984
491.1299	495.7281	500.0031
507.5510	517.6240	521.3460
524.3105	528.3149	532.5696
537.3425	552.2141	581.0403
589.3878	594.2654	597.5309
606.3629	611.6962	618.2417
629.7151	630.2434	644.2547
654.3765	694.5993	712.9735
715.7574	724.7211	728.7571
741.7023	752.3405	764.6359
767.7723	772.7776	777.2791
780.0113	785.5966	791.1571
802.2938	810.5765	831.6941
834.6410	839.7625	842.5237
855.1883	876.4244	883.4324
884.3301	896.1784	900.3598

910.8740	917.2932	920.1262
920.3310	945.1100	951.3892
955.7590	962.7537	970.7915
979.3327	982.4235	989.0790
1005.9607	1010.4104	1013.1513
1016.5075	1019.4144	1022.0191
1022.9536	1024.4872	1035.1170
1040.8031	1044.1957	1045.8717
1049.1155	1053.4417	1056.8831
1061.6917	1062.0981	1063.7304
1067.0633	1068.8952	1073.7346
1087.6227	1112.8110	1113.7710
1116.6511	1135.5033	1145.6023
1157.7514	1162.1817	1172.4225
1174.4179	1178.1825	1190.7219
1191.1311	1192.0264	1197.4580
1200.2449	1205.3606	1215.6302
1220.9632	1226.1185	1227.2644
1239.3158	1248.2172	1252.0462
1256.6003	1271.4555	1282.1325
1285.4024	1287.2539	1298.8811
1307.6942	1327.3629	1331.4118
1342.3109	1345.0932	1350.0329
1356.4908	1356.5655	1360.9976
1369.2711	1374.9005	1375.8774
1377.7808	1383.4099	1410.7316
1415.1117	1420.7768	1423.5991
1432.5499	1451.1285	1466.4639
1469.2133	1472.6043	1480.4390
1481.3009	1484.0238	1490.1959
1492.2504	1494.7257	1495.2539
1495.7370	1497.4551	1501.3357
1505.1446	1505.7238	1515.1345
1517.2147	1519.5650	1520.1252
1535.1015	1539.5127	1545.6644
1547.2595	1552.1962	1581.2301
1628.7940	1668.0631	1674.8403
1678.2470	1683.7227	1688.0489
1692.1734	1694.5767	1696.2271
1698.1315	1700.9262	1801.2685
3064.3741	3069.6396	3074.4713
3077.3244	3082.8818	3085.7698
3089.4492	3135.7129	3142.7563
3143.5756	3144.3230	3146.4767

3160.9497	3163.8056	3163.9811
3171.3171	3174.3866	3175.5014
3186.3455	3188.0470	3189.3156
3191.0269	3195.0081	3197.9507
3198.3243	3200.2381	3202.1762
3202.5275	3205.4274	3205.6983
3207.0494	3209.0830	3211.6049
3219.0426	3220.3017	3220.5168
3230.4120	3232.4596	3239.4005

TS5SR

Zero-point correction= 0.736746
Thermal correction to Energy= 0.779862
Thermal correction to Enthalpy= 0.780806
Thermal correction to Gibbs Free Energy= 0.659602
Sum of electronic and zero-point Energies= -2196.958300
Sum of electronic and thermal Energies= -2196.915184
Sum of electronic and thermal Enthalpies= -2196.914240
Sum of electronic and thermal Free Energies= -2197.035443
Cartesian coordinates

C	4.905839	-0.953196	-0.679029
C	3.523383	-0.810150	-0.765297
C	2.738618	-1.762497	-1.412201
C	3.366153	-2.855006	-2.003474
C	4.755327	-2.991712	-1.939792
C	5.532009	-2.046219	-1.274820
C	5.528853	0.163534	0.115358
H	1.656862	-1.669238	-1.455424
H	2.766861	-3.604670	-2.510835
H	5.232342	-3.849508	-2.402617
H	6.609286	-2.165479	-1.209876
H	6.139183	0.810519	-0.521828
C	2.371217	-0.483762	2.151208
C	3.793564	-0.358382	2.588146
C	4.343785	0.964779	0.705349
C	3.053494	0.426630	-0.025502
C	0.680349	-0.171437	0.792783
H	3.853977	-0.361070	3.676343
H	2.652831	1.210072	-0.671080
N	1.357295	-1.018800	2.759343
N	0.315355	-0.833980	1.900031
N	2.009817	0.049099	0.942714
C	-0.921359	-1.518735	2.190303
C	-1.739376	-1.013892	3.196700

C	-1.198574	-2.690368	1.481534
C	-2.899811	-1.728818	3.491120
C	-2.373686	-3.363154	1.809631
C	-3.231871	-2.899622	2.810104
H	-3.564258	-1.353557	4.266041
H	-2.623216	-4.272331	1.269775
O	4.262783	0.886379	2.116945
H	4.387188	-1.196935	2.196673
H	4.443086	2.028006	0.500190
H	6.179334	-0.196839	0.919058
C	-1.378413	0.258975	3.911226
H	-0.495246	0.119537	4.542340
H	-2.203925	0.594800	4.540446
H	-1.145568	1.047779	3.189290
C	-4.479785	-3.669801	3.157106
H	-5.181415	-3.050725	3.723713
H	-4.235580	-4.547063	3.767249
H	-4.983955	-4.027063	2.253828
C	-0.293147	-3.186086	0.386320
H	0.762573	-3.118985	0.670064
H	-0.443649	-2.602132	-0.531301
H	-0.517298	-4.227446	0.148098
C	-0.301755	0.113084	-0.315856
O	-1.497753	-0.031540	-0.012755
C	0.118926	0.574519	-1.582018
C	-0.837500	0.287235	-2.726457
H	1.175243	0.594201	-1.828896
H	-1.786609	0.803382	-2.545663
H	-0.410120	0.683659	-3.654069
C	-1.102218	-1.197100	-2.863773
C	-0.143116	-2.051985	-3.419168
C	-2.293284	-1.747562	-2.381423
C	-0.361357	-3.426573	-3.478178
H	0.783822	-1.634024	-3.807851
C	-2.515650	-3.122310	-2.442097
H	-3.035603	-1.084594	-1.945635
C	-1.549430	-3.966165	-2.985469
H	0.388600	-4.076113	-3.918668
H	-3.444567	-3.534385	-2.058388
H	-1.721901	-5.036938	-3.030913
N	-2.692906	2.482958	-1.086640
N	-3.730623	2.482411	-0.347432
C	-4.875867	2.164015	-1.109314
O	-4.935536	1.728468	-2.238854

O	-5.959220	2.384479	-0.346901
C	-7.200793	2.062479	-0.967669
H	-7.222853	1.009494	-1.255536
H	-7.969758	2.269374	-0.225543
H	-7.356266	2.675859	-1.858122
C	-1.495402	2.691697	-0.462655
C	-0.349746	2.673992	-1.296829
C	-1.319460	2.796993	0.954024
C	0.891014	3.223191	-0.770733
H	-0.521273	2.764083	-2.366301
C	-0.091596	3.046545	1.483647
H	-2.190126	2.651934	1.584786
C	1.952195	3.587112	-1.615693
C	1.036083	3.351116	0.631329
H	0.046085	3.115832	2.559717
C	3.134461	4.083634	-1.090720
H	1.830096	3.479654	-2.690735
C	2.254507	3.831832	1.147966
C	3.281671	4.208902	0.299831
H	3.943359	4.378054	-1.751184
H	2.370171	3.926647	2.224275
H	4.208046	4.597723	0.711891

Vibrational frequencies

-336.7254	9.8930	17.7512
26.7746	34.0708	39.5266
39.8754	49.3488	51.5596
62.9715	65.4402	68.4694
79.3573	80.3775	87.9091
93.2846	98.3967	99.7785
104.8287	116.7027	129.2893
132.5584	152.5040	161.4856
170.9931	174.7193	183.2851
196.9116	201.3212	205.2840
210.1240	215.8796	228.4873
233.4694	238.6122	242.0234
244.4161	252.7578	263.6888
272.4567	283.5596	294.4074
306.1697	326.5613	337.2013
341.7887	359.6278	373.9679
380.4704	401.9378	404.2342
408.5295	411.6943	414.3670
422.0592	442.2218	454.9677
490.0728	506.8169	509.6921
514.7795	518.2885	522.4640

523.8778	528.3479	536.2548
545.1011	550.0043	571.4826
590.3765	594.1839	595.8422
598.0052	610.1743	619.8714
630.5504	635.0518	640.0221
662.3713	685.5352	705.4135
720.1357	722.5784	723.9420
743.6123	750.9959	769.4140
777.0516	777.7641	779.9435
781.5542	787.1857	791.3439
800.6098	811.4879	822.6154
831.7365	836.8945	841.3861
851.3665	868.2713	874.4095
877.7759	884.6837	888.5598
903.3665	910.1693	912.6474
920.2423	940.8877	962.4074
967.5430	969.0755	971.7497
979.5844	983.2915	996.9338
1004.5345	1011.1505	1017.8169
1020.0174	1022.3209	1022.9573
1028.4837	1028.9151	1038.6761
1042.9645	1043.2100	1047.3987
1055.2711	1058.7256	1061.7601
1062.9845	1063.2012	1068.7619
1069.3431	1070.1118	1071.2419
1072.8128	1103.5226	1117.4223
1123.1226	1136.9623	1144.3374
1153.7107	1161.4349	1174.6119
1175.4522	1177.8291	1183.0533
1188.1328	1193.6524	1201.8646
1207.8943	1212.8397	1216.6180
1221.7077	1228.9171	1230.2388
1243.5703	1247.2526	1254.7368
1261.4162	1264.1801	1277.3918
1284.7466	1290.2513	1308.0795
1314.2382	1322.6889	1338.1694
1340.1958	1346.6175	1347.1371
1347.8618	1361.5550	1363.1541
1367.3343	1367.8988	1372.6086
1377.7894	1380.1194	1409.9021
1416.2438	1425.8630	1429.3910
1449.8719	1454.2317	1458.1315
1468.4905	1476.8621	1483.3202
1483.5006	1489.1539	1489.6494

1490.3447	1493.4152	1494.1594
1495.3628	1497.0240	1497.8888
1500.1721	1503.2983	1507.3439
1508.3127	1513.8786	1518.9897
1524.5649	1531.8534	1540.9471
1549.4267	1555.3345	1560.4376
1631.0959	1672.4291	1675.7264
1679.5319	1680.5258	1692.9054
1694.3217	1696.5271	1698.6766
1699.4028	1701.7428	1823.6521
3056.5482	3059.4622	3067.0722
3068.2045	3069.0834	3088.2646
3091.4344	3125.5600	3126.0607
3130.8443	3133.2247	3138.2098
3149.7092	3157.7775	3170.8754
3171.0719	3173.6764	3180.6582
3190.5163	3192.2977	3195.5142
3198.9711	3200.3377	3201.1383
3203.5850	3204.2388	3205.5869
3206.7613	3207.0238	3210.9013
3213.6906	3216.5328	3216.8217
3219.5204	3228.0529	3228.9020
3229.4835	3231.7753	3237.6101

TS5SRb

Zero-point correction= 0.736796
Thermal correction to Energy= 0.779913
Thermal correction to Enthalpy= 0.780858
Thermal correction to Gibbs Free Energy= 0.659924
Sum of electronic and zero-point Energies= -2196.958269
Sum of electronic and thermal Energies= -2196.915152
Sum of electronic and thermal Enthalpies= -2196.914208
Sum of electronic and thermal Free Energies= -2197.035141
Cartesian coordinates

C	-4.905445	0.957127	-0.673083
C	-3.523185	0.813609	-0.761771
C	-2.738550	1.768965	-1.404396
C	-3.366016	2.865253	-1.988652
C	-4.754997	3.002689	-1.922349
C	-5.531548	2.054004	-1.261795
C	-5.528499	-0.163908	0.115143
H	-1.656933	1.675093	-1.449702
H	-2.766826	3.617273	-2.492637
H	-5.231886	3.863475	-2.379732

H	-6.608668	2.173625	-1.194893
H	-6.140557	-0.806136	-0.525178
C	-2.370362	0.468304	2.153192
C	-3.792164	0.338674	2.590638
C	-4.343435	-0.970240	0.698200
C	-3.053262	-0.427635	-0.029510
C	-0.680251	0.167367	0.791348
H	-3.851353	0.332740	3.678894
H	-2.652695	-1.207201	-0.679766
N	-1.356708	1.000964	2.763863
N	-0.315234	0.823300	1.902464
N	-2.009325	-0.056038	0.940886
C	0.920722	1.508177	2.195598
C	1.736039	1.002553	3.203006
C	1.196408	2.684534	1.493559
C	2.893819	1.719640	3.505242
C	2.366519	3.359755	1.829895
C	3.225424	2.892784	2.828184
H	3.553547	1.346162	4.284154
H	2.612047	4.276659	1.299188
O	-4.261403	-0.902530	2.110304
H	-4.386593	1.180002	2.206484
H	-4.443477	-2.031862	0.485123
H	-6.177389	0.192107	0.922082
C	1.374735	-0.271180	3.916937
H	0.491764	-0.131510	4.548467
H	2.200381	-0.608054	4.545426
H	1.140624	-1.059040	3.194062
C	4.494986	3.638887	3.148162
H	4.313455	4.715034	3.209956
H	5.244266	3.477316	2.366920
H	4.922017	3.305287	4.096073
C	0.290051	3.184940	0.401231
H	-0.765730	3.113214	0.684607
H	0.441881	2.607360	-0.520061
H	0.511584	4.228414	0.169888
C	0.301569	-0.110250	-0.319290
O	1.497525	0.035333	-0.016474
C	-0.118838	-0.568633	-1.586655
C	0.837151	-0.276916	-2.730315
H	-1.175127	-0.588852	-1.833576
H	1.786977	-0.792231	-2.550920
H	0.410322	-0.671287	-3.659052
C	1.099662	1.208226	-2.863216

C	0.138815	2.063440	-3.415065
C	2.290237	1.758943	-2.379966
C	0.354832	3.438565	-3.469587
H	-0.787764	1.645337	-3.804444
C	2.510383	3.134241	-2.436154
H	3.033909	1.095695	-1.947945
C	1.542381	3.978388	-2.975871
H	-0.397454	4.088390	-3.907373
H	3.438887	3.546531	-2.052688
H	1.713107	5.049581	-3.017768
N	2.694720	-2.475085	-1.094400
N	3.732022	-2.476702	-0.354476
C	4.877686	-2.155617	-1.114407
O	4.938176	-1.716100	-2.242384
O	5.960585	-2.378670	-0.351036
C	7.202554	-2.054938	-0.970065
H	7.224705	-1.001241	-1.256306
H	7.971014	-2.263613	-0.227908
H	7.358793	-2.666059	-1.861942
C	1.497026	-2.685920	-0.471687
C	0.351760	-2.668010	-1.306440
C	1.320429	-2.794780	0.944688
C	-0.888728	-3.219911	-0.782349
H	0.524003	-2.755344	-2.376029
C	0.092602	-3.048204	1.473001
H	2.190556	-2.650141	1.576294
C	-1.949202	-3.582614	-1.628713
C	-1.034294	-3.351839	0.619300
H	-0.045645	-3.119379	2.548822
C	-3.131171	-4.081771	-1.105559
H	-1.826778	-3.472180	-2.703414
C	-2.252475	-3.835036	1.134155
C	-3.278903	-4.210842	0.284586
H	-3.939483	-4.375258	-1.767162
H	-2.368520	-3.932677	2.210167
H	-4.205128	-4.601503	0.695235

Vibrational frequencies

-337.1890	13.3293	17.9741
27.0301	34.5933	40.1714
41.1270	49.9736	53.2956
63.2471	65.7520	70.3074
76.9636	79.8142	81.0283
87.9123	94.0640	99.1053
104.9840	116.5659	130.1356

133.0898	153.1253	162.8344
171.9375	175.6964	184.1180
197.1817	201.8194	205.2032
210.5030	215.6615	229.2327
234.3483	239.3147	242.8587
244.4189	253.1582	263.9029
272.8704	281.1895	294.7437
306.3894	326.6359	337.5066
341.8840	359.5972	373.8894
380.6687	401.8961	403.0108
408.9723	411.6527	414.0420
422.6213	443.0834	454.8170
490.2121	506.1915	510.0150
514.7667	518.7925	522.4611
524.7717	528.4013	536.1168
544.2097	549.2532	569.8584
589.6425	593.8943	595.3196
597.9894	610.0883	623.4453
630.5187	635.0175	638.8368
662.4372	685.5432	705.3086
720.1445	722.4614	724.3306
743.5785	750.9847	769.2736
776.8104	777.7880	780.0617
781.6456	787.0385	791.3113
800.5753	811.5108	822.4399
831.6054	836.7910	841.3984
851.3138	868.3817	874.4776
879.6748	885.2041	888.4108
903.2098	911.2491	912.5527
920.0594	941.0139	962.5687
965.8658	969.1134	971.7018
979.4486	983.4261	996.6739
1005.0715	1011.2146	1017.8082
1019.9534	1022.5827	1022.8414
1028.6395	1028.7004	1036.1229
1042.0394	1043.0718	1047.1063
1055.6549	1059.2984	1061.7796
1062.6439	1063.2638	1065.9916
1068.9855	1069.2994	1071.1474
1072.3863	1103.4615	1117.3641
1123.0826	1136.7539	1144.2156
1153.8695	1161.2883	1174.5545
1175.6363	1177.5487	1183.0637
1188.2815	1193.3316	1201.6937

1207.6652	1212.8705	1216.4635
1221.9356	1229.0722	1230.2577
1243.9168	1247.3889	1254.5597
1261.6843	1264.1896	1277.4919
1284.6278	1289.8454	1308.5176
1314.7670	1322.5479	1337.8971
1340.1115	1346.5122	1347.0731
1348.6888	1361.5031	1363.2153
1367.2000	1367.9001	1372.6608
1377.7585	1380.2549	1410.6506
1416.1249	1425.7981	1428.4788
1449.5566	1454.4168	1458.0818
1469.0883	1476.9074	1483.5185
1483.7427	1489.5970	1489.6382
1491.1752	1493.8177	1494.2270
1495.2423	1496.9988	1497.9060
1500.0503	1503.1982	1507.3556
1508.7513	1513.7927	1518.8923
1524.6300	1532.0086	1540.8878
1549.4348	1555.2584	1560.6263
1630.9472	1672.5351	1675.5795
1679.4896	1680.4988	1693.0636
1694.3886	1696.5176	1698.7485
1699.6330	1702.5589	1823.2812
3056.3684	3066.0156	3067.7888
3069.5005	3071.8667	3088.5238
3090.6612	3124.8451	3126.4445
3133.5876	3136.8540	3142.2489
3158.3796	3166.3292	3170.3123
3170.8436	3172.1972	3180.8916
3189.0573	3191.3236	3195.9115
3196.4194	3198.8381	3199.9744
3200.7953	3202.6529	3205.4035
3206.2569	3206.9771	3211.7078
3213.5713	3216.2876	3216.3960
3219.6509	3228.0506	3229.5593
3230.4997	3231.8317	3237.5514

TS5SRc

Zero-point correction= 0.736711
Thermal correction to Energy= 0.779478
Thermal correction to Enthalpy= 0.780422
Thermal correction to Gibbs Free Energy= 0.660839
Sum of electronic and zero-point Energies= -2196.957897

Sum of electronic and thermal Energies= -2196.915130
Sum of electronic and thermal Enthalpies= -2196.914186
Sum of electronic and thermal Free Energies= -2197.033769
Cartesian coordinates

C	-1.132356	1.335415	3.845122
C	-1.322628	1.090066	2.484253
C	-1.915898	2.045636	1.660162
C	-2.305020	3.260348	2.220600
C	-2.115924	3.508131	3.581757
C	-1.533164	2.546277	4.402694
C	-0.468540	0.179073	4.542162
H	-2.086804	1.860873	0.603186
H	-2.768699	4.009827	1.587656
H	-2.430528	4.457266	4.004027
H	-1.389635	2.736893	5.462013
H	-1.014912	-0.141995	5.432200
C	1.681483	-0.298226	1.804222
C	1.892974	-0.995419	3.110406
C	-0.446516	-0.942667	3.478978
C	-0.795663	-0.277841	2.104500
C	0.584423	0.426928	0.057313
H	2.701662	-1.715910	2.984436
H	-1.506316	-0.902504	1.570136
N	2.587661	0.233040	1.030194
N	1.891089	0.694571	-0.039399
N	0.430431	-0.164594	1.270309
C	2.566411	1.573744	-0.966341
C	3.523869	1.045155	-1.827964
C	2.283648	2.940873	-0.872712
C	4.201228	1.943832	-2.653668
C	2.994165	3.793433	-1.711442
C	3.948764	3.313731	-2.612811
H	4.948438	1.556669	-3.341880
H	2.796623	4.861312	-1.661001
O	0.730906	-1.718947	3.445956
H	2.171521	-0.271375	3.885345
H	-1.243741	-1.659012	3.686878
H	0.540231	0.446082	4.872271
C	3.831718	-0.423460	-1.843146
H	4.455328	-0.692334	-0.983577
H	4.378217	-0.695700	-2.747886
H	2.927888	-1.036433	-1.779995
C	4.671306	4.261157	-3.532942
H	4.902752	5.206080	-3.021364

H	4.044868	4.504253	-4.405471
H	5.606474	3.823648	-3.904562
C	1.238638	3.472944	0.071036
H	1.320428	3.023752	1.066885
H	0.238589	3.253092	-0.319756
H	1.338410	4.554260	0.179010
C	-0.382537	0.610531	-1.086139
O	-0.041507	1.414223	-1.973557
C	-1.513784	-0.233420	-1.118756
C	-2.576773	0.131309	-2.128287
H	-1.879604	-0.667965	-0.196920
H	-2.103002	0.366620	-3.086715
H	-3.258432	-0.709537	-2.277280
C	-3.358890	1.322701	-1.618843
C	-4.460632	1.127883	-0.780158
C	-2.942983	2.630616	-1.891526
C	-5.131424	2.211594	-0.219588
H	-4.786811	0.113021	-0.561688
C	-3.613405	3.716469	-1.331565
H	-2.077784	2.783823	-2.529066
C	-4.708612	3.510915	-0.493686
H	-5.984221	2.042203	0.430737
H	-3.281208	4.726609	-1.552387
H	-5.229365	4.357779	-0.057443
N	1.380133	-2.562390	-0.523644
N	2.016918	-2.856314	0.552761
C	3.398902	-2.934528	0.325242
O	3.970158	-3.225684	-0.703257
O	4.045681	-2.720176	1.488473
C	5.464419	-2.852613	1.419142
H	5.883786	-2.128063	0.717880
H	5.831912	-2.662102	2.425726
H	5.737523	-3.859222	1.096244
C	0.029498	-2.678910	-0.480556
C	-0.674172	-2.264111	-1.642771
C	-0.718227	-3.188883	0.637297
C	-1.963233	-2.873641	-1.895760
H	-0.080390	-1.939894	-2.493725
C	-2.035561	-3.494340	0.493009
H	-0.197741	-3.330507	1.580394
C	-2.529344	-2.903253	-3.182557
C	-2.673252	-3.430584	-0.803696
H	-2.608646	-3.884390	1.329806
C	-3.781195	-3.454940	-3.387296

H	-1.970211	-2.478969	-4.012321
C	-3.958240	-3.958529	-1.028795
C	-4.503988	-3.970644	-2.300071
H	-4.208521	-3.480171	-4.384085
H	-4.508964	-4.378560	-0.191607
H	-5.491568	-4.391442	-2.459524

Vibrational frequencies

-328.0372	11.1762	20.4877
29.4729	29.8776	41.9754
43.5331	50.2355	56.0899
61.2073	67.3586	75.3278
78.5462	85.9525	88.5121
97.2441	104.4213	110.8146
118.8776	121.4441	125.6843
142.3979	162.4874	165.0233
178.2182	192.0105	198.4260
203.4454	213.8449	220.0166
224.2677	225.1839	230.1931
240.6198	248.1991	253.1354
255.1406	265.2133	265.7859
283.5126	292.1603	299.5808
310.9279	329.3324	337.4621
343.1609	356.6518	363.1573
383.2011	392.4667	398.6440
405.9619	409.1934	416.6814
425.3155	444.1922	455.9780
480.1975	491.8932	509.9871
515.1912	520.9496	523.9204
528.1988	529.5831	534.9826
548.6949	553.0680	566.2013
587.3557	591.8682	596.9655
603.6793	607.7498	627.6201
629.8993	630.4063	636.7735
650.6581	659.4453	687.6352
709.5801	718.1502	719.5849
735.8371	744.7002	763.6279
773.1906	776.6155	777.4328
780.0774	784.1230	787.6884
794.9295	805.7426	826.7619
832.8688	836.4970	838.7034
847.7645	859.9490	871.8680
883.2853	886.7473	898.0136
900.6090	912.6993	913.8575
917.4101	937.3563	954.0640

962.7021	970.1677	977.1536
977.9698	983.1726	995.8852
1001.8764	1005.1343	1012.8581
1016.4343	1018.5907	1019.5149
1022.4425	1026.7101	1030.8169
1039.8051	1046.2836	1050.7869
1053.2683	1059.1779	1063.6316
1065.5202	1068.5352	1069.9797
1072.6585	1072.8780	1077.1157
1089.8201	1106.5925	1112.0786
1127.6446	1137.0386	1146.2242
1162.1869	1170.9949	1171.7296
1175.4912	1175.6386	1176.6486
1191.8556	1194.7026	1197.6571
1199.9531	1205.1959	1213.0437
1217.3782	1226.8399	1230.3819
1239.4340	1243.5289	1254.0025
1256.0623	1261.1381	1286.1254
1287.3427	1289.7733	1307.2894
1322.6864	1329.3020	1332.5444
1343.0004	1345.7495	1352.0658
1355.4522	1356.1096	1358.1497
1365.8497	1369.2482	1369.7858
1379.2870	1382.6949	1405.1174
1418.7769	1421.9425	1428.9084
1437.1227	1447.6834	1451.0090
1469.3399	1471.2731	1478.0816
1479.1901	1482.1472	1487.9686
1492.9326	1496.5447	1499.3030
1499.8713	1501.1048	1501.6150
1504.3812	1505.1969	1507.1250
1509.7954	1512.4748	1514.5996
1526.0814	1533.9163	1540.5196
1546.7287	1552.0420	1556.5097
1627.9105	1660.3925	1673.0487
1675.7107	1678.8450	1680.8773
1692.4170	1693.9208	1698.1689
1698.6748	1699.4068	1819.0648
3022.7191	3062.0744	3076.0565
3082.7906	3086.8500	3087.2593
3090.9031	3099.8708	3119.1814
3132.1823	3136.8314	3146.4373
3146.5470	3148.6163	3169.7513
3172.2862	3174.1604	3181.7217

3188.4460	3191.6345	3193.5958
3194.9119	3196.0559	3196.4859
3198.6209	3204.2325	3205.2466
3206.0853	3206.9663	3214.6128
3215.5273	3215.6473	3218.1685
3220.2742	3221.4426	3224.5921
3231.2762	3233.9237	3258.2143

TS5SSb

Zero-point correction= 0.736678
Thermal correction to Energy= 0.780126
Thermal correction to Enthalpy= 0.781070
Thermal correction to Gibbs Free Energy= 0.659129
Sum of electronic and zero-point Energies= -2196.948974
Sum of electronic and thermal Energies= -2196.905526
Sum of electronic and thermal Enthalpies= -2196.904582
Sum of electronic and thermal Free Energies= -2197.026523
Cartesian coordinates

C	-4.144600	-1.851262	1.146285
C	-2.835413	-1.396025	1.284364
C	-2.204121	-1.359736	2.524512
C	-2.918143	-1.779346	3.644271
C	-4.236001	-2.225126	3.515176
C	-4.856784	-2.265540	2.268698
C	-4.589408	-1.812628	-0.292651
H	-1.176551	-1.015255	2.618746
H	-2.447954	-1.760754	4.621728
H	-4.779530	-2.550447	4.396390
H	-5.876723	-2.625228	2.172496
H	-5.317732	-1.011598	-0.456328
C	-0.879504	-2.911581	-0.673296
C	-2.143877	-3.580806	-1.102616
C	-3.314184	-1.512780	-1.113073
C	-2.264884	-0.996944	-0.058811
C	0.321159	-1.194176	-0.021353
H	-1.915507	-4.432883	-1.742519
H	-2.171015	0.077939	-0.176878
N	0.345315	-3.341076	-0.691602
N	1.081044	-2.272400	-0.272086
N	-0.946110	-1.608445	-0.266631
C	2.495152	-2.496305	-0.082732
C	2.971240	-2.684433	1.215909
C	3.294737	-2.606387	-1.216717
C	4.324834	-2.975908	1.358902

C	4.644920	-2.897610	-1.020408
C	5.174839	-3.085866	0.255363
H	4.727576	-3.119617	2.358637
H	5.294986	-2.976584	-1.888143
O	-2.860028	-2.628999	-1.862773
H	-2.716305	-3.927628	-0.231153
H	-3.496386	-0.726304	-1.845472
H	-5.043793	-2.749376	-0.630132
C	2.067720	-2.540399	2.409733
H	1.878709	-1.480012	2.610370
H	2.528971	-2.977979	3.296415
H	1.102308	-3.030609	2.248168
C	6.629205	-3.430928	0.445111
H	7.037079	-2.942666	1.333415
H	7.223560	-3.129354	-0.419819
H	6.755477	-4.510506	0.576736
C	2.716834	-2.424210	-2.593384
H	2.062500	-1.548712	-2.625613
H	2.118889	-3.293195	-2.884785
H	3.511546	-2.289908	-3.329188
C	0.910406	0.088400	0.547551
O	2.152038	0.136641	0.538480
C	0.053472	1.083137	1.054127
C	0.496254	1.902840	2.263144
H	-1.009732	0.882639	1.058861
H	-0.404908	2.357081	2.685702
H	0.869325	1.196709	3.019046
C	1.538597	2.992338	2.112049
C	2.901899	2.686504	2.070571
C	1.152270	4.334951	2.074075
C	3.852427	3.697720	1.970852
H	3.203361	1.644058	2.079338
C	2.101586	5.351441	1.967836
H	0.095849	4.588679	2.129509
C	3.456720	5.033800	1.912490
H	4.907216	3.442680	1.931428
H	1.781342	6.388178	1.934464
H	4.199400	5.821266	1.831177
N	-2.369999	2.330890	-0.983985
N	-3.384348	1.715150	-1.478222
C	-4.589205	2.192655	-0.934882
O	-4.786758	3.179036	-0.260352
O	-5.569837	1.345935	-1.309839
C	-6.871046	1.697054	-0.844131

H	-7.159754	2.680488	-1.220866
H	-7.543028	0.931300	-1.227718
H	-6.896323	1.714492	0.247666
C	-1.157278	1.930392	-1.439306
C	-0.029156	2.456617	-0.751061
C	-0.946190	0.913567	-2.429008
C	1.272094	2.341052	-1.374433
H	-0.204025	3.291501	-0.077967
C	0.313408	0.606719	-2.843219
H	-1.809718	0.418120	-2.859607
C	2.348143	3.175717	-1.024502
C	1.452534	1.366967	-2.389910
H	0.467544	-0.149128	-3.609157
C	3.577940	3.033614	-1.639198
H	2.199474	3.945217	-0.275124
C	2.718517	1.223834	-2.987480
C	3.767828	2.042794	-2.614457
H	4.398428	3.686095	-1.358169
H	2.853058	0.478722	-3.766901
H	4.738080	1.928133	-3.087530

Vibrational frequencies

-332.2979	18.1533	24.2976
25.7859	32.7435	35.0024
37.7705	45.9264	48.1657
55.8941	56.5900	64.3018
76.8581	78.6515	80.7031
89.8970	95.3626	103.7934
113.6414	119.6840	123.0296
127.7900	130.9357	150.6306
158.3196	164.0412	167.0220
188.2695	191.5730	201.3985
211.8981	215.6815	223.8271
226.0496	231.0945	241.8202
243.3380	248.7418	252.1381
272.2433	283.1481	299.6844
307.7945	313.7216	324.3072
339.4611	342.6051	360.6024
384.3464	399.4253	402.9124
411.5062	414.0191	419.7783
427.2441	435.5751	448.5681
490.5592	499.5070	505.6459
512.5134	517.4227	523.3213
528.4683	529.8257	530.7352
543.5683	553.6072	572.2196

590.7198 593.1216 599.2281
604.4755 609.3655 619.5037
630.4452 633.1795 644.5495
655.3689 678.0943 713.5474
721.5960 723.5825 724.3328
745.0432 753.4684 768.1464
769.1727 773.9220 779.3089
785.6673 788.2802 792.5185
798.6701 812.4219 821.3936
831.5751 837.3775 851.7877
859.0678 864.1137 876.9642
885.5283 886.4935 890.1111
913.7027 919.1134 920.6376
920.8801 939.3119 951.3742
958.3883 963.3466 969.9460
982.6551 988.2262 993.4193
1005.4812 1006.9080 1012.8773
1018.4810 1022.4641 1023.0458
1024.7207 1027.7290 1030.7304
1037.2927 1041.4429 1044.2193
1057.9380 1059.9184 1060.3103
1063.2315 1065.0770 1066.0476
1066.9430 1070.6635 1072.1859
1078.0582 1104.5386 1117.7344
1119.7211 1133.9414 1143.7008
1153.8023 1165.2392 1175.4486
1175.8887 1177.3603 1186.3100
1186.8908 1188.5954 1199.8606
1204.0157 1206.2191 1208.6218
1219.5773 1224.4221 1234.9093
1239.4403 1247.9884 1257.5386
1260.0539 1263.9949 1279.5794
1284.6040 1291.4879 1302.0972
1307.1720 1322.8562 1337.8295
1344.5091 1347.4272 1349.7949
1353.5277 1359.9628 1363.5720
1370.7890 1372.1946 1373.4249
1383.3213 1386.3917 1412.6618
1416.2358 1418.8728 1426.8564
1430.5445 1453.9805 1456.0694
1468.6091 1472.9129 1477.1097
1478.8036 1484.8586 1487.8563
1493.2520 1493.8442 1496.4563
1498.3093 1498.8549 1499.0927

1501.6926	1503.7997	1506.7580
1507.1657	1516.0756	1516.5156
1522.8107	1527.1491	1540.6276
1550.0113	1557.8195	1559.0437
1629.0891	1673.4762	1676.7193
1682.6697	1687.2636	1693.5315
1695.1377	1697.6629	1700.1739
1700.5999	1703.5464	1823.2546
3037.3580	3063.5940	3071.7097
3076.9568	3082.0574	3083.5544
3089.1040	3112.0754	3133.4969
3137.5806	3141.0648	3155.4015
3164.6407	3164.9582	3169.6988
3175.6175	3176.4654	3185.5823
3188.5169	3192.6282	3197.1380
3199.5473	3203.0570	3206.4656
3207.0170	3208.6485	3208.8206
3213.3818	3213.9235	3215.1726
3217.4214	3228.9395	3229.0566
3229.2150	3233.4029	3233.4810
3246.3474	3260.7909	3261.9764

TS5SSc

Zero-point correction= 0.736336
Thermal correction to Energy= 0.779789
Thermal correction to Enthalpy= 0.780733
Thermal correction to Gibbs Free Energy= 0.658531
Sum of electronic and zero-point Energies= -2196.956925
Sum of electronic and thermal Energies= -2196.913473
Sum of electronic and thermal Enthalpies= -2196.912528
Sum of electronic and thermal Free Energies= -2197.034731
Cartesian coordinates

C	0.018303	-3.028118	3.188430
C	0.064558	-1.890967	2.385711
C	0.255919	-0.625274	2.936314
C	0.387100	-0.511875	4.317245
C	0.330293	-1.648162	5.128441
C	0.147359	-2.911103	4.570500
C	-0.171872	-4.277261	2.370101
H	0.304138	0.263914	2.313121
H	0.535409	0.467610	4.760688
H	0.436491	-1.545884	6.203592
H	0.115090	-3.793506	5.202166
H	-1.152831	-4.725009	2.554517

C	2.253576	-2.350211	0.154980
C	2.290740	-3.772266	0.612498
C	-0.059989	-3.826270	0.893864
C	-0.078650	-2.252040	0.921221
C	1.287715	-0.449370	-0.321251
H	3.101145	-4.303643	0.113810
H	-1.004690	-1.895920	0.468189
N	3.214640	-1.588365	-0.275853
N	2.603649	-0.404448	-0.556706
N	1.053159	-1.693642	0.158673
C	3.429949	0.751185	-0.818001
C	3.584310	1.684372	0.210310
C	4.074487	0.851401	-2.049112
C	4.432922	2.762812	-0.036191
C	4.918690	1.942212	-2.240510
C	5.106880	2.907534	-1.249265
H	4.573932	3.505279	0.745287
H	5.435245	2.043870	-3.191682
O	1.069548	-4.368317	0.234339
H	2.452436	-3.816520	1.699157
H	-0.909682	-4.174329	0.307669
H	0.576048	-5.047275	2.585625
C	2.853910	1.554040	1.520666
H	1.799681	1.842343	1.409491
H	3.290900	2.219646	2.267151
H	2.893563	0.530599	1.909255
C	5.999233	4.095633	-1.497414
H	5.446768	4.890282	-2.008948
H	6.848848	3.826059	-2.128970
H	6.380273	4.506682	-0.560102
C	3.815022	-0.145284	-3.143754
H	2.790282	-0.023586	-3.510458
H	3.922094	-1.174255	-2.790454
H	4.498852	0.011873	-3.979062
C	0.382503	0.715939	-0.635694
O	0.868625	1.565429	-1.401190
C	-0.941777	0.715293	-0.150400
C	-1.597809	2.075565	-0.040944
H	-1.207559	0.014039	0.632553
H	-1.564441	2.586144	-1.008146
H	-2.651732	1.961255	0.228905
C	-0.852029	2.896350	0.990905
C	-1.024974	2.651887	2.358513
C	0.089573	3.851084	0.595617

C	-0.269926	3.337527	3.306866
H	-1.756337	1.912889	2.680356
C	0.842213	4.543322	1.543492
H	0.241956	4.032831	-0.463730
C	0.668522	4.286420	2.901113
H	-0.422848	3.140019	4.363847
H	1.569331	5.281114	1.217379
H	1.255271	4.823584	3.639584
N	-4.053654	0.723274	-1.374476
N	-5.237872	0.527763	-0.925347
C	-5.943886	1.744384	-0.859637
O	-5.533575	2.871995	-1.034678
O	-7.216711	1.469507	-0.519505
C	-8.055699	2.612877	-0.385689
H	-8.132276	3.146633	-1.335833
H	-9.031205	2.235671	-0.083661
H	-7.659623	3.294966	0.369772
C	-3.242781	-0.364144	-1.444835
C	-1.911926	-0.118001	-1.884634
C	-3.619332	-1.690297	-1.040110
C	-1.126347	-1.266208	-2.325612
H	-1.717076	0.830524	-2.381191
C	-2.797380	-2.747694	-1.267705
H	-4.591673	-1.820531	-0.578642
C	0.058695	-1.098981	-3.064625
C	-1.545307	-2.571231	-1.971115
H	-3.092229	-3.753903	-0.981184
C	0.842961	-2.190773	-3.400135
H	0.356458	-0.093157	-3.349885
C	-0.728911	-3.665515	-2.316824
C	0.454165	-3.479685	-3.007219
H	1.752468	-2.054010	-3.975733
H	-1.043745	-4.667501	-2.036042
H	1.072689	-4.334410	-3.260855

Vibrational frequencies

-379.0760	18.6314	21.8659
28.1541	30.6432	33.0323
42.4785	44.2516	46.8689
58.2269	62.0225	67.2766
77.9499	79.5912	83.1832
85.6064	90.0573	94.7263
100.4922	108.3177	111.9349
119.4740	133.8497	136.3488
150.8687	161.3220	168.0145

192.5927 199.5600 206.1061
213.4888 216.3485 220.2963
234.7906 240.9495 244.4829
246.4555 249.6263 264.5719
273.7214 284.4736 297.4936
309.1176 323.8599 334.8318
342.6210 352.7839 360.1718
377.2614 395.4965 407.8359
409.0830 412.3465 414.4435
416.7393 447.0478 459.5403
492.1827 504.2182 512.7569
517.8629 519.2842 523.0786
525.6239 529.3643 533.2933
543.3512 550.9747 572.0407
588.8830 589.6918 597.6710
600.1061 611.4118 625.3357
630.2020 633.4900 635.0723
652.0672 687.9081 704.1185
713.4616 720.3676 722.3231
743.0002 748.0400 764.2349
777.0640 779.4330 783.8314
785.1846 789.0258 792.0125
801.3654 814.6893 825.7761
831.8640 836.4545 844.2419
866.1694 868.7745 873.6160
879.1599 886.9454 893.3646
908.1218 914.0947 920.4601
927.2065 928.8465 947.9465
963.5219 966.2534 970.3964
982.9874 988.1489 992.4446
1004.4791 1016.6084 1017.0148
1019.1713 1023.6819 1027.9659
1029.0932 1036.1531 1037.3304
1043.1677 1044.2720 1053.1403
1060.5465 1061.4109 1064.0730
1064.8229 1065.8881 1067.7287
1069.3884 1071.3590 1072.8156
1076.4500 1109.5793 1112.7370
1122.5751 1137.9286 1146.2364
1159.2512 1160.2249 1171.3108
1175.6793 1177.6235 1181.4773
1190.2207 1192.7311 1199.9703
1201.2721 1207.8801 1214.9214
1221.5106 1225.9503 1228.6694

1240.4063	1247.6643	1250.0487
1255.2361	1266.4946	1283.8287
1284.5572	1289.9185	1310.0562
1316.7354	1321.4304	1326.2619
1341.3246	1341.7264	1343.3396
1344.2752	1356.0311	1358.2386
1366.0768	1367.4617	1371.0140
1378.5019	1381.6487	1411.1783
1417.5161	1419.8175	1429.8967
1435.8655	1449.0490	1456.2384
1461.5973	1467.2934	1471.5798
1479.6095	1485.2003	1487.6099
1489.2249	1492.7171	1495.5735
1496.6601	1498.7745	1499.4235
1500.8947	1503.3490	1504.3480
1508.2761	1511.7075	1515.4184
1523.8062	1535.6668	1542.3567
1548.0674	1550.5321	1561.2225
1629.2201	1671.8416	1679.4419
1679.6910	1684.1046	1690.6855
1693.9633	1694.4014	1696.3794
1697.1880	1701.1403	1819.9013
3051.4876	3066.9681	3067.1619
3077.4459	3085.3786	3085.7700
3094.5402	3119.5608	3138.3261
3139.8049	3140.9261	3148.1523
3159.2037	3164.1767	3165.4061
3170.2819	3172.4676	3176.5878
3181.1561	3189.4220	3189.8825
3196.5618	3197.0984	3197.6144
3198.3034	3199.7376	3204.6693
3207.0723	3209.5558	3216.3930
3216.8497	3217.0957	3221.2583
3223.9985	3229.0657	3231.0349
3236.6872	3240.5580	3257.5169

TS5SS(TS5S)

Zero-point correction= 0.735819
Thermal correction to Energy= 0.778991
Thermal correction to Enthalpy= 0.779935
Thermal correction to Gibbs Free Energy= 0.660159
Sum of electronic and zero-point Energies= -2196.960909
Sum of electronic and thermal Energies= -2196.917738
Sum of electronic and thermal Enthalpies= -2196.916793

Sum of electronic and thermal Free Energies= -2197.036569

Cartesian coordinates

C	4.202127	-1.463766	-1.978079
C	2.913245	-0.933858	-1.915829
C	2.330314	-0.301250	-3.007132
C	3.078318	-0.180466	-4.177858
C	4.376614	-0.689317	-4.241831
C	4.946848	-1.337033	-3.145150
C	4.561589	-2.132422	-0.671649
H	1.310094	0.073725	-2.960827
H	2.644888	0.303470	-5.046601
H	4.943877	-0.593407	-5.162033
H	5.948962	-1.749850	-3.210030
H	5.201578	-1.480812	-0.065589
C	0.587771	-2.854357	-0.942786
C	1.707064	-3.796093	-1.239082
C	3.203937	-2.340720	0.027984
C	2.324414	-1.190515	-0.545649
C	-0.194587	-0.935277	-0.260197
H	1.349823	-4.824777	-1.194908
H	2.380942	-0.325552	0.113553
N	-0.698221	-3.036189	-0.857194
N	-1.170218	-1.830018	-0.428911
N	0.928687	-1.578974	-0.603193
C	-2.590140	-1.600364	-0.356602
C	-3.223146	-1.106553	-1.498281
C	-3.248551	-1.873678	0.839570
C	-4.598848	-0.900759	-1.419230
C	-4.625611	-1.653871	0.866166
C	-5.312647	-1.171788	-0.249250
H	-5.122511	-0.512510	-2.288934
H	-5.170421	-1.853228	1.786820
O	2.692939	-3.644684	-0.235658
H	2.107451	-3.597440	-2.242294
H	3.254148	-2.263566	1.114231
H	5.076668	-3.087949	-0.793677
C	-2.436074	-0.759710	-2.734046
H	-1.868257	0.167370	-2.575138
H	-3.103740	-0.591605	-3.580436
H	-1.730900	-1.554256	-2.997524
C	-6.799079	-0.933859	-0.203305
H	-7.037164	0.099232	-0.502331
H	-7.199072	-1.100249	0.804944
H	-7.323717	-1.605473	-0.900190

C	-2.476177	-2.310527	2.051604
H	-1.870748	-1.467560	2.407883
H	-1.789034	-3.127879	1.813553
H	-3.146822	-2.629923	2.850977
C	-0.463283	0.476622	0.185270
O	-1.372457	0.584693	1.019046
C	0.327360	1.546578	-0.297358
C	-0.405962	2.871941	-0.394716
H	1.037242	1.329326	-1.095375
H	-0.862493	3.092280	0.575454
H	0.301362	3.676126	-0.617560
C	-1.477649	2.804983	-1.462616
C	-1.154624	2.992958	-2.811298
C	-2.798569	2.489117	-1.127655
C	-2.126354	2.872818	-3.801734
H	-0.129887	3.237789	-3.082872
C	-3.773336	2.371600	-2.117155
H	-3.050591	2.318771	-0.084795
C	-3.441374	2.562294	-3.456395
H	-1.859632	3.026674	-4.843040
H	-4.794663	2.127930	-1.838769
H	-4.200700	2.469624	-4.226701
N	1.060678	-0.213293	2.443204
N	0.591210	-0.920293	3.408862
C	0.586691	-2.277651	3.061939
O	0.862693	-2.801738	1.996475
O	0.171365	-2.982233	4.128514
C	0.109422	-4.391608	3.931357
H	1.086274	-4.783069	3.639686
H	-0.201260	-4.812163	4.886069
H	-0.617032	-4.642032	3.154197
C	1.004988	1.130793	2.543163
C	1.622482	1.834694	1.464216
C	0.272768	1.854435	3.546144
C	1.749269	3.278164	1.580360
H	2.434596	1.342893	0.941638
C	0.261108	3.209618	3.555057
H	-0.276343	1.275702	4.280598
C	2.561130	4.004606	0.691183
C	1.030945	3.963542	2.589623
H	-0.301100	3.758120	4.304936
C	2.650596	5.381735	0.776225
H	3.107542	3.464025	-0.078453
C	1.123374	5.367297	2.649681

C	1.917266	6.065935	1.758662
H	3.279090	5.933154	0.084853
H	0.568430	5.896786	3.419272
H	1.980093	7.147627	1.823150

Vibrational frequencies

-420.9055	20.8050	29.4756
33.0208	39.6572	42.4038
45.5692	52.2377	57.2423
59.9049	65.6874	71.6851
75.4618	78.0588	84.6408
93.0755	98.7949	105.1020
106.1690	119.7992	128.2287
132.7417	151.1184	155.0086
162.2268	170.5139	179.1941
188.4706	199.0808	203.0804
207.4421	212.4988	221.4018
232.1946	242.4365	245.9436
246.9105	251.2218	258.5436
270.0790	284.1578	294.9584
304.6751	318.6819	336.8903
344.3882	352.3231	368.4187
374.5966	375.5201	404.4690
409.2316	414.2640	417.0570
420.2364	429.2201	440.2552
494.6644	498.2903	507.7071
514.3780	515.2104	524.8462
527.3153	529.8655	532.6918
536.9491	552.3803	577.1492
590.9045	593.3297	597.1856
602.1873	613.9113	619.4263
628.1168	636.4825	640.2589
662.7322	699.6450	718.2306
720.0112	722.2332	732.8161
744.2788	754.3351	762.6431
769.4605	773.8730	778.9331
779.6891	790.5414	792.8317
801.5361	807.2185	825.3985
828.4324	834.5007	843.8552
848.4163	853.0197	873.9303
879.5152	886.3635	901.9927
904.8311	915.2047	916.7145
923.7779	934.1658	948.0597
955.7960	966.0079	966.6726
980.6432	982.4655	990.6258

995.8035	1001.5814	1010.7669
1013.5605	1015.6575	1017.8070
1019.5040	1026.5125	1031.4011
1035.5225	1039.3664	1047.9040
1052.9871	1057.2215	1059.2173
1063.2115	1066.1705	1067.4742
1068.3355	1072.0044	1073.2944
1077.8010	1108.4364	1112.9820
1114.5836	1134.5106	1141.6651
1153.1097	1161.2378	1172.3805
1173.9298	1177.0250	1180.8281
1183.4677	1190.3720	1193.9165
1199.4929	1208.2617	1217.7556
1222.4339	1225.5911	1228.7189
1234.6585	1243.5925	1251.8118
1257.2797	1274.3775	1281.1688
1285.0281	1287.0004	1294.6233
1305.0832	1323.8709	1327.9672
1342.0087	1342.9235	1344.7929
1352.0222	1356.2683	1358.0726
1374.9720	1375.8914	1379.2403
1382.4884	1382.8682	1404.6311
1413.0943	1417.8364	1429.6428
1435.7853	1450.6911	1465.8869
1468.9469	1470.5445	1475.3701
1478.8149	1481.1085	1482.7455
1488.9994	1491.2096	1492.6717
1494.0194	1497.7471	1500.0672
1504.4223	1505.1253	1506.4171
1512.9750	1514.0718	1526.4218
1537.6218	1544.5815	1546.7576
1556.1846	1557.7801	1581.7993
1631.5289	1671.8977	1681.2227
1686.1478	1690.4476	1690.8827
1693.6319	1695.2721	1698.7315
1700.4180	1703.2214	1781.9122
3017.3735	3045.1479	3058.4541
3077.8708	3080.8965	3085.5566
3085.6256	3087.5773	3114.6792
3118.6307	3131.7601	3141.1805
3148.7032	3164.9124	3165.8888
3166.4592	3169.1172	3174.1026
3180.5855	3185.9163	3190.9023
3192.2406	3193.1066	3194.7451

3200.8898	3202.3937	3204.4783
3204.6089	3206.2821	3206.7929
3209.2071	3216.5510	3217.5426
3217.8838	3227.5457	3229.5746
3229.6481	3232.0560	3247.9925

M5RR(M5R)

preTS6

Zero-point correction= 0.740677

Thermal correction to Energy= 0.783107

Thermal correction to Enthalpy= 0.784051

Thermal correction to Gibbs Free Energy= 0.665909

Sum of electronic and zero-point Energies= -2197.011623

Sum of electronic and thermal Energies= -2196.969193

Sum of electronic and thermal Enthalpies= -2196.968249

Sum of electronic and thermal Free Energies= -2197.086391

Cartesian coordinates

C	-5.192573	0.642946	-1.095309
C	-3.819484	0.841639	-0.973865
C	-3.238459	2.084342	-1.203006
C	-4.066972	3.142448	-1.569539
C	-5.444291	2.950155	-1.702725
C	-6.016975	1.701428	-1.466385
C	-5.559594	-0.787570	-0.786909
H	-2.166692	2.227574	-1.094136
H	-3.639309	4.123507	-1.749742
H	-6.076222	3.785603	-1.985339
H	-7.089282	1.559278	-1.561368
H	-5.786568	-1.335364	-1.707704
C	-2.623015	-0.169974	1.830765
C	-4.079738	-0.379575	2.074531
C	-4.306310	-1.384765	-0.109299
C	-3.135968	-0.441509	-0.557384
C	-0.856324	-0.093399	0.557847
H	-4.256271	-0.622003	3.122484
H	-2.576219	-0.902932	-1.372326
N	-1.628559	-0.025361	2.658327
N	-0.533883	0.032657	1.845876
N	-2.194953	-0.208899	0.538677
C	0.761835	0.320306	2.396390
C	1.554062	-0.743707	2.834002
C	1.158449	1.657545	2.432098
C	2.834425	-0.423434	3.280385
C	2.452548	1.921415	2.876712

C	3.305621	0.894258	3.287087
H	3.486030	-1.223421	3.623306
H	2.801992	2.950732	2.897248
O	-4.473778	-1.493173	1.299747
H	-4.642965	0.526382	1.812126
H	-4.093183	-2.403822	-0.440609
H	-6.424171	-0.884628	-0.124674
C	1.029018	-2.154662	2.831852
H	0.597660	-2.421689	1.860688
H	0.231016	-2.262177	3.574189
H	1.827229	-2.855390	3.078669
C	4.719146	1.190420	3.712107
H	5.418158	0.948268	2.902208
H	5.003218	0.591259	4.582295
H	4.846882	2.247075	3.958897
C	0.229458	2.748755	1.972308
H	-0.757568	2.642869	2.432373
H	0.100288	2.725811	0.882268
H	0.633146	3.728701	2.227316
C	-0.026250	0.053298	-0.694330
O	-0.656239	0.259190	-1.713888
C	1.489701	0.039670	-0.701521
C	1.964441	1.017821	-1.794189
H	1.877508	0.385599	0.260231
H	3.041626	0.886148	-1.919938
H	1.481629	0.765308	-2.741956
C	1.686036	2.450550	-1.408373
C	0.560324	3.134132	-1.878253
C	2.553207	3.108827	-0.529324
C	0.304919	4.444490	-1.473630
H	-0.114056	2.632324	-2.566156
C	2.305675	4.419107	-0.130268
H	3.431519	2.582759	-0.159085
C	1.176914	5.090158	-0.600237
H	-0.572780	4.962305	-1.849203
H	2.991714	4.916897	0.547787
H	0.980891	6.111494	-0.289710
N	0.103447	-2.700013	-1.699980
N	-0.307761	-2.493569	-0.423654
C	-1.424259	-3.201731	-0.113613
O	-2.083630	-3.997320	-0.771319
O	-1.770491	-2.908512	1.185776
C	-2.691137	-3.810598	1.784268
H	-2.248523	-4.807988	1.863837

H	-2.896417	-3.411961	2.778352
H	-3.620563	-3.874520	1.216893
C	1.268628	-2.181095	-1.953438
C	2.049188	-1.430721	-0.904355
C	1.833845	-2.344356	-3.279351
C	3.533379	-1.365173	-1.183238
H	1.880796	-1.935665	0.052602
C	3.124515	-2.056429	-3.534680
H	1.177675	-2.745545	-4.046682
C	4.412214	-0.983842	-0.169999
C	4.031579	-1.616030	-2.474816
H	3.539833	-2.199436	-4.527828
C	5.774301	-0.839195	-0.420807
H	4.019097	-0.795860	0.827803
C	5.403875	-1.464101	-2.718004
C	6.269926	-1.076225	-1.702851
H	6.446812	-0.545542	0.379470
H	5.786280	-1.658173	-3.716735
H	7.329576	-0.962662	-1.909027

Vibrational frequencies

17.1611	18.6741	27.7952
38.0427	42.9836	46.4613
52.9346	63.3369	66.9858
70.3879	72.0865	79.2307
88.8933	95.0961	96.2442
103.9089	115.2521	117.7926
126.6220	139.6741	144.9641
147.4059	162.5859	165.0461
182.3014	186.1208	197.3223
202.2673	212.6049	220.0522
230.1082	239.4626	243.8079
252.1515	255.2237	269.0068
278.7514	286.2784	294.4857
298.5967	314.5878	316.0719
326.7507	345.3732	356.9381
361.3497	387.1362	395.4708
406.2032	409.4084	418.1513
423.2605	434.3994	441.9451
448.2986	453.4737	489.0836
495.0220	499.7292	507.8633
516.0853	522.1767	525.7877
527.9259	542.0151	552.4008
563.4213	570.7798	588.5807
591.6758	597.6334	602.7732

610.5179 622.1532 627.5669
635.1467 645.5703 655.4405
697.3784 712.7967 718.0162
721.9767 728.7474 738.0567
747.4667 754.4290 763.3848
771.0810 774.3393 778.1797
779.5449 794.6372 801.4816
808.7253 814.4389 834.6187
838.4845 856.1335 863.1072
871.6292 876.4541 879.8458
885.0269 896.0604 910.3989
918.2321 920.1686 926.7913
940.5015 957.9078 963.8702
966.8334 978.3178 982.8374
987.6561 992.4494 1004.1072
1010.1578 1016.7837 1016.8591
1021.3526 1022.7286 1023.3420
1028.2851 1029.0848 1038.6714
1044.2490 1047.1333 1058.7293
1062.3117 1064.5784 1067.4311
1068.1010 1068.2377 1072.2839
1078.2922 1081.1993 1108.1627
1113.7239 1119.6205 1120.8804
1137.5103 1152.7285 1159.2476
1164.7339 1168.2874 1179.0513
1179.4662 1191.1158 1193.6478
1195.1646 1200.8119 1202.8647
1208.1139 1216.7834 1222.2126
1230.6827 1236.2419 1244.8578
1245.7947 1249.6580 1254.9575
1270.4215 1276.4172 1278.8629
1281.0806 1282.1243 1300.3867
1310.6382 1324.0514 1329.0235
1334.5614 1342.5678 1344.0175
1346.2281 1348.4592 1353.8005
1354.9889 1360.0511 1371.8600
1376.6762 1380.0132 1385.8008
1405.4376 1419.6386 1422.7745
1429.5193 1431.4714 1456.9205
1464.6079 1469.3622 1474.4119
1478.8747 1483.3403 1484.4717
1494.1941 1494.8024 1495.4125
1496.8144 1500.0795 1500.7494
1501.3679 1509.9121 1516.5045

1523.1695	1526.4367	1538.0361
1542.0993	1545.6725	1545.8588
1547.0751	1592.3709	1632.9051
1648.8652	1670.9771	1682.1624
1684.3465	1689.4814	1692.8906
1695.3954	1696.3550	1698.9222
1708.4941	1761.3692	1793.6841
3058.4429	3061.6512	3065.7940
3067.9007	3079.7309	3084.8560
3100.9384	3107.1923	3131.0999
3132.7961	3136.2471	3138.5907
3141.9759	3149.3980	3160.5703
3163.3273	3165.0417	3169.2495
3170.6263	3178.3698	3179.8918
3182.7509	3184.1414	3191.6180
3193.5596	3195.9113	3196.0035
3201.5178	3204.6908	3206.5656
3207.2808	3209.5595	3211.6420
3213.8159	3219.6680	3222.8581
3224.1284	3226.5156	3235.9978

M5SS(M5S)

Zero-point correction= 0.739687
Thermal correction to Energy= 0.782708
Thermal correction to Enthalpy= 0.783652
Thermal correction to Gibbs Free Energy= 0.663593
Sum of electronic and zero-point Energies= -2196.986669
Sum of electronic and thermal Energies= -2196.943647
Sum of electronic and thermal Enthalpies= -2196.942703
Sum of electronic and thermal Free Energies= -2197.062762
Cartesian coordinates

C	-3.417026	2.615222	-2.051608
C	-2.439882	1.635506	-1.871996
C	-2.311657	0.572895	-2.759619
C	-3.205653	0.484363	-3.826601
C	-4.201952	1.446935	-3.994998
C	-4.310698	2.521304	-3.112393
C	-3.310929	3.678172	-0.985298
H	-1.514669	-0.158950	-2.655452
H	-3.119112	-0.332763	-4.534874
H	-4.888776	1.366880	-4.831259
H	-5.072314	3.280789	-3.260213
H	-4.085632	3.539821	-0.222762
C	0.569723	2.645823	-1.409402

C	-0.117298	3.858737	-1.941166
C	-1.916856	3.463934	-0.361808
C	-1.629054	1.951657	-0.634347
C	0.628040	0.786457	-0.282948
H	0.617412	4.629773	-2.171979
H	-1.931702	1.397554	0.255381
N	1.836225	2.352872	-1.317334
N	1.855412	1.188090	-0.618624
N	-0.202750	1.701850	-0.804111
C	3.125177	0.537049	-0.395597
C	3.622845	-0.265634	-1.421027
C	3.802026	0.785331	0.799227
C	4.880053	-0.835381	-1.224795
C	5.053690	0.190223	0.943865
C	5.604688	-0.619430	-0.052143
H	5.297758	-1.465061	-2.006548
H	5.610995	0.364065	1.860933
O	-0.955464	4.355251	-0.917993
H	-0.676878	3.607465	-2.851930
H	-1.883677	3.647510	0.711147
H	-3.402948	4.695693	-1.372702
C	2.815053	-0.521050	-2.664056
H	2.495579	0.415184	-3.131760
H	1.918870	-1.107796	-2.424012
H	3.395774	-1.092532	-3.389191
C	6.946104	-1.275681	0.148699
H	7.456599	-1.430071	-0.804530
H	6.825765	-2.255223	0.623013
H	7.588605	-0.672740	0.793952
C	3.183285	1.613311	1.889099
H	2.443329	1.014137	2.433888
H	2.650132	2.479153	1.488013
H	3.943474	1.953657	2.594705
C	0.394404	-0.511311	0.465454
O	1.291286	-0.853201	1.199620
C	-0.791966	-1.427777	0.143521
C	-0.292697	-2.877652	0.295908
H	-1.071743	-1.268827	-0.905468
H	0.091080	-3.013155	1.311266
H	-1.149908	-3.543375	0.174917
C	0.755136	-3.243521	-0.730732
C	0.364191	-3.510317	-2.049146
C	2.109744	-3.337286	-0.403359
C	1.300196	-3.872879	-3.013025

H	-0.690412	-3.451681	-2.313115
C	3.048363	-3.709702	-1.364263
H	2.427916	-3.115556	0.611392
C	2.647544	-3.979589	-2.669914
H	0.978118	-4.083629	-4.028099
H	4.095386	-3.788136	-1.088021
H	3.379108	-4.271208	-3.417178
N	-0.981346	0.686321	2.167035
N	-0.428839	1.332050	3.212077
C	0.164975	2.465283	2.782502
O	0.230890	2.963681	1.649776
O	0.767992	3.093645	3.838264
C	1.350419	4.350166	3.536360
H	0.613051	5.037158	3.112675
H	1.726107	4.742593	4.481672
H	2.175106	4.249901	2.825109
C	-1.598216	-0.438124	2.341366
C	-2.046784	-1.085309	1.040609
C	-1.747660	-1.152276	3.594385
C	-2.969321	-2.271140	1.229169
H	-2.625521	-0.348828	0.472846
C	-2.419038	-2.318156	3.655708
H	-1.285358	-0.709066	4.469386
C	-3.686091	-2.771389	0.143873
C	-3.098664	-2.884930	2.488004
H	-2.512726	-2.853435	4.596851
C	-4.504064	-3.890443	0.279156
H	-3.596248	-2.277686	-0.822556
C	-3.922929	-4.010544	2.613488
C	-4.615209	-4.516553	1.519661
H	-5.052300	-4.269317	-0.577202
H	-4.022200	-4.483176	3.587087
H	-5.248654	-5.390162	1.635103

Vibrational frequencies

7.9657	29.4365	34.4055
40.8576	46.2490	46.4336
50.7901	53.9567	64.4469
67.4319	70.9349	80.6567
84.9372	92.2279	97.1546
99.7425	105.7685	114.5067
119.5856	123.4211	135.1740
144.0950	159.3372	160.8601
168.5088	172.3917	176.8508
189.3165	195.6901	200.0220

213.0757 222.5298 232.3306
235.5660 242.5207 245.7015
253.0085 273.9688 284.5799
291.5428 312.6959 319.3433
326.7291 338.5730 351.5352
363.7630 377.2283 384.2834
394.0007 410.6402 412.7564
421.9534 423.2704 433.8057
437.7410 441.8532 485.7831
496.9718 499.2910 509.4155
510.6240 521.3408 526.1073
528.0147 532.4425 541.1933
555.0734 578.8691 590.9195
593.1873 599.3440 608.4996
616.0845 620.7746 630.9902
637.1412 648.6497 661.1987
678.8229 714.5024 719.9375
720.3694 732.1488 740.6597
747.7625 753.1864 759.9353
766.4899 768.5041 775.9396
783.6430 798.2972 802.3388
812.2735 816.4556 837.1976
844.6250 853.4279 858.6483
872.4351 876.1459 878.9488
883.5322 894.7985 910.1585
911.5535 916.6012 918.9578
938.4771 954.0261 961.6392
968.7341 980.4702 981.7512
985.9510 987.9717 1004.1124
1011.1180 1012.6190 1017.3716
1018.4618 1021.0224 1022.7957
1023.8898 1030.6887 1040.1001
1043.2258 1044.9982 1052.6506
1060.6374 1063.0043 1066.0933
1066.6682 1071.2961 1073.0775
1074.2559 1083.4779 1094.1618
1115.1524 1118.9310 1120.1821
1141.6868 1153.4671 1159.9963
1169.0651 1174.0027 1177.5951
1188.0698 1189.3872 1192.8181
1195.8229 1201.1922 1209.1429
1211.4487 1221.4061 1226.8771
1236.0043 1242.2003 1243.7576
1253.2535 1254.3214 1261.1538

1271.1472	1284.1691	1285.3727
1289.6735	1303.8505	1306.4655
1312.2453	1317.1957	1323.8334
1338.7790	1342.3928	1343.4841
1347.4496	1348.3695	1350.9172
1357.3874	1358.7850	1375.8710
1377.6974	1382.8855	1387.0266
1391.5656	1411.3245	1420.3655
1423.8513	1429.8610	1444.0676
1465.9918	1467.0356	1476.5643
1480.8672	1484.9850	1488.1883
1493.4593	1494.1016	1495.6158
1497.0118	1500.0622	1500.4395
1504.1804	1504.8359	1517.3285
1523.1650	1523.6630	1541.1838
1543.5056	1547.9389	1549.0567
1551.6713	1581.5441	1639.1876
1652.9390	1674.6178	1683.8897
1686.9764	1694.8296	1695.0252
1696.9059	1697.3756	1701.4964
1706.8645	1720.6688	1837.4395
3056.9208	3063.5499	3072.9794
3074.8531	3075.5377	3076.3131
3086.0542	3088.6775	3100.4303
3127.9286	3137.7972	3145.0054
3146.5895	3147.2833	3154.3914
3166.6430	3168.9729	3172.3941
3172.7145	3173.2805	3179.9091
3180.4051	3187.8442	3188.6694
3189.6727	3193.1653	3194.1933
3196.0158	3200.5755	3201.4161
3207.6147	3212.0772	3212.1775
3215.4875	3221.9510	3222.2151
3226.0435	3235.0460	3235.4094

TS6a

Zero-point correction= 0.740409

Thermal correction to Energy= 0.782239

Thermal correction to Enthalpy= 0.783184

Thermal correction to Gibbs Free Energy= 0.666894

Sum of electronic and zero-point Energies= -2197.004432

Sum of electronic and thermal Energies= -2196.962602

Sum of electronic and thermal Enthalpies= -2196.961658

Sum of electronic and thermal Free Energies= -2197.077948

Cartesian coordinates

C	-5.304921	0.690921	-0.160215
C	-3.919288	0.821831	-0.202189
C	-3.286612	2.017353	0.119081
C	-4.080780	3.099908	0.493029
C	-5.472081	2.979209	0.535262
C	-6.095039	1.776525	0.206710
C	-5.729248	-0.702264	-0.550633
H	-2.203085	2.104538	0.070669
H	-3.610267	4.042873	0.751402
H	-6.074510	3.832211	0.831101
H	-7.176357	1.685509	0.246103
H	-6.173991	-0.707920	-1.551193
C	-2.470418	-1.420755	1.504390
C	-3.889009	-1.796799	1.770472
C	-4.428196	-1.537680	-0.542758
C	-3.267920	-0.479067	-0.611205
C	-0.842353	-0.704332	0.234245
H	-3.939882	-2.532724	2.572225
H	-2.833969	-0.430529	-1.606943
N	-1.391208	-1.677508	2.180515
N	-0.383582	-1.215085	1.382441
N	-2.180979	-0.819404	0.316714
C	0.941049	-1.251459	1.950808
C	1.765806	-2.353479	1.722144
C	1.258463	-0.224758	2.851579
C	2.999407	-2.362939	2.380091
C	2.490186	-0.295202	3.495015
C	3.378870	-1.349126	3.257475
H	3.671395	-3.200704	2.210474
H	2.765281	0.491109	4.193374
O	-4.360181	-2.404832	0.582503
H	-4.484503	-0.916527	2.045446
H	-4.369680	-2.206726	-1.401988
H	-6.459915	-1.143761	0.133464
C	1.365261	-3.500233	0.831851
H	1.825075	-3.403494	-0.156241
H	0.285447	-3.539423	0.677271
H	1.698814	-4.441672	1.273757
C	4.737017	-1.368001	3.906094
H	5.481265	-0.941126	3.224954
H	5.050662	-2.387943	4.139403
H	4.746590	-0.779118	4.825508
C	0.286563	0.891938	3.128433

H	-0.583173	0.517631	3.677764
H	-0.083275	1.351073	2.204344
H	0.760632	1.673351	3.724753
C	-0.139646	-0.064948	-0.977348
O	-0.923051	0.501174	-1.758768
C	1.247975	0.581991	-0.706966
C	1.305090	1.942157	-1.424009
H	1.330547	0.757085	0.372071
H	2.352433	2.262395	-1.452429
H	0.964612	1.817170	-2.453914
C	0.499049	3.018326	-0.739636
C	-0.555320	3.666639	-1.385985
C	0.826339	3.410718	0.563324
C	-1.260046	4.686909	-0.750105
H	-0.829173	3.356105	-2.390148
C	0.112954	4.415873	1.210801
H	1.660983	2.928478	1.071104
C	-0.932049	5.061619	0.551465
H	-2.076570	5.181343	-1.267892
H	0.380360	4.703223	2.223194
H	-1.484155	5.853725	1.048169
N	1.244637	-1.461897	-2.868599
N	0.438632	-1.762915	-1.802400
C	-0.461180	-2.743377	-2.138435
O	-0.498706	-3.422739	-3.147417
O	-1.335346	-2.955619	-1.110906
C	-2.198861	-4.077219	-1.282495
H	-1.623152	-5.006148	-1.276398
H	-2.890061	-4.046036	-0.440376
H	-2.740140	-4.006731	-2.228163
C	2.261037	-0.735026	-2.541316
C	2.455580	-0.311189	-1.114924
C	3.190018	-0.313582	-3.575075
C	3.780578	0.362517	-0.839238
H	2.382783	-1.217860	-0.500809
C	4.308890	0.366092	-3.268646
H	2.945199	-0.584441	-4.597433
C	4.134207	0.675903	0.471329
C	4.657192	0.699738	-1.886556
H	5.002161	0.669708	-4.048225
C	5.336239	1.317587	0.758986
H	3.456655	0.410744	1.278041
C	5.864496	1.345264	-1.588497
C	6.205580	1.655036	-0.277556

H	5.590176	1.554216	1.787868
H	6.537018	1.602449	-2.402553
H	7.144269	2.156032	-0.064525

Vibrational frequencies

-93.0394	24.0534	30.1937
32.5356	36.7523	41.7240
46.8533	54.1621	63.7656
68.9190	73.2903	77.9923
84.6451	85.2022	92.1981
101.0603	106.6256	110.6442
120.4602	122.2454	131.0824
141.9777	153.7039	154.7607
166.2667	173.7396	179.7849
190.3183	200.9024	216.3673
219.4825	224.5127	238.6318
242.8111	246.6047	259.2653
280.8136	288.1667	292.3447
298.2674	325.4279	330.4267
333.5377	350.5794	367.9974
379.0314	395.8080	402.6705
417.2572	418.6108	420.3398
431.9927	437.1215	441.3332
450.4854	461.7449	489.3998
495.7409	497.8242	508.6277
512.6450	521.0444	525.2301
528.6720	537.5318	553.0875
556.1119	570.8706	586.9422
590.7661	600.0902	604.8120
610.3077	624.3215	627.6874
632.4175	644.2434	652.9751
699.1787	716.2058	720.1802
725.2325	730.6382	742.9082
751.8325	755.6493	765.9751
769.4223	775.7340	778.5170
783.1648	790.8761	799.0040
813.0194	817.1232	836.8086
838.2695	856.8115	864.9678
878.0451	880.9459	883.5918
884.2038	893.6775	909.9842
916.1204	923.0972	929.1757
942.1715	955.5804	960.6075
970.1168	978.3496	983.0412
988.7011	990.6904	1005.4416
1014.6748	1017.5257	1020.5800

1024.0277	1025.7171	1026.8263
1029.3655	1039.2512	1042.0895
1050.1279	1051.2063	1056.5641
1061.0645	1062.3015	1063.3535
1064.3267	1070.6076	1072.0151
1082.2523	1091.3558	1096.2522
1107.4180	1117.2005	1126.0294
1141.1352	1145.3534	1152.1860
1162.7427	1173.7959	1177.0143
1181.9400	1188.8963	1193.4603
1198.4140	1201.8058	1205.6914
1211.9391	1212.5385	1221.6806
1224.7983	1231.5513	1235.0584
1246.7486	1247.1884	1252.1296
1262.6740	1276.5214	1278.9061
1281.5743	1291.7310	1296.3971
1303.9168	1307.3114	1324.3889
1334.5834	1335.7771	1340.7749
1350.3371	1351.0279	1353.0886
1360.0620	1363.1140	1371.1016
1374.6065	1384.1854	1389.7499
1398.4448	1419.5423	1419.6860
1424.1088	1432.5047	1456.1634
1461.5041	1465.8065	1477.2341
1479.1483	1479.6391	1485.7822
1486.7486	1494.6496	1496.8108
1498.5629	1500.5115	1501.6625
1506.9481	1512.1163	1516.3469
1516.9011	1521.4157	1524.0163
1534.6169	1538.3436	1550.4552
1556.5634	1575.1225	1628.5874
1654.8753	1674.9444	1679.1602
1682.7754	1683.6384	1690.6387
1696.8973	1699.1961	1700.4791
1700.8617	1719.6407	1800.5136
3063.9356	3071.5314	3078.7579
3081.1664	3081.5261	3084.6592
3090.2382	3094.4181	3102.9481
3131.4252	3137.7938	3143.5475
3154.5254	3155.4234	3158.9458
3161.7942	3168.7428	3172.8773
3178.0801	3181.2511	3188.7033
3191.7604	3193.2595	3194.3362
3195.0979	3196.5859	3196.7354

3206.7691	3207.3405	3210.1270
3211.9429	3212.4976	3216.9273
3218.9364	3223.5217	3230.6505
3233.8438	3235.6634	3236.1279

M6a

Zero-point correction= 0.740707
Thermal correction to Energy= 0.783019
Thermal correction to Enthalpy= 0.783963
Thermal correction to Gibbs Free Energy= 0.665757
Sum of electronic and zero-point Energies= -2197.008306
Sum of electronic and thermal Energies= -2196.965994
Sum of electronic and thermal Enthalpies= -2196.965050
Sum of electronic and thermal Free Energies= -2197.083256
Cartesian coordinates

C	5.222115	0.583003	-0.306042
C	3.839159	0.718668	-0.197023
C	3.177674	1.838900	-0.687883
C	3.932995	2.821733	-1.326359
C	5.317336	2.687677	-1.449333
C	5.974040	1.571655	-0.932592
C	5.689621	-0.702976	0.326886
H	2.100973	1.952862	-0.569251
H	3.437275	3.701255	-1.723154
H	5.887597	3.462394	-1.952169
H	7.051248	1.470935	-1.027152
H	6.180958	-0.506767	1.285584
C	2.368116	-1.763760	-1.414915
C	3.781470	-2.173785	-1.662837
C	4.402990	-1.529758	0.549323
C	3.231983	-0.485050	0.487448
C	0.775185	-0.946989	-0.150222
H	3.809025	-3.031633	-2.333997
H	2.817979	-0.258423	1.469855
N	1.270301	-2.155067	-1.989034
N	0.289446	-1.625790	-1.197780
N	2.111153	-1.011581	-0.305021
C	-1.075057	-1.778039	-1.618848
C	-1.838036	-2.842849	-1.142976
C	-1.561983	-0.833217	-2.534345
C	-3.182016	-2.881447	-1.529124
C	-2.903090	-0.919978	-2.887319
C	-3.735321	-1.918765	-2.369097
H	-3.807852	-3.686926	-1.152841

H	-3.316149	-0.186101	-3.575282
O	4.282637	-2.582960	-0.401159
H	4.371961	-1.354834	-2.093040
H	4.401939	-2.037046	1.515215
H	6.394660	-1.266833	-0.291195
C	-1.279005	-3.916391	-0.248997
H	-1.720132	-3.855530	0.750232
H	-0.195045	-3.838104	-0.149813
H	-1.517784	-4.899914	-0.662020
C	-5.199794	-1.932662	-2.717694
H	-5.710804	-1.099018	-2.225048
H	-5.676955	-2.860520	-2.397324
H	-5.348517	-1.817643	-3.794537
C	-0.658290	0.213775	-3.133621
H	0.113397	-0.257328	-3.750384
H	-0.137795	0.807448	-2.373471
H	-1.231421	0.895630	-3.764458
C	0.075234	-0.273140	1.107295
O	0.957000	0.204953	1.907660
C	-1.029060	0.763288	0.635987
C	-0.949254	2.009172	1.539550
H	-0.790125	1.062890	-0.390258
H	-1.932428	2.494462	1.542310
H	-0.724708	1.688978	2.558143
C	0.069132	3.025444	1.086192
C	1.203991	3.323565	1.843641
C	-0.137434	3.720543	-0.110265
C	2.093965	4.311981	1.430838
H	1.386330	2.759255	2.752750
C	0.756265	4.701175	-0.534196
H	-1.023597	3.500950	-0.704228
C	1.871062	5.007413	0.244014
H	2.969635	4.535851	2.032652
H	0.575049	5.234906	-1.462449
H	2.567179	5.775962	-0.078121
N	-1.828705	-1.226953	2.528061
N	-0.722884	-1.505867	1.744039
C	0.011651	-2.551361	2.289359
O	-0.356741	-3.304764	3.163026
O	1.184839	-2.706933	1.641907
C	1.934923	-3.867345	1.999721
H	1.321441	-4.764869	1.895592
H	2.773029	-3.892432	1.302480
H	2.288861	-3.791146	3.029670

C	-2.678985	-0.409422	2.014829
C	-2.459196	0.179812	0.650888
C	-3.859997	-0.069706	2.793312
C	-3.520828	1.163336	0.203064
H	-2.489884	-0.668678	-0.043123
C	-4.779088	0.783755	2.313501
H	-3.959447	-0.533670	3.769182
C	-3.403649	1.812520	-1.026381
C	-4.644381	1.428732	1.005642
H	-5.659496	1.028473	2.901456
C	-4.381174	2.699435	-1.470071
H	-2.535707	1.619176	-1.651394
C	-5.624489	2.321188	0.552348
C	-5.499627	2.953319	-0.678186
H	-4.268524	3.189580	-2.431846
H	-6.488211	2.517499	1.182123
H	-6.265917	3.642655	-1.017076

Vibrational frequencies

18.5843	20.6173	32.8088
33.3534	34.9875	42.7801
47.0455	56.4161	62.6340
69.0606	77.1046	87.2408
90.3453	98.5995	100.8706
102.8379	115.8351	118.4586
122.7091	126.5213	141.9805
147.1266	157.0686	164.9969
168.2427	178.9228	185.6734
195.5377	206.4156	211.4236
223.1378	232.9879	243.9461
247.8027	264.5032	266.9037
279.4123	282.7973	296.9572
316.2896	330.8264	333.3148
343.4233	353.7147	369.0551
380.0694	405.8686	407.2480
410.0983	414.2195	428.7065
437.5241	439.7403	449.4578
454.0237	481.4407	493.2196
494.8559	498.3539	513.8830
516.5163	522.4795	526.5463
533.0028	537.0470	557.2889
564.6376	578.5580	589.9440
597.8697	603.2114	610.4995
619.1213	622.0059	626.7708
632.5572	654.0046	669.1274

700.1228 710.9747 717.2879
730.6208 735.3577 744.7090
751.6461 757.0083 763.4707
772.0350 776.4517 785.4111
796.4015 803.5880 804.6699
814.0266 826.5347 837.4891
844.0175 856.2892 861.9543
868.7367 877.1729 882.7205
889.5585 891.8199 914.5214
917.3506 923.0895 925.3211
934.2436 946.6242 953.5253
967.3947 977.6278 987.1321
988.0571 989.9726 1000.5509
1013.8591 1018.5897 1020.7838
1021.1573 1022.7600 1026.6287
1028.5388 1038.9181 1046.1965
1047.3259 1052.2778 1055.3198
1056.6204 1060.2776 1061.9596
1064.2860 1065.3631 1070.1275
1073.3615 1085.4026 1093.7542
1112.3440 1116.6542 1123.5855
1132.1796 1145.7888 1151.2881
1169.8807 1171.1592 1178.7705
1181.6780 1187.6767 1191.6031
1200.1869 1204.8412 1205.8878
1209.7717 1216.3846 1224.4023
1230.9087 1231.8598 1239.4724
1244.1347 1247.0997 1251.1255
1267.8739 1272.5129 1279.3783
1282.6166 1285.8688 1303.1802
1306.1075 1310.4628 1323.1446
1329.6387 1333.0848 1338.2500
1345.8389 1349.2071 1350.7531
1356.3665 1362.9656 1372.8929
1374.5913 1379.9891 1382.3725
1390.3593 1416.7765 1419.7809
1422.7395 1429.1929 1432.9341
1459.1230 1459.2626 1467.7683
1469.3895 1478.1299 1479.8681
1484.0535 1491.5242 1492.1499
1493.1395 1493.4114 1496.5160
1500.0032 1507.7619 1507.9281
1511.2434 1513.7774 1515.4315
1519.5276 1529.0227 1536.4002

1548.1553	1553.4157	1570.1779
1655.2156	1677.2360	1680.8085
1688.8743	1689.9287	1694.1338
1698.8275	1700.1213	1700.5055
1717.4597	1736.6481	1834.6179
3064.8439	3072.5871	3073.4864
3077.8670	3083.1943	3084.8032
3086.9767	3110.4195	3115.2667
3131.1230	3133.0255	3145.1898
3149.5551	3151.9701	3158.1749
3167.2490	3169.1311	3172.3587
3175.2872	3181.7207	3182.3253
3188.4255	3190.8356	3191.8121
3196.3382	3197.5424	3198.4836
3206.1204	3208.8191	3208.9916
3209.1149	3214.3005	3215.3050
3217.5688	3217.9887	3227.1503
3229.5900	3231.5711	3237.0593

TS7a

Zero-point correction= 0.740538
Thermal correction to Energy= 0.782206
Thermal correction to Enthalpy= 0.783150
Thermal correction to Gibbs Free Energy= 0.666388
Sum of electronic and zero-point Energies= -2197.000125
Sum of electronic and thermal Energies= -2196.958457
Sum of electronic and thermal Enthalpies= -2196.957513
Sum of electronic and thermal Free Energies= -2197.074275
Cartesian coordinates

C	-4.459363	0.866061	1.574784
C	-3.454783	0.898741	0.603361
C	-2.689924	2.042239	0.401417
C	-2.935226	3.158185	1.201745
C	-3.934227	3.127301	2.176252
C	-4.706801	1.982240	2.366415
C	-5.152309	-0.471614	1.598871
H	-1.941676	2.061623	-0.383156
H	-2.350182	4.059615	1.046194
H	-4.120595	4.006715	2.785125
H	-5.492656	1.963889	3.116069
H	-6.237920	-0.399987	1.696648
C	-2.487828	-2.492883	0.954638
C	-3.850555	-3.099518	1.082638
C	-4.739160	-1.077076	0.240653

C	-3.381474	-0.421929	-0.131240
C	-0.943749	-1.059038	0.269599
H	-3.792169	-4.157628	0.822439
H	-3.224904	-0.322647	-1.204751
N	-1.362200	-3.045771	1.298447
N	-0.428718	-2.141810	0.876057
N	-2.281626	-1.272387	0.370259
C	0.950452	-2.339015	1.215827
C	1.767036	-3.129738	0.408989
C	1.433877	-1.627566	2.326031
C	3.140959	-3.099876	0.673931
C	2.803068	-1.648773	2.559621
C	3.675879	-2.345447	1.714844
H	3.805660	-3.674002	0.032513
H	3.206818	-1.077141	3.391973
O	-4.731206	-2.489325	0.164394
H	-4.216138	-3.022865	2.113426
H	-5.456486	-0.754700	-0.517547
H	-4.789254	-1.070080	2.441989
C	1.230600	-3.971911	-0.717096
H	1.662354	-3.659336	-1.672225
H	0.143427	-3.906000	-0.789448
H	1.497773	-5.019776	-0.552977
C	5.163983	-2.246445	1.921756
H	5.525917	-1.274945	1.566696
H	5.696177	-3.026579	1.374205
H	5.421730	-2.325159	2.981026
C	0.504147	-0.797670	3.172163
H	-0.369063	-1.376360	3.487734
H	0.130147	0.067888	2.611932
H	1.020329	-0.430199	4.060372
C	-0.285726	-0.022366	-1.212444
O	-1.284799	0.426855	-1.805738
C	0.753766	0.986293	-0.680750
C	0.974727	2.088388	-1.750915
H	0.319392	1.436283	0.217300
H	2.035010	2.369433	-1.731753
H	0.767812	1.679333	-2.743493
C	0.154335	3.334380	-1.521841
C	-0.969592	3.635157	-2.294000
C	0.526290	4.220817	-0.505460
C	-1.700650	4.798786	-2.059608
H	-1.279170	2.937497	-3.066681
C	-0.197252	5.386424	-0.271589

H	1.402559	3.993172	0.099110
C	-1.314698	5.680395	-1.052378
H	-2.573301	5.018488	-2.667038
H	0.112817	6.067362	0.515337
H	-1.881296	6.589026	-0.874302
N	1.747162	-1.095073	-2.320692
N	0.431633	-1.169943	-1.917594
C	-0.310760	-2.076163	-2.670669
O	0.075253	-2.671043	-3.650401
O	-1.507633	-2.284770	-2.099230
C	-2.358049	-3.217654	-2.763206
H	-1.893966	-4.206226	-2.787930
H	-3.274367	-3.236620	-2.172549
H	-2.565043	-2.889799	-3.783513
C	2.549284	-0.413501	-1.581108
C	2.075197	0.289223	-0.338710
C	3.946739	-0.345933	-1.980361
C	3.106405	1.160159	0.340932
H	1.840768	-0.509134	0.366964
C	4.823938	0.400691	-1.289719
H	4.238227	-0.912737	-2.858506
C	2.766091	1.896574	1.475761
C	4.436300	1.186340	-0.115990
H	5.865192	0.445324	-1.597521
C	3.715486	2.667401	2.143284
H	1.744777	1.868522	1.848100
C	5.385049	1.961545	0.562552
C	5.030496	2.702566	1.683085
H	3.428748	3.235661	3.022155
H	6.408848	1.977781	0.198465
H	5.775143	3.300712	2.197688

Vibrational frequencies

-182.8164	11.1210	23.3797
31.1095	36.2660	42.1415
49.0580	52.1789	55.8477
62.2506	66.3866	74.0230
82.1489	89.5541	92.2904
95.4971	105.5249	109.5669
117.5620	131.7806	141.9307
159.1900	166.7154	176.3537
183.7921	190.2282	195.7681
212.0704	216.6966	224.2185
230.3775	236.7945	239.4198
246.8909	260.8954	275.9908

276.4399	285.0651	292.9995
307.9516	323.0496	333.0623
342.5089	349.1853	360.2957
369.0859	385.3560	390.4703
414.5814	415.4233	419.7137
422.5776	434.9708	442.9654
455.6147	471.3277	482.1557
494.2923	500.0853	510.7767
520.9381	521.9048	529.8178
532.0314	536.7833	544.1329
552.8416	569.9216	586.4439
593.4614	596.0258	602.1097
605.1248	623.6195	627.3722
632.0479	633.3260	653.6232
660.8627	676.2478	712.1470
717.7133	718.2860	734.9592
736.5880	752.1676	757.8035
767.7625	773.7676	776.1902
780.5816	791.4855	807.4154
815.4061	826.2943	832.3376
838.7367	850.5439	865.1608
875.8982	883.2172	884.1818
887.3246	903.7740	904.5832
917.8305	919.4038	921.5659
936.3979	945.9110	970.1287
974.4320	978.1999	986.2398
999.5352	1006.2225	1008.2223
1015.2163	1015.9298	1018.0195
1018.8548	1024.1782	1029.5458
1034.3357	1043.5715	1047.3488
1049.7544	1055.4907	1057.8776
1060.5564	1061.8546	1064.5377
1067.2169	1070.5284	1085.2174
1093.9259	1097.9577	1117.2620
1120.4171	1121.7888	1128.9298
1133.1623	1158.0407	1164.4433
1169.0124	1171.1774	1178.2569
1185.3275	1186.4010	1187.7538
1199.0146	1203.3004	1206.7453
1216.0289	1217.6122	1221.7317
1235.9844	1238.2105	1244.2789
1245.5209	1252.1391	1257.1148
1258.9210	1275.7649	1277.6820
1280.5810	1295.3463	1304.0994

1312.3913	1314.1788	1318.5797
1330.3377	1335.0234	1342.3279
1348.3721	1351.0308	1354.1249
1361.8589	1365.3426	1369.9442
1370.7149	1380.0718	1381.6245
1393.7835	1395.8474	1416.4397
1419.0172	1420.1135	1430.1725
1458.5393	1460.1361	1467.8958
1484.8745	1485.7418	1488.2665
1489.7313	1491.7895	1494.0176
1499.5935	1501.8408	1502.5409
1507.5010	1508.4103	1510.1608
1511.5345	1513.1000	1515.6993
1521.2512	1532.5774	1551.8374
1553.3510	1560.6103	1615.4827
1657.4819	1675.0773	1677.2942
1679.8792	1683.4451	1691.3946
1697.0911	1699.3451	1702.6871
1718.5679	1737.5290	1843.5085
3061.0808	3071.7213	3073.8166
3077.4465	3078.7764	3083.9397
3090.7827	3103.4082	3131.8280
3138.0620	3138.6327	3141.5752
3150.2080	3150.5635	3152.1671
3167.2018	3170.5583	3171.5691
3173.2932	3179.8007	3187.1774
3188.0461	3190.5290	3191.9396
3194.9024	3195.3622	3198.4798
3199.5458	3199.6332	3206.1312
3206.3411	3208.0300	3213.1238
3217.0386	3218.0272	3226.4617
3237.3077	3243.1341	3243.7099

M7a

Zero-point correction= 0.738977
Thermal correction to Energy= 0.782855
Thermal correction to Enthalpy= 0.783800
Thermal correction to Gibbs Free Energy= 0.656085
Sum of electronic and zero-point Energies= -2197.005594
Sum of electronic and thermal Energies= -2196.961715
Sum of electronic and thermal Enthalpies= -2196.960771
Sum of electronic and thermal Free Energies= -2197.088486
Cartesian coordinates

C	-6.748350	0.479883	0.909429

C	-5.465770	0.985282	1.136567
C	-4.806945	0.770263	2.341146
C	-5.458810	0.040816	3.333298
C	-6.743832	-0.461860	3.114462
C	-7.396014	-0.246974	1.901634
C	-7.224216	0.827487	-0.478840
H	-3.808000	1.161440	2.499430
H	-4.967603	-0.134439	4.286806
H	-7.239389	-1.023189	3.900971
H	-8.395937	-0.639817	1.738404
H	-8.276463	1.117868	-0.526630
C	-4.305762	0.643950	-2.228659
C	-5.516696	1.157617	-2.944992
C	-6.285009	1.998786	-0.855286
C	-4.971933	1.733975	-0.075348
C	-2.921055	0.326443	-0.476061
H	-5.232189	1.539560	-3.927300
H	-4.442053	2.658834	0.166864
N	-3.352232	-0.097047	-2.711282
N	-2.527798	-0.269116	-1.618880
N	-4.086737	0.907418	-0.903237
C	-1.362307	-1.090391	-1.745191
C	-0.143022	-0.498879	-2.065914
C	-1.491294	-2.459757	-1.491890
C	0.983293	-1.325299	-2.119484
C	-0.336612	-3.239071	-1.532346
C	0.911483	-2.684647	-1.827692
H	1.942658	-0.889345	-2.390562
H	-0.409396	-4.302670	-1.311688
O	-6.089825	2.237640	-2.233057
H	-6.237490	0.346041	-3.093213
H	-6.712405	2.924846	-0.464142
H	-7.086637	-0.027402	-1.151492
C	-0.035216	0.986495	-2.280351
H	0.920105	1.240890	-2.746874
H	-0.092924	1.509522	-1.318385
H	-0.845842	1.359001	-2.910237
C	2.151448	-3.535957	-1.772309
H	2.439737	-3.705205	-0.727327
H	2.991582	-3.050456	-2.280961
H	1.990146	-4.514933	-2.229210
C	-2.831806	-3.044605	-1.140328
H	-3.556478	-2.869146	-1.940950
H	-3.234506	-2.572325	-0.237364

H	-2.754030	-4.120713	-0.968530
C	3.956941	1.387876	1.555376
O	5.006527	1.863687	1.912624
C	3.739907	-0.086864	1.295805
C	3.677352	-0.344238	-0.224150
H	4.605494	-0.594377	1.725454
H	3.405424	-1.396791	-0.369939
H	2.861493	0.255105	-0.644905
C	4.968159	-0.033603	-0.937269
C	5.263189	1.275475	-1.330592
C	5.895854	-1.043279	-1.195372
C	6.465511	1.565982	-1.969305
H	4.548741	2.069864	-1.129548
C	7.098301	-0.756319	-1.837516
H	5.670301	-2.064775	-0.893759
C	7.385327	0.551264	-2.224667
H	6.684893	2.587434	-2.268294
H	7.811017	-1.550312	-2.034256
H	8.320975	0.777114	-2.726673
N	1.520787	1.638540	1.190569
N	2.800477	2.162960	1.315937
C	2.812792	3.575866	1.196748
O	1.855713	4.265310	1.428903
O	3.981644	4.014417	0.746383
C	4.084004	5.441783	0.643286
H	3.918499	5.900753	1.618033
H	5.095149	5.634554	0.293678
H	3.349052	5.822569	-0.067159
C	1.338178	0.396139	1.477374
C	2.439459	-0.506366	1.991445
C	-0.007012	-0.130529	1.308668
C	2.130968	-1.990260	1.903639
H	2.540457	-0.263004	3.063645
C	-0.242172	-1.446472	1.419492
H	-0.806543	0.554993	1.034916
C	3.132240	-2.939724	2.117466
C	0.815119	-2.423829	1.671396
H	-1.253003	-1.819909	1.268094
C	2.838847	-4.301741	2.096986
H	4.151755	-2.620755	2.312886
C	0.531207	-3.793942	1.658127
C	1.532345	-4.730699	1.866878
H	3.631420	-5.025070	2.264174
H	-0.491171	-4.113117	1.470235

H	1.300666	-5.790818	1.851303

Vibrational frequencies

6.4103	14.0716	16.8044
18.7168	24.1627	28.6846
29.4706	36.3176	39.4392
44.7627	49.3997	61.1729
66.3288	68.6484	74.7910
89.0887	100.7907	105.7924
112.9885	128.4065	140.4053
143.8008	144.4208	147.1007
152.1098	158.6827	163.3112
172.2590	178.1368	189.7461
207.0681	212.1408	228.2350
236.8246	237.1762	255.7457
262.9451	272.8377	282.8990
297.0880	300.7765	314.0588
321.8712	333.7643	335.9228
356.6414	366.5340	389.7712
391.8464	412.2587	417.4239
424.1900	426.6335	449.8479
453.1729	465.9902	478.5667
492.6207	498.5179	507.9097
508.5675	526.6519	527.7525
529.7461	536.9241	539.3957
563.8007	565.4066	589.4369
590.1960	597.6312	606.6549
621.5193	623.9028	625.5528
630.9770	634.7729	652.5214
686.5440	690.2567	710.4764
715.5225	720.1516	734.5573
734.8879	750.3676	762.0880
775.9290	777.6060	778.2368
780.6446	790.5483	800.0632
819.3448	826.5502	833.9489
850.5462	857.5313	869.6020
874.7058	880.2570	889.1125
895.6098	899.6412	904.8658
914.3928	921.1938	929.0675
934.3583	946.0558	964.9364
974.0293	977.8861	979.4235
997.8339	999.4431	1005.4960
1018.0451	1019.8137	1021.6289
1023.8659	1025.8263	1028.0363
1034.4962	1037.2092	1042.9205

1049.7063	1052.3257	1060.5312
1061.8567	1064.9036	1065.6282
1069.7612	1071.6148	1082.3640
1087.6013	1091.2876	1097.5826
1119.6339	1130.0062	1135.0228
1146.8761	1164.4103	1168.6950
1177.0176	1181.0155	1183.0684
1188.5545	1191.0070	1197.2608
1200.5576	1206.4078	1208.4810
1210.9388	1221.8794	1230.2706
1235.5277	1244.5135	1245.6151
1248.3488	1257.1658	1262.7458
1273.6806	1280.9807	1285.5984
1290.7465	1293.6207	1308.4222
1310.5265	1323.2777	1330.8962
1339.2533	1340.3237	1344.8566
1346.5168	1348.2987	1349.5437
1360.2897	1362.0802	1369.9344
1371.9345	1376.0015	1376.2807
1387.0055	1392.6692	1413.9233
1415.7682	1424.1347	1428.9779
1447.4109	1448.9622	1465.1938
1478.9272	1484.0753	1486.3098
1487.5838	1490.7317	1491.0828
1493.7125	1493.9725	1495.7954
1501.9780	1508.9212	1510.8014
1513.1600	1513.2281	1521.0732
1528.0764	1540.6976	1549.3341
1556.7646	1573.9068	1658.4599
1676.2738	1679.4285	1682.2828
1690.4973	1692.5737	1698.7396
1702.4995	1709.3572	1719.2022
1732.1188	1871.6070	1882.7070
3010.4903	3052.6380	3057.8109
3058.5507	3072.0667	3075.9368
3087.2221	3106.8218	3122.4691
3122.7111	3125.2618	3127.2067
3132.5272	3139.0178	3140.5679
3150.0040	3155.7781	3157.6929
3158.1217	3158.7445	3179.1174
3182.9048	3184.4002	3191.8956
3192.5518	3193.8189	3197.5517
3201.5997	3201.8118	3204.1052
3205.2361	3207.5202	3214.6057

3217.8260	3221.4798	3225.2223
3225.9344	3231.1771	3235.3322

TS8a

Zero-point correction= 0.735055
Thermal correction to Energy= 0.777890
Thermal correction to Enthalpy= 0.778834
Thermal correction to Gibbs Free Energy= 0.657034
Sum of electronic and zero-point Energies= -2196.997761
Sum of electronic and thermal Energies= -2196.954925
Sum of electronic and thermal Enthalpies= -2196.953981
Sum of electronic and thermal Free Energies= -2197.075781
Cartesian coordinates

C	-1.792805	1.367501	0.004414
O	-2.313194	1.574771	-1.072144
C	-1.856619	0.031320	0.711238
C	-3.043914	0.073673	1.712423
H	-2.081818	-0.698301	-0.073955
H	-3.044216	-0.870679	2.266373
H	-2.856995	0.874717	2.437842
C	-4.368855	0.278693	1.025430
C	-4.927683	1.553262	0.906981
C	-5.036856	-0.803508	0.444825
C	-6.133182	1.742673	0.235929
H	-4.404451	2.404519	1.337018
C	-6.243073	-0.619164	-0.226018
H	-4.607316	-1.800620	0.525325
C	-6.796118	0.656206	-0.329822
H	-6.555251	2.739502	0.154689
H	-6.753365	-1.471736	-0.664503
H	-7.738572	0.801419	-0.848012
N	-0.230109	2.137143	1.789201
N	-1.111992	2.364358	0.722115
C	-1.107264	3.717836	0.323499
O	-0.173383	4.462649	0.497568
O	-2.272332	4.083264	-0.203681
C	-2.316726	5.432599	-0.676138
H	-1.549538	5.594257	-1.435247
H	-3.309062	5.559309	-1.103000
H	-2.160524	6.128963	0.149460
C	0.010786	0.891466	2.087438
C	-0.534136	-0.260221	1.394001
C	1.048370	0.666443	3.086191
C	-0.353117	-1.578910	2.014595

H	0.529960	-0.350084	0.450227
C	1.383510	-0.584639	3.461308
H	1.539025	1.541393	3.501393
C	-1.103804	-2.705896	1.638765
C	0.674636	-1.756298	2.973292
H	2.172770	-0.739116	4.193484
C	-0.842463	-3.955825	2.185834
H	-1.900537	-2.605824	0.907306
C	0.942327	-3.028594	3.496170
C	0.192686	-4.129037	3.108395
H	-1.446537	-4.806661	1.884400
H	1.738165	-3.137441	4.228710
H	0.398285	-5.108898	3.525922
C	5.002346	1.804934	-0.581117
C	3.811513	1.464931	0.061067
C	2.789774	2.396612	0.224161
C	2.977111	3.685823	-0.270913
C	4.170356	4.031403	-0.909381
C	5.191131	3.095959	-1.066168
C	5.940999	0.630840	-0.669058
H	1.861805	2.146156	0.730680
H	2.183024	4.414745	-0.147465
H	4.305743	5.040514	-1.286017
H	6.118001	3.368048	-1.562498
H	6.962995	0.874120	-0.369084
C	3.392033	-1.751082	-1.240397
C	4.844952	-2.097708	-1.321570
C	5.312785	-0.409067	0.287062
C	3.824373	0.017150	0.496843
C	1.597870	-0.754820	-0.412515
H	4.955922	-3.174534	-1.455686
H	3.493658	-0.122448	1.529071
N	2.399277	-2.270002	-1.902867
N	1.309006	-1.633016	-1.375219
N	2.947355	-0.818032	-0.340802
C	-0.019145	-1.880779	-1.853025
C	-0.595568	-3.133629	-1.636679
C	-0.693930	-0.822543	-2.474562
C	-1.929693	-3.294586	-2.014836
C	-2.022568	-1.035006	-2.831952
C	-2.659851	-2.255933	-2.594716
H	-2.409786	-4.254932	-1.842495
H	-2.577269	-0.219445	-3.286924
O	5.469943	-1.760918	-0.100228

H	5.312725	-1.598259	-2.178014
H	5.803597	-0.340100	1.259667
H	5.993058	0.257311	-1.697242
C	0.193604	-4.261955	-1.028775
H	-0.475155	-5.054885	-0.688568
H	0.780703	-3.919004	-0.172092
H	0.887963	-4.683123	-1.761783
C	-4.106552	-2.436520	-2.974376
H	-4.720636	-1.649494	-2.526851
H	-4.487755	-3.403661	-2.639546
H	-4.234729	-2.376835	-4.059470
C	-0.005177	0.486926	-2.764494
H	0.931322	0.317514	-3.305755
H	0.241721	1.034073	-1.849750
H	-0.652339	1.125037	-3.366795

Vibrational frequencies

-1259.4083	13.1972	15.8157
23.8282	26.4611	32.0288
38.2626	39.6297	45.3408
48.5236	50.6064	62.7448
67.1000	73.2598	79.3372
86.2374	93.9497	99.9440
115.4239	128.7658	131.9165
141.5624	157.0494	162.4420
166.6496	185.2424	190.2656
198.8126	201.1308	210.4842
213.4435	223.5221	227.7883
234.4049	242.0810	253.4903
267.6276	269.7194	280.2392
284.8352	308.6629	313.1773
325.8903	332.4547	338.2986
344.8558	356.8981	369.8947
400.9239	406.0552	420.0725
420.3072	425.7307	442.0111
449.9301	463.7506	470.9246
481.9104	494.4667	503.3829
507.8719	511.7383	523.0306
525.3224	528.7336	534.1236
561.2235	563.7283	570.5515
585.8774	597.0778	598.6722
606.1425	620.3278	623.7738
630.2723	631.4444	639.2883
656.9007	699.6796	708.0194
709.5314	719.8006	721.0922

726.1153	735.1992	750.8639
753.5537	775.5784	781.8303
782.5913	784.8538	797.9834
801.6368	815.6286	833.3980
836.5975	845.9038	849.8426
860.7738	874.4201	877.9850
885.6689	890.4599	893.8854
909.4864	911.2015	920.8629
924.2819	949.5018	962.2881
964.8636	977.2873	978.1958
981.2366	1000.9270	1002.5093
1014.9155	1017.7523	1018.7559
1023.2791	1023.8428	1030.8692
1037.3542	1038.0196	1039.4545
1043.3749	1052.2423	1054.4994
1056.2259	1062.0478	1063.2185
1063.8873	1067.9804	1069.6519
1083.5042	1091.2924	1104.1773
1110.0905	1117.0466	1132.5297
1136.1692	1167.3115	1168.6928
1173.9629	1178.8871	1179.8654
1183.8095	1189.0966	1192.1797
1194.3672	1197.9868	1202.6501
1208.3545	1211.0796	1232.7549
1237.0260	1242.1497	1247.2359
1255.2691	1261.1942	1262.3349
1278.8337	1285.2037	1300.7465
1301.6730	1315.9441	1319.3439
1327.0421	1327.9257	1335.6550
1340.9911	1343.1519	1349.0758
1351.8073	1354.8516	1357.0209
1360.2404	1364.0418	1369.4868
1370.8666	1373.2230	1381.9405
1401.5007	1413.2928	1417.6688
1418.8046	1420.7735	1430.8907
1437.2640	1462.7118	1465.4198
1473.5722	1483.8586	1488.3709
1490.2771	1491.0013	1494.1871
1495.4150	1497.1337	1498.9945
1503.1239	1507.4927	1509.4486
1511.2016	1511.5889	1519.8359
1522.7488	1532.3742	1539.3123
1550.8324	1552.0928	1571.0839
1635.1214	1662.1225	1675.6104

1677.6015	1683.4596	1685.7992
1695.8304	1697.2193	1699.6224
1699.8590	1714.0887	1836.5915
1854.5172	3068.0396	3068.6815
3069.3621	3076.2145	3081.8499
3094.0948	3096.6167	3108.9558
3124.0151	3130.7703	3131.0470
3136.6906	3140.7568	3152.0475
3152.1674	3164.6636	3166.9638
3177.3978	3180.7894	3182.6620
3185.8296	3186.7448	3198.0643
3199.9706	3200.2228	3201.2794
3203.0901	3207.7343	3213.8773
3214.0895	3217.4599	3218.5421
3218.9588	3220.8450	3220.9777
3226.9989	3230.7238	3240.9730

M8a

Zero-point correction= 0.738831
Thermal correction to Energy= 0.782464
Thermal correction to Enthalpy= 0.783409
Thermal correction to Gibbs Free Energy= 0.657531
Sum of electronic and zero-point Energies= -2197.025745
Sum of electronic and thermal Energies= -2196.982111
Sum of electronic and thermal Enthalpies= -2196.981167
Sum of electronic and thermal Free Energies= -2197.107044
Cartesian coordinates

H	1.146852	0.455528	-0.507861
C	-2.587391	-0.697994	-1.074107
O	-3.019076	-1.426639	-1.949223
C	-3.163003	-0.618470	0.318946
C	-3.887735	0.739312	0.525523
H	-3.891048	-1.430545	0.377864
H	-4.284041	0.743659	1.546186
H	-3.132752	1.531115	0.459280
C	-4.989019	0.979337	-0.474744
C	-4.704992	1.550897	-1.719093
C	-6.303661	0.594658	-0.199101
C	-5.711209	1.736592	-2.663249
H	-3.683186	1.844061	-1.949895
C	-7.313884	0.782398	-1.139152
H	-6.534774	0.147710	0.765044
C	-7.019835	1.355347	-2.374633
H	-5.473862	2.182689	-3.624245

H	-8.331416	0.483862	-0.906232
H	-7.805954	1.504245	-3.108113
N	-0.651082	0.600875	-0.188585
N	-1.468781	0.128323	-1.246800
C	-0.888306	0.310694	-2.502439
O	0.310584	0.421191	-2.684083
O	-1.793627	0.408061	-3.471099
C	-1.257768	0.522207	-4.791813
H	-0.638916	-0.345587	-5.027388
H	-2.120506	0.565302	-5.452827
H	-0.657994	1.429473	-4.880645
C	-0.887406	-0.006639	0.996569
C	-2.026689	-0.767849	1.297260
C	0.109295	0.167725	2.022108
C	-2.134031	-1.468642	2.531043
C	0.020860	-0.497956	3.203985
H	0.935097	0.848512	1.828361
C	-3.253942	-2.276772	2.879394
C	-1.079279	-1.363176	3.490505
H	0.792897	-0.372464	3.959913
C	-3.303839	-2.953269	4.076943
H	-4.084592	-2.368941	2.187179
C	-1.160932	-2.068629	4.710767
C	-2.248058	-2.858765	5.008344
H	-4.169769	-3.566791	4.308323
H	-0.341589	-1.970658	5.419430
H	-2.298987	-3.397733	5.948513
C	2.884660	-3.454386	-0.531367
C	1.950641	-2.536557	-1.018299
C	0.642813	-2.508810	-0.551972
C	0.272890	-3.416806	0.438836
C	1.198911	-4.341251	0.926267
C	2.507492	-4.372760	0.441913
C	4.234157	-3.245523	-1.174508
H	-0.069871	-1.790216	-0.942701
H	-0.738104	-3.394482	0.833699
H	0.895732	-5.045439	1.694565
H	3.219723	-5.096768	0.825937
H	4.733852	-4.173447	-1.460082
C	4.297783	0.121154	-1.310256
C	5.417811	-0.608072	-1.988768
C	3.883542	-2.383094	-2.407948
C	2.597860	-1.613483	-2.018016
C	2.252674	0.488063	-0.654598

H	6.026661	0.100507	-2.552425
H	1.970006	-1.334734	-2.865520
N	4.361533	1.218470	-0.608525
N	3.074579	1.424734	-0.205881
N	3.016719	-0.357081	-1.357355
C	2.717960	2.537479	0.631463
C	1.850762	3.506154	0.124695
C	3.235214	2.566981	1.932139
C	1.513411	4.560033	0.977010
C	2.868716	3.641081	2.736433
C	2.010108	4.644816	2.276230
H	0.842633	5.331517	0.609209
H	3.254224	3.692512	3.751639
O	4.904887	-1.544301	-2.909885
H	6.056769	-1.082212	-1.233451
H	3.620272	-3.040428	-3.239187
H	4.902881	-2.714142	-0.486177
C	1.278634	3.410988	-1.263673
H	0.844333	4.367920	-1.558869
H	0.493707	2.646951	-1.292732
H	2.041070	3.134768	-1.997575
C	1.608485	5.776618	3.184470
H	0.842779	5.442846	3.894562
H	1.197721	6.614739	2.615373
H	2.463128	6.134843	3.767669
C	4.126651	1.467416	2.446926
H	5.095884	1.471423	1.942246
H	3.673602	0.484185	2.276676
H	4.292522	1.586191	3.518405

Vibrational frequencies

7.0377	14.5743	17.0839
20.3222	25.0950	32.4229
38.8331	40.4070	43.7703
52.3531	61.8067	62.0825
73.6724	79.7737	83.7018
90.9243	95.8027	101.6314
108.2748	114.4910	121.9221
135.2996	147.0985	149.5229
160.8952	167.6992	173.8237
191.1748	193.2719	203.3806
208.5854	217.9621	228.6156
234.8417	245.2744	253.0774
258.3325	274.9405	284.3272
295.3212	306.2956	316.9702

323.5067	331.8424	351.0940
353.8091	365.8206	388.5534
398.8601	413.7388	413.7855
423.0582	427.6639	446.8386
467.1113	467.8231	490.9856
498.2764	506.8250	510.4052
511.9794	525.9328	528.1983
533.8834	544.0513	551.2548
557.6834	569.5726	586.7215
587.6609	589.3734	604.0500
617.6452	624.5428	629.7583
630.9726	634.1102	653.1903
687.6093	705.9774	707.6410
714.0605	717.7992	727.7307
733.4286	748.0342	752.5897
763.3307	775.7724	777.2620
781.3277	783.5774	796.2849
808.6548	822.2023	835.1020
835.5860	849.5513	851.8327
873.3644	874.1218	886.7439
888.2387	896.3108	900.1858
919.5615	919.8282	921.1001
948.3322	963.7434	968.5913
970.4218	974.7567	979.3934
988.0552	995.7431	995.9354
1000.8303	1005.3146	1017.3753
1022.6967	1026.0954	1028.1579
1037.6441	1043.0800	1045.4325
1049.1579	1051.6127	1063.8151
1066.0371	1067.1568	1068.4250
1069.2319	1070.1299	1075.2332
1094.5855	1101.2540	1105.5517
1108.2498	1119.2770	1131.6873
1133.4936	1168.2989	1172.5498
1175.1849	1176.8623	1182.0035
1188.7365	1189.7810	1193.0854
1198.2288	1198.9354	1199.4327
1208.8680	1213.4769	1230.9934
1242.0689	1242.9983	1246.2838
1248.8022	1264.4297	1268.8792
1278.1731	1284.7781	1286.4669
1302.4574	1309.1341	1321.7788
1327.1542	1328.8798	1334.3553
1342.5048	1346.4556	1350.9272

1353.9600	1357.3513	1358.7631
1362.2039	1367.4346	1374.4258
1382.0414	1384.9964	1406.7488
1417.1883	1419.2251	1421.6911
1428.4023	1431.3188	1446.7762
1463.4767	1466.2462	1471.9055
1482.7365	1487.3392	1488.7137
1490.0615	1490.4616	1492.1889
1495.2343	1500.8144	1501.8120
1505.5148	1506.7114	1508.0675
1513.6560	1519.5576	1524.7452
1534.7758	1539.7357	1550.2441
1552.7698	1573.9678	1604.0292
1635.0148	1667.9676	1677.1161
1679.7082	1690.7901	1691.3394
1696.8021	1697.0309	1704.2719
1706.9509	1795.7379	1820.4524
2703.3182	3057.9409	3065.9735
3069.4514	3073.5684	3074.2526
3087.5068	3097.4291	3124.9379
3128.5370	3137.8972	3138.4604
3140.4543	3143.5145	3148.9206
3152.1639	3164.0984	3167.1541
3175.1334	3178.1285	3182.9632
3184.2719	3186.7205	3186.9195
3194.4473	3194.7574	3203.0333
3204.6036	3205.5949	3207.3321
3208.3304	3213.8600	3214.4443
3217.1384	3218.7891	3225.4912
3231.3911	3232.4309	3269.7503

TS9a

Zero-point correction= 0.734627

Thermal correction to Energy= 0.778108

Thermal correction to Enthalpy= 0.779052

Thermal correction to Gibbs Free Energy= 0.654820

Sum of electronic and zero-point Energies= -2197.024280

Sum of electronic and thermal Energies= -2196.980799

Sum of electronic and thermal Enthalpies= -2196.979855

Sum of electronic and thermal Free Energies= -2197.104087

Cartesian coordinates

H	0.818724	0.507359	-0.343258
C	-2.489798	-0.451804	-1.244094
O	-2.961471	-0.931227	-2.255507

C	-3.084835	-0.645247	0.127744
C	-3.795218	0.656723	0.588109
H	-3.827253	-1.436039	0.004690
H	-4.171240	0.479050	1.601047
H	-3.038244	1.447148	0.652627
C	-4.917535	1.066644	-0.330195
C	-4.658257	1.820122	-1.479115
C	-6.229542	0.658851	-0.077656
C	-5.686854	2.160970	-2.352859
H	-3.638604	2.133062	-1.693987
C	-7.262024	1.000645	-0.947467
H	-6.442220	0.071660	0.812749
C	-6.992914	1.754030	-2.087992
H	-5.467632	2.745827	-3.240848
H	-8.277170	0.680902	-0.733307
H	-7.796739	2.022559	-2.766019
N	-0.504780	0.520641	-0.098094
N	-1.328462	0.335197	-1.244522
C	-0.793672	0.875360	-2.414475
O	0.386201	1.127657	-2.554664
O	-1.724461	1.148047	-3.323031
C	-1.225413	1.666808	-4.559894
H	-0.518231	0.966467	-5.007212
H	-2.099340	1.786702	-5.196217
H	-0.732142	2.626412	-4.396677
C	-0.791802	-0.316800	0.951840
C	-1.984880	-1.020609	1.083984
C	0.206059	-0.441700	1.976881
C	-2.183117	-1.926785	2.165803
C	0.037489	-1.316433	3.007230
H	1.095621	0.178175	1.922842
C	-3.385175	-2.665404	2.348911
C	-1.143727	-2.105410	3.126792
H	0.808026	-1.414970	3.767872
C	-3.527689	-3.545029	3.396061
H	-4.206905	-2.537593	1.652302
C	-1.319329	-3.018506	4.192511
C	-2.485118	-3.734246	4.329621
H	-4.454993	-4.098863	3.507066
H	-0.510530	-3.139625	4.908968
H	-2.609855	-4.433872	5.149328
C	2.950321	-3.288726	-1.138874
C	1.964839	-2.344842	-1.439657
C	0.659751	-2.491829	-0.990071

C	0.348547	-3.593542	-0.194003
C	1.329676	-4.536979	0.114139
C	2.633882	-4.398606	-0.363683
C	4.275648	-2.894566	-1.743262
H	-0.100522	-1.763126	-1.251005
H	-0.660655	-3.709384	0.189759
H	1.073069	-5.393552	0.729345
H	3.388337	-5.143882	-0.129977
H	4.818321	-3.728196	-2.194109
C	4.211485	0.419545	-1.268894
C	5.332063	-0.110379	-2.111559
C	3.853233	-1.845620	-2.797097
C	2.556043	-1.211572	-2.239775
C	2.150371	0.559749	-0.483940
H	5.880189	0.720516	-2.558670
H	1.900369	-0.801173	-3.009836
N	4.266313	1.366212	-0.378010
N	2.980434	1.428331	0.094413
N	2.946210	-0.097384	-1.354632
C	2.643922	2.346783	1.144480
C	1.810150	3.428659	0.857295
C	3.164753	2.102506	2.420975
C	1.503610	4.295205	1.908056
C	2.830675	2.998030	3.432734
C	2.002198	4.097969	3.194413
H	0.860069	5.148489	1.709343
H	3.222789	2.831127	4.433095
O	4.825303	-0.891748	-3.172285
H	6.029055	-0.679605	-1.483918
H	3.586982	-2.362559	-3.721827
H	4.926868	-2.456734	-0.977168
C	1.250664	3.646048	-0.522130
H	0.833322	4.650751	-0.608422
H	0.460403	2.917720	-0.729375
H	2.017612	3.517171	-1.291008
C	1.642364	5.035687	4.317400
H	0.907670	4.574213	4.984672
H	1.212639	5.963829	3.935481
H	2.520815	5.283010	4.918875
C	4.042721	0.907946	2.686609
H	5.018136	1.022476	2.205817
H	3.593277	-0.008582	2.288368
H	4.196008	0.778451	3.759018

Vibrational frequencies

-1209.8343	14.6267	16.9936
22.4634	26.5851	29.6042
30.8263	33.0927	44.9549
52.8931	57.4837	60.0268
70.8730	79.1112	81.5601
82.6349	89.8719	91.7537
93.1156	97.2696	100.6645
113.2733	138.3625	144.8631
148.1977	160.0015	161.2038
169.7435	189.9839	197.6033
201.6844	217.5945	224.2516
233.7272	237.7849	242.7470
250.5717	261.7475	281.8854
285.0801	293.9148	312.4217
316.0477	327.1079	332.3070
349.1407	360.8624	372.0803
393.3786	403.8745	411.5748
421.3087	425.1287	427.6195
446.4896	460.2554	467.2064
493.4290	496.6946	508.5417
510.0362	512.0339	524.3829
531.1690	539.7660	545.0598
553.6844	556.4549	573.4774
588.2146	588.5414	593.6800
606.1326	622.9619	627.9546
632.5826	633.9677	638.8027
655.4282	688.8397	708.5860
709.7823	715.5201	720.5786
734.5862	738.4475	751.8206
757.9022	765.6946	776.9502
778.6787	782.8730	783.6106
802.5183	817.3052	830.7679
833.8144	834.8425	848.9650
852.3931	877.3908	882.7442
882.9027	887.9274	895.8047
900.9062	910.6884	915.7376
921.1504	949.5333	966.8605
970.0048	971.7549	973.4974
982.3607	987.2912	1000.2422
1003.9139	1008.3115	1017.8418
1021.4737	1024.6386	1024.9417
1037.9559	1040.8800	1042.1685
1046.5374	1051.4701	1058.0789
1062.4341	1063.6518	1065.2633

1066.8900	1067.0870	1070.6918
1071.6613	1096.8549	1108.4908
1110.3535	1120.0120	1134.0523
1134.5132	1167.4041	1170.8656
1175.2759	1180.4293	1184.1431
1189.4536	1192.6190	1193.9147
1200.0946	1201.0425	1206.4443
1210.4934	1215.2312	1228.2785
1243.5319	1243.8221	1246.6640
1254.2580	1266.7828	1267.2716
1278.6113	1285.1832	1298.6170
1303.4485	1312.3871	1322.2509
1325.0391	1333.0420	1335.8895
1339.1039	1341.9823	1348.9512
1354.6471	1358.5758	1360.8334
1362.6785	1369.9570	1374.5553
1384.3221	1386.6683	1408.3262
1415.8522	1419.4176	1421.5328
1428.2969	1429.6959	1441.2918
1458.6888	1467.3312	1476.9606
1485.4364	1486.1047	1487.7329
1490.6688	1492.0981	1492.4710
1493.3023	1494.8749	1497.2983
1498.7585	1507.3773	1512.9251
1514.9375	1519.8774	1522.0834
1526.2787	1535.0185	1537.4763
1555.3735	1572.5266	1576.7300
1627.8743	1652.3411	1676.5406
1676.9335	1681.0912	1689.1083
1693.4856	1702.4222	1703.3888
1705.7794	1709.1070	1815.2655
1839.4201	3067.1691	3074.4077
3075.3196	3077.3389	3078.2737
3088.6451	3097.9056	3125.5530
3134.4022	3138.7436	3144.1368
3145.9882	3147.9078	3151.9901
3153.5271	3167.8074	3171.2116
3171.7437	3172.9803	3185.8918
3190.2624	3191.8108	3192.2924
3196.4214	3198.1042	3199.0118
3202.7236	3203.8414	3204.9419
3212.7676	3214.2067	3215.8097
3217.0597	3223.8647	3225.5360
3228.8913	3232.4218	3236.7583

P+NHC

Zero-point correction= 0.739545

Thermal correction to Energy= 0.783103

Thermal correction to Enthalpy= 0.784047

Thermal correction to Gibbs Free Energy= 0.660176

Sum of electronic and zero-point Energies= -2197.033835

Sum of electronic and thermal Energies= -2196.990278

Sum of electronic and thermal Enthalpies= -2196.989333

Sum of electronic and thermal Free Energies= -2197.113204

Cartesian coordinates

H	0.513947	-0.527736	1.026862
C	-2.354293	0.883573	1.856714
O	-3.156656	1.036143	2.749124
C	-2.507636	1.515362	0.482250
C	-2.973988	0.459732	-0.559188
H	-3.291320	2.263108	0.616368
H	-3.153951	0.995228	-1.497900
H	-2.151200	-0.241042	-0.732044
C	-4.207828	-0.292077	-0.134083
C	-4.090596	-1.472305	0.605999
C	-5.484952	0.178911	-0.449177
C	-5.222760	-2.172028	1.014436
H	-3.097143	-1.845760	0.849184
C	-6.620594	-0.518392	-0.043918
H	-5.586100	1.096689	-1.024014
C	-6.491437	-1.697503	0.687075
H	-5.115471	-3.090125	1.583843
H	-7.606057	-0.143319	-0.302009
H	-7.375252	-2.244695	0.999114
N	-0.299440	0.088503	0.882153
N	-1.178922	0.128118	1.983878
C	-0.787698	-0.662471	3.063169
O	0.245197	-1.300864	3.044058
O	-1.658889	-0.659573	4.059875
C	-1.292304	-1.494349	5.166823
H	-0.343614	-1.163040	5.591322
H	-2.096800	-1.381660	5.889456
H	-1.204485	-2.532724	4.843913
C	-0.089727	1.312541	0.244692
C	-1.194795	2.116299	0.045410
C	1.191807	1.691313	-0.237529
C	-1.063855	3.360113	-0.634526
C	1.331988	2.880429	-0.899357

H	2.045794	1.047332	-0.054812
C	-2.162228	4.226696	-0.888850
C	0.224578	3.746443	-1.111288
H	2.311670	3.187470	-1.256270
C	-1.985745	5.412139	-1.558883
H	-3.155299	3.948961	-0.552015
C	0.373743	4.981172	-1.792985
C	-0.704086	5.800961	-2.013304
H	-2.837976	6.058975	-1.741845
H	1.363705	5.264169	-2.141055
H	-0.579207	6.743525	-2.535905
C	4.793752	0.925143	0.750793
C	4.000414	-0.010167	1.421114
C	3.094113	0.373000	2.403125
C	2.992586	1.728496	2.713474
C	3.782190	2.669571	2.049224
C	4.687947	2.276776	1.063753
C	5.664091	0.248609	-0.282542
H	2.459424	-0.360870	2.891191
H	2.288465	2.057190	3.471293
H	3.686878	3.721291	2.300228
H	5.299477	3.014112	0.552020
H	6.681654	0.642279	-0.329168
C	3.600615	-2.094759	-1.460737
C	5.028858	-2.228411	-1.895132
C	5.628387	-1.224048	0.186267
C	4.246305	-1.386438	0.857709
C	1.912848	-1.584395	-0.066540
H	5.180015	-3.180856	-2.406172
H	4.225134	-2.190142	1.596946
N	2.533813	-2.264928	-2.180691
N	1.518292	-1.940689	-1.303323
N	3.267187	-1.690539	-0.193849
C	0.162473	-1.995236	-1.765080
C	-0.740860	-2.858741	-1.131426
C	-0.213711	-1.185415	-2.842254
C	-2.039836	-2.921208	-1.634261
C	-1.526871	-1.284877	-3.306265
C	-2.452044	-2.147045	-2.720392
H	-2.752938	-3.592568	-1.160813
H	-1.833818	-0.659505	-4.141410
O	5.899818	-2.216593	-0.781445
H	5.271903	-1.422930	-2.600606
H	6.387763	-1.363871	0.959133

H	5.220789	0.360285	-1.280091
C	-0.347739	-3.682567	0.066534
H	-1.104762	-4.444076	0.264958
H	-0.244165	-3.049161	0.954396
H	0.615823	-4.177009	-0.084838
C	-3.877792	-2.210981	-3.202512
H	-4.535658	-1.664020	-2.516731
H	-4.234001	-3.243864	-3.242759
H	-3.981938	-1.770103	-4.196347
C	0.751208	-0.218105	-3.477110
H	1.487923	-0.738601	-4.094484
H	1.299876	0.341502	-2.712827
H	0.211468	0.494839	-4.103534

Vibrational frequencies

12.0775	16.0133	20.7044
24.7493	29.2611	38.9633
44.4201	48.4841	52.7426
61.7099	66.5998	67.1101
73.0026	78.3422	79.7136
84.4997	86.3463	92.5927
100.6268	124.5980	136.3144
143.3189	147.0356	150.0115
163.2675	173.8376	177.0808
181.5657	203.3767	208.0914
217.1878	218.8602	221.5597
243.1194	247.4086	251.0699
259.9599	278.2840	281.3014
291.0662	295.6649	319.5777
321.2422	332.4297	342.9009
361.1233	380.9557	391.7856
399.2389	408.5453	411.5034
420.6139	433.2986	445.8870
455.0980	462.2138	477.4461
494.8603	508.6330	510.4112
512.1151	526.5125	530.1976
532.3459	540.5996	547.1312
559.4122	570.4292	586.7557
590.3955	593.5297	605.3663
619.2666	626.0057	629.6976
632.4348	635.9860	651.9309
682.6081	687.9372	692.0868
706.3061	717.0251	721.5120
735.0669	744.0439	757.3072
759.6064	768.3055	772.8406

774.5063 788.0934 795.4219
802.1497 818.8023 823.0550
825.7889 845.3201 850.6102
855.9006 873.1940 886.6763
887.9777 889.0516 898.4501
904.9139 913.1807 921.9546
922.6509 949.2250 964.2198
971.6880 975.5375 978.2341
979.6564 990.4420 995.7719
1001.6302 1004.7997 1014.7095
1017.8537 1018.3567 1021.1524
1026.3146 1037.2564 1037.8769
1043.6844 1050.9164 1051.9181
1060.4907 1062.0582 1063.6152
1064.6117 1066.3813 1067.3826
1067.5486 1087.7114 1098.2589
1108.1077 1114.6779 1132.2840
1133.7312 1166.5015 1166.9915
1176.4195 1177.8314 1182.2616
1188.3178 1188.8727 1198.7335
1199.9113 1200.4988 1207.1863
1208.8001 1220.9517 1236.5818
1238.3038 1245.4992 1247.8551
1252.4744 1264.4680 1268.8102
1273.3026 1281.7166 1294.2316
1300.8923 1306.6269 1309.9351
1322.6557 1326.6247 1337.0969
1342.8975 1345.3100 1351.1579
1357.2376 1357.8020 1360.0340
1370.7060 1372.8788 1375.9464
1388.1016 1396.9792 1409.2330
1415.1693 1418.4053 1425.4448
1428.7766 1430.3902 1442.3206
1449.2191 1464.4874 1472.2150
1484.0920 1484.5255 1486.1081
1488.2794 1489.8265 1492.7383
1493.0907 1494.1152 1497.5016
1500.9951 1506.5745 1506.5842
1509.1465 1521.9206 1522.1701
1526.5327 1538.2235 1547.0709
1550.5543 1562.4313 1593.3199
1669.7861 1679.3612 1680.0170
1680.9985 1688.8303 1692.9916
1697.2373 1699.8479 1705.5515

1715.8136	1820.3156	1862.7699
3061.2867	3065.1258	3066.1230
3070.5814	3080.0154	3081.2356
3099.6657	3132.9875	3133.9909
3137.5188	3138.9579	3144.6204
3146.6079	3148.0073	3157.2736
3159.1248	3161.5332	3164.9916
3166.0058	3176.0497	3184.6714
3190.0324	3190.7142	3194.2354
3195.1705	3198.2819	3199.0457
3204.0562	3204.6062	3207.8369
3209.1765	3215.7432	3218.9689
3219.3898	3224.6702	3226.9296
3227.6463	3234.8643	3290.3652

TS8a1

Zero-point correction= 0.617398

Thermal correction to Energy= 0.650694

Thermal correction to Enthalpy= 0.651638

Thermal correction to Gibbs Free Energy= 0.553364

Sum of electronic and zero-point Energies= -1516.052235

Sum of electronic and thermal Energies= -1516.018939

Sum of electronic and thermal Enthalpies= -1516.017995

Sum of electronic and thermal Free Energies= -1516.116269

Cartesian coordinates

N	2.232597	-1.080482	1.003293
C	1.913022	-2.549013	0.930971
C	1.799828	-3.020192	-0.520066
C	0.644036	-2.937306	1.685743
H	2.743578	-3.076900	1.410065
H	2.602622	-2.647133	-1.160053
H	1.844238	-4.112453	-0.534870
H	0.844993	-2.720341	-0.960137
H	0.738211	-2.825092	2.767633
H	-0.228284	-2.371120	1.357101
H	0.448460	-3.993302	1.481539
C	3.591344	-0.772799	0.395705
C	4.655076	-1.854675	0.617498
C	4.170741	0.569064	0.845796
H	3.390115	-0.700462	-0.680407
H	4.417581	-2.805570	0.138608
H	5.592121	-1.496497	0.184062
H	4.829889	-2.034092	1.682309

H	3.464695	1.394018	0.773645
H	4.553900	0.517456	1.869066
H	5.013544	0.802962	0.190601
C	2.000210	-0.508535	2.354936
C	2.824584	-1.103409	3.491741
H	0.932158	-0.632143	2.557380
H	2.172843	0.567583	2.281558
H	2.477260	-0.684205	4.439330
H	2.720789	-2.189748	3.550570
H	3.886685	-0.869633	3.394874
C	-1.490917	-0.562182	0.267834
O	-2.046662	-0.945248	1.278901
C	-0.789098	0.766796	0.157402
C	-1.690978	1.759472	-0.624742
H	-0.681676	1.116033	1.188163
H	-1.141818	2.701644	-0.719359
H	-1.834811	1.362164	-1.636579
C	-3.021428	1.992968	0.042007
C	-4.107318	1.153294	-0.222291
C	-3.180783	3.024517	0.970862
C	-5.326050	1.343221	0.422924
H	-3.990161	0.338914	-0.934236
C	-4.398524	3.218578	1.617918
H	-2.340858	3.682482	1.183398
C	-5.475612	2.378297	1.343564
H	-6.160395	0.683773	0.205200
H	-4.507928	4.027281	2.333824
H	-6.426878	2.529865	1.843624
N	-0.545330	-1.097639	-1.970545
N	-1.428612	-1.325793	-0.902505
C	-2.149270	-2.532563	-1.056019
O	-1.727632	-3.486362	-1.660706
O	-3.353835	-2.456496	-0.498889
C	-4.116316	-3.666491	-0.553104
H	-3.575360	-4.477029	-0.061903
H	-5.042737	-3.450516	-0.025805
H	-4.317453	-3.940291	-1.590019
C	0.384188	-0.209142	-1.763726
C	0.554978	0.553948	-0.531632
C	1.362806	-0.047987	-2.833599
C	1.418989	1.749012	-0.615059
H	1.376068	-0.365998	0.243165
C	2.290056	0.927208	-2.776621
H	1.294582	-0.728122	-3.676404

C	1.408207	2.747158	0.374001
C	2.334185	1.887694	-1.685389
H	3.013814	1.040792	-3.579989
C	2.299391	3.812370	0.332400
H	0.699834	2.684705	1.194721
C	3.238239	2.958357	-1.705568
C	3.233228	3.915797	-0.701841
H	2.267949	4.566192	1.113073
H	3.941077	3.033800	-2.531631
H	3.934916	4.742486	-0.728121

Vibrational frequencies

-1357.0668	21.2949	27.7553
30.8731	39.4667	51.2173
56.7017	65.1958	77.3229
85.2984	92.7362	98.0488
100.3821	128.7573	134.3766
141.4522	156.0870	168.8866
169.2595	176.6176	181.2598
192.3756	201.1083	221.4902
231.2517	240.3124	246.0889
250.4260	260.7097	275.8477
282.0628	300.0568	307.6865
320.8830	325.3108	345.1187
365.8745	374.4201	383.5227
404.8893	418.2798	421.5063
423.3830	431.3407	447.0159
458.0197	468.2630	479.5929
485.6253	497.1662	502.1566
515.1023	531.9408	563.2571
566.4046	599.2738	624.6288
629.9552	633.0465	656.9657
705.7804	714.5892	721.4827
730.7317	747.7475	756.5321
775.7990	778.2796	784.8105
799.2617	801.3494	821.7698
836.7996	846.3199	862.2360
867.4091	878.9435	886.5376
905.7866	908.5184	926.3368
935.5723	951.6112	953.3811
961.0865	962.9619	973.9125
977.2368	980.8567	983.4919
1001.2673	1009.4981	1018.4015
1024.5379	1024.7563	1038.5161
1050.6771	1072.3057	1077.1160

1087.0427	1103.5138	1108.3171
1115.8730	1136.2582	1137.7741
1146.6913	1158.3112	1164.8335
1166.4533	1173.9644	1176.9351
1190.2955	1191.3727	1193.2870
1206.9889	1209.1490	1210.0077
1221.7757	1236.4717	1239.7751
1240.3513	1245.4275	1260.4571
1293.1712	1316.4481	1329.7360
1340.2524	1347.8837	1349.8430
1358.0707	1358.9508	1361.6697
1367.1034	1371.4998	1375.8537
1381.6468	1389.5982	1402.2214
1418.6005	1424.1458	1428.3754
1436.6294	1441.6558	1446.9277
1453.1604	1489.8557	1491.2491
1492.7378	1496.1170	1497.9077
1498.0773	1501.3167	1501.7679
1504.9691	1508.9455	1510.2410
1510.7110	1517.7146	1519.5101
1523.5611	1530.9481	1533.4401
1542.7082	1543.9509	1555.6590
1567.3368	1633.0083	1658.2252
1679.2090	1691.2486	1701.5094
1716.1421	1827.7012	1863.6378
3076.5635	3079.5528	3082.0213
3083.0796	3087.6281	3092.8509
3096.3112	3098.9044	3106.7753
3109.8778	3111.4225	3133.3969
3148.3304	3153.6059	3157.7904
3161.5945	3163.8557	3168.0960
3170.4406	3174.3859	3177.9270
3185.7495	3187.7830	3189.8603
3192.9989	3199.9475	3200.7828
3207.3699	3210.5236	3212.4146
3212.6216	3214.3622	3217.0000
3223.8847	3224.4334	3228.3682

M8a1

Zero-point correction= 0.620026

Thermal correction to Energy= 0.654049

Thermal correction to Enthalpy= 0.654993

Thermal correction to Gibbs Free Energy= 0.553625

Sum of electronic and zero-point Energies= -1516.074238

Sum of electronic and thermal Energies= -1516.040215
Sum of electronic and thermal Enthalpies= -1516.039271
Sum of electronic and thermal Free Energies= -1516.140639
Cartesian coordinates

N	-3.216402	0.355661	0.461817
C	-4.520206	0.406451	-0.304764
C	-4.578617	-0.747722	-1.300955
C	-4.688521	1.728654	-1.047304
H	-5.322637	0.304475	0.430727
H	-4.468115	-1.730444	-0.838113
H	-5.546883	-0.726333	-1.805420
H	-3.798599	-0.619939	-2.057509
H	-4.851097	2.572605	-0.373649
H	-3.814626	1.934823	-1.669781
H	-5.569686	1.646740	-1.687533
C	-3.061910	-0.922074	1.278041
C	-4.316182	-1.338701	2.042239
C	-1.848757	-0.847947	2.198146
H	-2.845888	-1.685924	0.525449
H	-5.143800	-1.604728	1.381994
H	-4.068235	-2.227723	2.627009
H	-4.657711	-0.568545	2.736212
H	-0.953156	-0.515014	1.668019
H	-2.021300	-0.194042	3.057715
H	-1.648770	-1.853343	2.575352
C	-2.916710	1.624415	1.203807
C	-3.898758	1.992472	2.305163
H	-2.876053	2.403665	0.443118
H	-1.904609	1.530205	1.601959
H	-3.678339	3.010375	2.634589
H	-4.935770	1.973206	1.959155
H	-3.809972	1.339496	3.175182
H	-2.385568	0.255113	-0.283447
C	0.769065	0.929097	0.382458
O	0.945931	1.720552	1.284240
C	1.615365	-0.300965	0.171593
C	2.755600	0.064297	-0.830277
H	2.066344	-0.524434	1.144526
H	3.226474	-0.875210	-1.137196
H	2.291139	0.496891	-1.723932
C	3.788943	0.998807	-0.255945
C	3.615916	2.385121	-0.306959
C	4.927439	0.487309	0.372594
C	4.561174	3.238421	0.256215

H	2.727372	2.794072	-0.782143
C	5.874067	1.337722	0.938455
H	5.077826	-0.589595	0.408135
C	5.692673	2.717701	0.880808
H	4.414044	4.313039	0.206765
H	6.755413	0.922953	1.417713
H	6.430123	3.384194	1.316776
N	-1.032959	0.044686	-1.086617
N	-0.221290	1.117169	-0.605435
C	-0.607605	2.369521	-1.047514
O	-1.637820	2.593902	-1.649351
O	0.311246	3.306281	-0.781591
C	-0.045021	4.628066	-1.191675
H	-0.953914	4.952892	-0.681459
H	0.796468	5.256280	-0.906953
H	-0.204340	4.663776	-2.270453
C	-0.451245	-1.178516	-0.939909
C	0.776900	-1.449753	-0.328442
C	-1.215305	-2.290817	-1.447393
C	1.251011	-2.789315	-0.202020
C	-0.779907	-3.572574	-1.323930
H	-2.151055	-2.071502	-1.951472
C	2.492147	-3.113629	0.415874
C	0.465388	-3.872546	-0.695143
H	-1.375016	-4.391684	-1.720259
C	2.914818	-4.418403	0.532218
H	3.122823	-2.321810	0.807934
C	0.925742	-5.200991	-0.565114
C	2.130770	-5.481500	0.037640
H	3.866635	-4.629981	1.010375
H	0.303354	-6.003519	-0.953997
H	2.477169	-6.505117	0.132455

Vibrational frequencies

14.1598	21.5475	26.0549
40.1391	42.2357	53.4399
62.4834	64.9069	80.6671
85.0110	98.1321	99.9040
110.9680	117.1852	130.4819
136.0773	139.6876	145.7614
154.5157	160.2082	177.1808
193.1929	211.3260	217.8713
221.5778	234.2833	251.5084
279.0171	286.0899	289.6239
294.4600	303.3016	314.9182

317.5748 345.6568 356.2066
364.2270 366.8145 370.6144
407.4283 415.6007 420.9664
428.3268 436.9193 450.7824
454.6291 467.0252 484.3377
488.5386 506.3737 510.3667
537.4880 555.0526 557.4445
575.7938 622.8383 630.5147
635.6668 643.0562 683.5765
704.4440 720.4022 724.3062
745.8680 754.9961 763.4741
773.0834 775.9649 780.5538
799.8436 815.2149 827.9056
831.8036 849.2601 861.5792
875.0394 881.4179 898.4418
902.0638 922.8969 931.3537
949.5161 949.8242 957.4279
967.6952 969.5180 969.8870
974.8245 981.4824 982.8137
997.7115 1006.9456 1017.9654
1019.7449 1024.9735 1047.7863
1068.2843 1071.8599 1080.7634
1095.5262 1104.7556 1118.9431
1130.6152 1136.6015 1144.6950
1153.3110 1166.5261 1176.3070
1180.0878 1185.5560 1187.5445
1195.4193 1196.2886 1206.8288
1208.4054 1210.0933 1215.2345
1226.7855 1232.7560 1240.4983
1244.1056 1271.4146 1293.1496
1312.9712 1334.4190 1335.1337
1347.5596 1351.0729 1359.4768
1363.7867 1366.0353 1371.3111
1375.8030 1386.5966 1392.8382
1407.0895 1414.0780 1420.1695
1421.8511 1428.8278 1432.1344
1435.6687 1443.9952 1447.8687
1468.1742 1484.6004 1489.7309
1490.7606 1491.7823 1496.3214
1496.8885 1498.0388 1500.9120
1502.8815 1507.4082 1509.0375
1509.9922 1513.3567 1517.0919
1524.1463 1528.0789 1552.1044
1554.9722 1555.3377 1571.0870

1642.6837	1679.9217	1686.1657
1690.7638	1700.1461	1703.1052
1817.8699	1841.9856	1956.8911
3071.5848	3080.8554	3081.2625
3082.6706	3084.5950	3090.3540
3091.7652	3095.8894	3127.8964
3128.1385	3131.6357	3139.7200
3159.6082	3161.0520	3163.4352
3165.1354	3165.8294	3170.0961
3175.9502	3177.9181	3179.4609
3180.1119	3183.3239	3183.5060
3183.8525	3186.1551	3193.3051
3194.8100	3196.0849	3205.4190
3209.7348	3210.8459	3214.2769
3221.4252	3222.4202	3226.8917

TS8a2

Zero-point correction= 0.632625
Thermal correction to Energy= 0.665772
Thermal correction to Enthalpy= 0.666716
Thermal correction to Gibbs Free Energy= 0.568298
Sum of electronic and zero-point Energies= -1516.486765
Sum of electronic and thermal Energies= -1516.453618
Sum of electronic and thermal Enthalpies= -1516.452674
Sum of electronic and thermal Free Energies= -1516.551092
Cartesian coordinates

N	3.280523	-0.357416	0.024546
C	4.109335	-0.515442	1.262123
C	3.596196	-1.662997	2.129004
C	4.137532	0.758705	2.105309
H	5.141221	-0.743925	0.964801
H	3.525727	-2.613914	1.595167
H	4.282942	-1.813122	2.965079
H	2.617763	-1.411088	2.553306
H	4.699175	1.566720	1.631871
H	3.123027	1.109912	2.310457
H	4.627977	0.535154	3.055684
C	3.317768	-1.582978	-0.847209
C	4.688024	-2.251342	-1.014500
C	2.687598	-1.328343	-2.217924
H	2.676422	-2.316209	-0.344737
H	5.072226	-2.656892	-0.076386
H	4.578440	-3.087171	-1.710345
H	5.435464	-1.570644	-1.425149

H	1.730415	-0.801733	-2.152809
H	3.347180	-0.746859	-2.868101
H	2.509010	-2.290577	-2.702936
C	3.602082	0.901755	-0.698120
C	5.017631	1.056192	-1.252017
H	3.402579	1.716237	-0.002532
H	2.878841	1.012780	-1.511362
H	5.149776	2.086647	-1.591687
H	5.778643	0.857528	-0.491951
H	5.205640	0.402568	-2.105893
H	1.676019	-0.300375	0.327048
C	-1.029647	0.908079	-1.314532
O	-1.218391	1.735722	-2.156784
C	-2.052622	-0.088160	-0.824530
C	-2.615567	0.387298	0.540428
H	-2.837037	-0.092556	-1.583163
H	-3.524859	-0.189525	0.737506
H	-1.902803	0.132239	1.333866
C	-2.900314	1.869754	0.576726
C	-2.103058	2.723124	1.343034
C	-3.934643	2.414703	-0.189774
C	-2.338418	4.098035	1.348607
H	-1.303021	2.309869	1.954339
C	-4.165660	3.785956	-0.190637
H	-4.564034	1.759979	-0.787544
C	-3.366493	4.631878	0.578402
H	-1.725425	4.748293	1.965031
H	-4.972326	4.196526	-0.789210
H	-3.551489	5.700894	0.581214
N	0.570374	-0.296036	0.107491
N	0.216473	0.855656	-0.590375
C	0.753550	2.026741	0.022107
O	1.299190	1.979082	1.096334
O	0.584066	3.082368	-0.736660
C	1.022197	4.321695	-0.149095
H	2.107228	4.311341	-0.038583
H	0.707927	5.093576	-0.846186
H	0.548769	4.457885	0.823416
C	-0.147370	-1.384115	0.108184
C	-1.404169	-1.471488	-0.712623
C	0.317880	-2.530557	0.836956
C	-2.341603	-2.591871	-0.311805
C	-0.505040	-3.590309	1.001481
H	1.286294	-2.493313	1.317501

C	-3.649598	-2.642695	-0.783387
C	-1.856752	-3.646929	0.479950
H	-0.161749	-4.435098	1.592445
C	-4.471414	-3.721748	-0.462044
H	-4.043791	-1.845342	-1.404685
C	-2.687156	-4.730818	0.791593
C	-3.992420	-4.768700	0.323572
H	-5.491501	-3.742158	-0.829904
H	-2.297176	-5.536116	1.406758
H	-4.634884	-5.606859	0.568571
H	-1.016203	-1.750004	-1.711353

Vibrational frequencies

-96.0802	12.6912	25.8269
32.2312	44.5763	51.8028
55.5098	65.4353	76.8616
84.9447	93.6821	100.1756
118.7167	133.3145	134.8219
141.7207	145.9575	158.4331
160.2029	168.5574	183.1218
193.8156	211.4424	218.1330
226.1168	242.7476	251.8730
265.3339	277.6470	289.5644
295.6078	312.2404	321.6046
331.2832	337.8698	348.1944
358.4440	364.8823	377.2598
395.0516	420.5037	421.3555
424.4420	438.0836	443.2825
452.8697	468.9859	475.4282
488.1004	495.1790	505.8899
522.5507	535.1193	554.3032
582.0352	598.2541	629.8400
635.8171	640.1402	657.1600
697.6575	708.4739	724.5938
727.3349	749.5934	765.3612
775.2222	781.7204	795.9568
809.4593	819.9479	829.9586
851.6165	858.8549	867.6029
880.2673	887.0250	901.3797
909.4849	912.9130	917.4597
929.2234	948.3126	958.4050
960.6017	966.9500	973.2499
986.4362	991.1507	1004.8153
1010.5793	1018.1763	1034.3409
1035.9290	1038.2564	1044.1777

1050.5612	1072.2623	1081.1047
1083.0906	1090.3970	1107.0709
1121.4187	1134.2646	1141.8805
1147.4967	1150.9514	1168.1600
1178.0333	1181.4630	1185.9737
1189.3709	1195.8702	1199.5492
1211.7382	1211.9700	1220.2666
1229.5216	1237.9947	1243.0497
1246.9288	1254.1628	1255.1908
1261.2607	1265.8804	1292.9673
1315.1036	1332.0315	1339.0262
1350.7507	1361.3644	1362.0821
1365.8082	1369.6538	1374.7770
1379.8429	1385.8554	1386.4469
1395.5713	1400.2318	1412.4264
1412.8640	1426.1082	1427.9014
1432.5733	1434.0281	1457.8900
1488.8656	1489.6852	1491.4147
1495.2615	1497.8505	1499.4812
1501.1507	1502.1480	1502.6618
1509.3096	1509.6712	1511.4556
1514.3165	1520.1574	1525.0526
1527.9969	1550.2780	1552.5379
1556.1658	1601.5616	1644.4276
1678.4447	1693.1928	1695.9387
1701.5856	1734.2444	1867.2103
1920.9436	1946.8407	2999.8072
3063.9228	3074.7775	3074.8748
3076.6357	3080.4926	3083.0557
3090.8411	3094.6305	3107.8560
3115.4473	3129.4330	3146.5324
3153.1369	3155.1297	3155.9511
3157.7085	3160.6978	3162.8488
3164.8003	3167.0321	3175.9599
3185.5677	3186.1940	3191.9591
3201.2554	3202.1098	3209.5783
3212.9759	3216.1202	3222.8467
3225.9537	3229.5234	3233.3095
3236.1115	3243.3564	3270.2011

M8a2

Zero-point correction= 0.633135

Thermal correction to Energy= 0.667564

Thermal correction to Enthalpy= 0.668508

Thermal correction to Gibbs Free Energy= 0.567120
Sum of electronic and zero-point Energies= -1516.487031
Sum of electronic and thermal Energies= -1516.452602
Sum of electronic and thermal Enthalpies= -1516.451657
Sum of electronic and thermal Free Energies= -1516.553045
Cartesian coordinates

N	-2.253139	0.967378	0.984820
C	-3.369443	1.210128	0.043631
C	-3.883439	-0.103713	-0.550891
C	-2.947567	2.139400	-1.096382
H	-4.210388	1.694850	0.565471
H	-4.283873	-0.788697	0.198765
H	-4.684307	0.110456	-1.262573
H	-3.086402	-0.622824	-1.095793
H	-2.752563	3.162058	-0.765015
H	-2.047136	1.761492	-1.594803
H	-3.745909	2.183158	-1.840705
C	-2.594145	0.009287	2.069140
C	-3.915557	0.267114	2.805390
C	-1.455818	-0.119525	3.079217
H	-2.683425	-0.967777	1.576040
H	-4.776283	0.266437	2.132465
H	-4.072521	-0.527939	3.540346
H	-3.902393	1.219071	3.341106
H	-0.480771	-0.210666	2.588173
H	-1.410076	0.741779	3.752799
H	-1.615996	-1.011347	3.690521
C	-1.572804	2.198971	1.417053
C	-2.400482	3.239964	2.175388
H	-1.156271	2.668286	0.522100
H	-0.705100	1.918949	2.018070
H	-1.829007	4.169569	2.252192
H	-3.340199	3.466028	1.662285
H	-2.636518	2.913069	3.190792
H	0.261639	1.202006	-3.019554
C	1.255320	0.866371	0.089020
O	1.762750	1.490827	0.977890
C	1.066245	-0.637586	0.086169
C	2.236679	-1.354069	-0.627607
H	1.076850	-0.921408	1.140762
H	2.002441	-2.424172	-0.630976
H	2.291384	-1.030465	-1.673377
C	3.551796	-1.102108	0.066898
C	4.395727	-0.072882	-0.353709

C	3.917176	-1.869984	1.175566
C	5.585788	0.186375	0.321418
H	4.121823	0.528836	-1.217548
C	5.105930	-1.613540	1.852009
H	3.265303	-2.675738	1.506336
C	5.942383	-0.583474	1.425949
H	6.234827	0.987728	-0.016382
H	5.381594	-2.218803	2.709483
H	6.870314	-0.383671	1.951660
N	0.249568	0.721610	-2.119541
N	0.745936	1.500824	-1.084586
C	0.691990	2.883287	-1.399455
O	0.290279	3.239111	-2.482572
O	1.093391	3.638096	-0.409522
C	1.001944	5.057445	-0.657418
H	-0.040290	5.330850	-0.827361
H	1.385976	5.524658	0.244879
H	1.606583	5.321334	-1.524735
C	-0.311191	-0.448718	-1.925612
C	-0.309624	-0.950931	-0.532827
C	-0.875146	-1.169244	-3.013946
C	-0.787593	-2.365590	-0.374332
C	-1.368402	-2.412420	-2.772202
H	-0.896068	-0.726850	-4.003197
C	-0.744273	-3.001041	0.865373
C	-1.333379	-3.051662	-1.476732
H	-1.806755	-2.969838	-3.595851
C	-1.230670	-4.297397	1.007380
H	-0.337278	-2.487458	1.731543
C	-1.828897	-4.356011	-1.319790
C	-1.776037	-4.977683	-0.083688
H	-1.185574	-4.779602	1.978000
H	-2.251971	-4.868545	-2.178359
H	-2.157180	-5.985160	0.037057
H	-1.051447	-0.267204	-0.005907

Vibrational frequencies

23.8478	28.8941	36.7694
38.8525	46.5454	52.6876
59.8824	67.7026	76.3693
83.0282	89.2346	94.9602
97.5189	108.0566	120.8437
124.9044	137.0701	141.9709
153.6006	162.9952	176.3421
186.7318	193.1292	207.1794

221.5486	226.5123	234.3508
244.4830	261.6461	275.9208
284.7861	297.8838	312.4583
329.7285	354.9941	361.7016
365.3850	368.2966	380.5400
390.6603	418.8763	420.6189
425.3270	438.3060	442.2213
448.7747	466.3692	477.0286
495.6100	498.6480	506.5806
519.3964	532.3925	540.5351
591.8008	612.4771	621.7554
624.0907	633.2386	695.6659
698.8566	712.2554	713.4471
720.9416	740.9719	755.9897
771.7579	774.2800	777.9150
792.0931	801.0410	813.4274
828.7663	847.5396	861.4970
862.9711	880.0560	888.8992
899.6234	906.8942	920.1872
923.7276	937.5498	949.9323
953.6182	955.3249	965.4546
971.0028	985.3701	1003.4982
1005.3043	1018.7959	1025.4136
1028.6307	1030.0573	1036.8483
1038.8863	1074.7932	1080.6081
1082.4570	1091.6091	1105.7450
1123.6449	1132.1803	1138.0127
1142.8622	1160.7938	1163.0395
1182.3177	1185.8220	1186.4013
1187.9668	1192.9013	1194.3921
1203.2999	1214.8232	1223.9065
1238.9557	1245.7136	1253.7003
1256.0927	1258.3090	1261.5020
1282.1424	1288.1327	1308.0717
1318.4670	1350.1890	1354.9610
1360.9076	1363.4029	1365.9793
1370.3474	1373.8800	1377.3839
1378.5335	1381.4877	1385.1772
1395.2028	1406.6322	1407.6767
1414.3954	1419.5751	1424.3111
1427.2846	1432.7700	1468.4731
1483.9903	1489.7614	1492.3702
1494.5623	1495.4754	1497.8563
1498.6429	1500.0518	1502.4820

1503.1244	1505.6523	1509.3090
1515.5757	1516.8123	1517.1620
1520.5974	1521.2929	1540.3377
1548.3015	1561.6323	1624.5055
1681.3064	1683.5964	1687.1958
1704.5394	1706.1607	1861.3159
1904.7992	2469.6755	3020.0795
3066.2705	3067.0607	3069.1597
3070.5606	3078.1172	3078.2996
3079.5482	3110.9091	3117.0802
3130.8999	3142.9763	3144.2742
3147.8915	3148.9212	3152.6750
3153.1567	3154.1755	3157.3575
3159.2586	3164.9449	3168.6795
3172.3477	3184.4011	3202.0934
3207.7785	3207.8365	3209.8791
3212.3482	3218.1838	3223.3549
3227.3484	3233.2929	3237.7940
3239.8440	3244.0069	3507.3139

TS7a3

Zero-point correction= 1.004071
Thermal correction to Energy= 1.058350
Thermal correction to Enthalpy= 1.059294
Thermal correction to Gibbs Free Energy= 0.918427
Sum of electronic and zero-point Energies= -2567.577319
Sum of electronic and thermal Energies= -2567.523040
Sum of electronic and thermal Enthalpies= -2567.522095
Sum of electronic and thermal Free Energies= -2567.662962
Cartesian coordinates

C	-5.886167	1.087627	-1.308157
C	-4.614731	1.220001	-0.755655
C	-4.246475	2.343789	-0.023253
C	-5.197702	3.345477	0.161133
C	-6.477913	3.220857	-0.385828
C	-6.830615	2.094522	-1.127808
C	-6.012822	-0.208947	-2.069069
H	-3.232952	2.417935	0.360479
H	-4.941483	4.233203	0.730454
H	-7.206765	4.010372	-0.231631
H	-7.826048	2.001689	-1.551904
H	-5.989427	-0.027261	-3.148823
C	-3.825148	-1.251962	1.022474
C	-5.218428	-1.629155	0.640566

C	-4.782196	-1.040420	-1.643472
C	-3.764102	0.010789	-1.075781
C	-1.830710	-0.497832	0.520127
H	-5.559033	-2.472458	1.239503
H	-2.978766	0.259719	-1.789443
N	-3.072647	-1.655658	2.002479
N	-1.831620	-1.160620	1.683503
N	-3.117351	-0.515131	0.126085
C	-0.790844	-1.359688	2.657737
C	-0.005222	-2.514317	2.563465
C	-0.687476	-0.452662	3.711560
C	0.976873	-2.702726	3.528681
C	0.326916	-0.679199	4.648830
C	1.170841	-1.781590	4.565848
H	1.607395	-3.586483	3.473489
H	0.443660	0.025852	5.469019
O	-5.131086	-2.058027	-0.709103
H	-5.913132	-0.788764	0.762355
H	-4.338374	-1.581826	-2.480418
H	-6.931757	-0.760510	-1.849995
C	-0.240289	-3.509085	1.459120
H	-0.101715	-3.050805	0.474501
H	-1.271423	-3.878225	1.486408
H	0.435734	-4.360665	1.555441
C	2.266755	-2.005664	5.575059
H	3.249098	-1.970757	5.091244
H	2.167349	-2.989186	6.045908
H	2.244864	-1.244629	6.359309
C	-1.645462	0.694228	3.903189
H	-2.349061	0.453981	4.706237
H	-2.228787	0.914513	3.007386
H	-1.105069	1.599147	4.190156
C	-0.792207	0.318837	-0.311763
O	-1.396706	1.430673	-0.606950
C	0.602361	0.464058	0.388879
C	0.497143	1.626897	1.427032
H	0.785127	-0.457311	0.957152
H	-0.554754	1.692298	1.724794
H	1.057230	1.350320	2.327409
C	0.947088	3.016864	1.009797
C	1.830721	3.721736	1.834768
C	0.519501	3.626517	-0.173337
C	2.292394	4.988758	1.488118
H	2.187303	3.254797	2.750300

C	0.981773	4.893166	-0.523966
H	-0.166971	3.078581	-0.810794
C	1.870631	5.579896	0.298873
H	2.987979	5.507007	2.141317
H	0.648134	5.342767	-1.455392
H	2.233336	6.564135	0.017416
N	0.176607	0.294223	-2.556891
N	-0.469340	-0.516761	-1.607698
C	-0.984317	-1.662798	-2.113268
O	-0.802357	-2.102919	-3.237944
O	-1.705533	-2.359835	-1.186499
C	-2.209992	-3.621658	-1.613661
H	-1.404670	-4.362135	-1.652825
H	-2.953750	-3.907015	-0.870585
H	-2.668425	-3.540700	-2.600004
C	1.206019	0.904492	-2.028431
C	1.712980	0.654138	-0.680145
C	1.900758	1.856448	-2.887795
C	2.913924	1.394559	-0.266166
H	2.496444	-0.615853	-0.967325
C	2.977681	2.538454	-2.451248
H	1.484596	2.018088	-3.877766
C	3.538681	1.135678	0.970600
C	3.542604	2.318999	-1.134537
H	3.463119	3.267336	-3.096541
C	4.707126	1.781044	1.342902
H	3.088797	0.415087	1.650920
C	4.710742	2.983846	-0.733958
C	5.297137	2.725439	0.493877
H	5.163666	1.555442	2.303270
H	5.161003	3.701240	-1.416459
H	6.205687	3.239809	0.789393
N	3.147458	-1.656277	-1.361488
C	3.903584	-1.136054	-2.556935
C	4.178971	-2.167713	-3.652867
C	5.189375	-0.404438	-2.172794
H	3.217719	-0.392828	-2.981077
H	3.259272	-2.588543	-4.062369
H	4.697107	-1.658143	-4.469417
H	4.819433	-2.983659	-3.308969
H	5.053269	0.274463	-1.328897
H	6.004043	-1.097113	-1.944622
H	5.499126	0.198377	-3.030367
C	3.975799	-2.136157	-0.211441

C	4.926601	-3.297740	-0.508933
C	3.080643	-2.457182	0.979584
H	4.580661	-1.269560	0.066395
H	5.623346	-3.068570	-1.315421
H	5.517951	-3.490069	0.391245
H	4.396847	-4.217457	-0.759229
H	2.360413	-1.657748	1.166235
H	2.529939	-3.392159	0.840515
H	3.698327	-2.565497	1.875702
C	1.973162	-2.491065	-1.736633
C	2.127691	-3.993509	-1.949026
H	1.552117	-2.021255	-2.630798
H	1.232238	-2.323260	-0.949844
H	1.195405	-4.343370	-2.402266
H	2.946220	-4.259648	-2.617866
H	2.260173	-4.533592	-1.008617

Vibrational frequencies

-1294.9132	18.7443	21.1233
24.7642	29.0136	36.8754
45.1430	47.0274	54.7397
57.8636	70.4022	77.5673
80.9984	82.9942	86.3936
90.3745	94.3011	98.1038
100.3258	105.2878	109.3465
110.2415	115.7238	120.4712
127.2045	130.5318	133.7698
146.7406	148.4480	156.6182
162.4460	168.0479	181.5112
191.6658	196.3650	201.7565
204.3879	209.8808	215.3993
219.1801	222.6560	231.1915
247.1360	249.3177	253.2210
259.4239	261.8061	270.6345
274.7867	281.0163	282.9374
286.4878	289.8344	295.8773
301.0024	317.4059	320.7077
325.8004	332.9732	345.1198
352.8295	355.1736	356.0979
369.6125	372.3433	387.5706
391.2514	401.9993	414.4190
421.3238	424.3539	427.4488
435.7909	443.6298	447.2244
448.9857	478.4006	489.8634
491.8556	494.6361	495.3141

503.5736	513.8202	515.9574
522.2659	529.1852	537.8444
546.6430	557.5990	565.6950
569.5845	584.9470	594.0035
597.0787	602.0114	608.7238
620.8485	627.6255	631.3022
644.7589	668.8657	682.0685
687.4101	700.4232	715.1491
720.1001	729.7414	735.2758
746.6466	748.1209	752.1111
759.6830	763.4345	764.9081
771.5227	777.9401	782.2601
792.7605	809.7466	814.1941
824.4398	834.6873	843.1564
850.2259	856.2949	864.0918
866.8398	880.0272	881.0706
884.2069	886.8683	897.4367
904.2487	906.7801	918.9180
926.6821	929.7484	931.6206
947.4164	951.2968	953.1436
960.0941	964.0698	966.2883
971.0418	972.4761	972.8845
978.1801	996.4293	998.4936
1000.5416	1002.2956	1004.4251
1012.2639	1013.5270	1018.8947
1019.6609	1032.1763	1037.3925
1040.0928	1041.7632	1047.7049
1048.1610	1053.0875	1055.4042
1059.5185	1063.1497	1065.3728
1068.5885	1071.3783	1079.2910
1080.5826	1094.4623	1098.3637
1111.7016	1114.6472	1115.1260
1116.5019	1128.8444	1135.9948
1145.6068	1148.5647	1162.0520
1165.9763	1167.1755	1174.8197
1175.4606	1181.7830	1182.1287
1189.4285	1190.7283	1200.5644
1200.8811	1203.7159	1205.3845
1207.3608	1222.7433	1229.7106
1233.3007	1234.2421	1236.6265
1238.2084	1240.2760	1246.0690
1261.7135	1274.8474	1277.9124
1286.3954	1287.7013	1289.7341
1301.9431	1304.6455	1321.7456

1334.8048	1336.5391	1339.1910
1344.1716	1350.2748	1356.6645
1358.5492	1361.5822	1368.3480
1371.2926	1371.7201	1373.9275
1375.9219	1377.0451	1380.9734
1389.5127	1403.1897	1409.1009
1410.5158	1412.1313	1413.1127
1414.4522	1418.7308	1420.0970
1421.2871	1428.8596	1435.1405
1441.1181	1453.1956	1454.6284
1465.3273	1469.4039	1474.5098
1475.7637	1482.3309	1484.3368
1485.5143	1486.3708	1490.1076
1491.1762	1493.4058	1493.5760
1494.1166	1496.4735	1496.9874
1500.0421	1503.8612	1505.0432
1506.1470	1507.9450	1511.2099
1516.1429	1517.1271	1519.6904
1520.9379	1523.4088	1526.4693
1532.0458	1534.6524	1535.9064
1541.3075	1542.2140	1546.4649
1567.2480	1573.3264	1583.9828
1623.1156	1640.0539	1671.1669
1680.7947	1690.1474	1692.5669
1695.4016	1695.6426	1696.8903
1699.3894	1716.8811	1791.0559
3059.3286	3059.9890	3069.6128
3075.4806	3076.8936	3078.0202
3078.1106	3080.7652	3081.3243
3082.3261	3084.5846	3085.8481
3089.8004	3098.6900	3110.5690
3122.5719	3131.7108	3133.2621
3134.5273	3139.5188	3147.3563
3148.4238	3152.6583	3153.3833
3155.9713	3157.9617	3158.8462
3161.4231	3168.2184	3169.2342
3169.9633	3173.4042	3177.9358
3178.0136	3179.6358	3180.1180
3181.1499	3184.5203	3185.4461
3186.0154	3187.5671	3189.3485
3194.4846	3195.1393	3195.9348
3199.5698	3200.5465	3203.6639
3203.9022	3208.2922	3211.8200
3212.6371	3216.0393	3219.1681

3224.2675 3224.3231 3236.6062

M7a3

Zero-point correction= 1.010162
Thermal correction to Energy= 1.064716
Thermal correction to Enthalpy= 1.065660
Thermal correction to Gibbs Free Energy= 0.923525
Sum of electronic and zero-point Energies= -2567.586399
Sum of electronic and thermal Energies= -2567.531845
Sum of electronic and thermal Enthalpies= -2567.530901
Sum of electronic and thermal Free Energies= -2567.673036
Cartesian coordinates

C	-6.099278	0.166911	-1.599147
C	-4.838311	0.567494	-1.165567
C	-4.540534	1.901839	-0.908566
C	-5.553299	2.843402	-1.079858
C	-6.824864	2.451056	-1.507708
C	-7.106462	1.112270	-1.775379
C	-6.142571	-1.322690	-1.834761
H	-3.530291	2.169408	-0.610937
H	-5.352863	3.892249	-0.885502
H	-7.601714	3.198447	-1.635440
H	-8.094820	0.812043	-2.110698
H	-6.147464	-1.544408	-2.907182
C	-3.889934	-1.087208	1.366585
C	-5.251139	-1.665418	1.168735
C	-4.851486	-1.868779	-1.183946
C	-3.909509	-0.618585	-1.040632
C	-1.957880	-0.404150	0.591558
H	-5.535836	-2.267671	2.030665
H	-3.129278	-0.594123	-1.800823
N	-3.105087	-1.106797	2.402824
N	-1.905233	-0.662334	1.906945
N	-3.240512	-0.635629	0.260729
C	-0.839416	-0.482910	2.857766
C	0.154084	-1.462662	2.956433
C	-0.878238	0.647780	3.673713
C	1.179891	-1.242956	3.869859
C	0.182253	0.829615	4.564868
C	1.223478	-0.091268	4.663147
H	1.968042	-1.986329	3.965292
H	0.188359	1.714820	5.195636
O	-5.125092	-2.528319	0.049681
H	-6.003306	-0.884109	1.002783

H	-4.368025	-2.632097	-1.795255
H	-7.017820	-1.811806	-1.396802
C	0.125183	-2.675901	2.068615
H	0.368261	-2.398568	1.034403
H	-0.870210	-3.128781	2.048723
H	0.845291	-3.421927	2.410807
C	2.385819	0.143667	5.591482
H	3.267798	0.458798	5.023751
H	2.651428	-0.770536	6.128300
H	2.161153	0.922809	6.322191
C	-2.025837	1.620978	3.627627
H	-2.846524	1.265505	4.258753
H	-2.421292	1.743403	2.616637
H	-1.711552	2.599600	3.994901
C	-0.957613	0.177202	-0.471781
O	-1.642440	1.003469	-1.207561
C	0.299337	0.789804	0.242141
C	-0.097918	2.203364	0.785520
H	0.548114	0.172298	1.112839
H	-1.193222	2.237702	0.819186
H	0.255403	2.314345	1.816342
C	0.374169	3.401905	-0.009767
C	1.063185	4.436019	0.627229
C	0.139900	3.503104	-1.386711
C	1.516634	5.546458	-0.083098
H	1.265999	4.359244	1.693335
C	0.602073	4.605613	-2.100119
H	-0.398887	2.693860	-1.872288
C	1.291622	5.631754	-1.453852
H	2.053394	6.336903	0.433295
H	0.422344	4.665778	-3.169877
H	1.650254	6.489503	-2.015195
N	0.389394	-0.558397	-2.405916
N	-0.375124	-1.006413	-1.302797
C	-0.746853	-2.303547	-1.401562
O	-0.277262	-3.134922	-2.169400
O	-1.717484	-2.653345	-0.503855
C	-2.046407	-4.037098	-0.462774
H	-1.222275	-4.618127	-0.036924
H	-2.930729	-4.101997	0.172257
H	-2.265386	-4.412759	-1.463324
C	1.326524	0.297361	-2.015917
C	1.486598	0.808662	-0.698728
C	2.293228	0.717680	-3.012997

C	2.694901	1.453241	-0.326462
H	3.359202	-0.791314	-1.178314
C	3.407952	1.421483	-2.675954
H	2.101772	0.425810	-4.042403
C	3.011017	1.787920	1.027950
C	3.686152	1.766205	-1.313079
H	4.127197	1.707944	-3.441229
C	4.211590	2.366901	1.367831
H	2.297355	1.545810	1.812411
C	4.896891	2.384782	-0.934731
C	5.173158	2.682138	0.382691
H	4.420784	2.587296	2.411416
H	5.620272	2.618479	-1.714331
H	6.111013	3.151173	0.660604
N	3.750741	-1.744224	-1.100380
C	4.628405	-1.859749	-2.347366
C	4.955105	-3.291527	-2.752154
C	5.867897	-0.980699	-2.237566
H	3.980232	-1.430260	-3.117707
H	4.062465	-3.848405	-3.039625
H	5.602343	-3.239094	-3.630959
H	5.489784	-3.844761	-1.978368
H	5.620527	0.025428	-1.893155
H	6.627864	-1.407003	-1.578783
H	6.304238	-0.895147	-3.235331
C	4.457517	-1.695745	0.249995
C	5.392317	-2.867668	0.520301
C	3.431943	-1.532430	1.369175
H	5.043762	-0.772448	0.194116
H	6.228019	-2.917986	-0.177107
H	5.810293	-2.723629	1.519967
H	4.869643	-3.825416	0.515680
H	2.649348	-0.815589	1.109212
H	2.969838	-2.487356	1.629924
H	3.948693	-1.154361	2.254906
C	2.497967	-2.593528	-1.182662
C	2.557401	-4.032771	-0.700626
H	2.168240	-2.534787	-2.221612
H	1.747787	-2.036364	-0.617257
H	1.591354	-4.465737	-0.975572
H	3.342501	-4.626654	-1.168612
H	2.660253	-4.113519	0.383019

Vibrational frequencies

13.6355	20.4883	26.2715

34.1534	36.0933	39.3509
48.3669	52.2358	55.3747
56.5171	64.0152	72.0305
73.3304	77.3695	87.8243
87.9734	90.1303	93.4597
102.8224	109.5183	112.7774
119.9250	127.6479	129.9323
137.5164	142.7114	144.9207
154.3256	156.4398	173.9451
180.2678	186.4528	188.2595
194.2619	198.1911	206.4508
213.2300	215.0302	223.2281
234.8303	237.9303	241.6978
245.2550	254.0465	256.0894
259.9093	263.1474	270.9605
273.8485	280.9354	285.3817
287.8680	288.7410	298.7157
307.6441	311.7647	331.7457
333.9807	338.4821	352.6653
356.2352	362.7448	364.9379
369.6716	382.6418	387.2956
389.0512	413.6814	417.8825
422.6822	423.8855	436.9916
438.4099	449.5517	451.2238
475.4578	478.2903	489.8107
495.0233	498.9313	506.7340
513.1191	515.1070	521.3646
525.2502	536.0387	545.9173
552.1500	553.7476	561.3363
586.3737	589.4745	593.5140
602.1054	608.1208	621.5461
628.6686	631.1409	647.7085
657.3911	660.6963	681.4346
702.4420	709.3429	717.2346
721.2551	731.2559	736.7681
745.5654	750.1964	755.2880
759.3480	764.8494	765.9638
773.9196	777.8094	780.5723
789.7893	794.2329	810.4667
831.7537	834.9215	838.9957
851.9571	852.3476	870.0118
876.7299	877.6948	880.4926
883.1645	886.7907	890.0824
907.3652	917.2119	923.3254

933.7437 944.1938 949.8496
951.2154 952.1360 958.3134
963.3670 964.0744 966.9200
972.4855 977.9380 984.0443
985.9622 987.6049 996.7390
1000.2191 1001.4610 1002.5738
1015.2660 1015.6994 1024.2113
1031.6587 1038.1195 1040.4710
1043.6846 1046.3396 1050.6949
1054.3619 1058.4835 1064.2247
1066.3609 1067.5716 1069.0028
1070.8777 1073.2394 1076.7096
1081.7150 1087.0008 1093.0933
1110.3742 1114.4474 1118.1360
1123.2127 1125.3194 1130.1550
1144.2861 1159.5332 1171.0735
1171.2091 1176.6549 1179.7065
1181.8884 1184.8323 1190.4705
1190.5989 1196.6666 1200.7076
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1228.2502 1232.1951 1235.7495
1238.9400 1245.4446 1259.0243
1279.0731 1281.5246 1287.3620
1288.9238 1290.7390 1298.6325
1307.3644 1320.9461 1332.9335
1337.4582 1341.2440 1344.6558
1348.5461 1352.9770 1357.7346
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1370.7779 1375.3802 1380.5569
1385.3881 1391.6546 1392.4293
1399.3273 1406.0101 1407.1005
1414.1305 1416.7338 1417.8952
1418.4774 1419.6076 1423.1795
1428.4839 1428.8407 1440.1362
1448.0137 1450.6998 1460.5962
1462.9730 1466.1783 1471.8903
1473.8184 1476.2251 1478.2651
1482.3042 1487.4901 1488.9409
1491.2249 1491.6544 1492.8812
1494.6092 1494.9077 1496.7294
1497.5017 1499.3139 1499.5400
1503.5177 1503.7198 1509.2023
1511.1219 1513.0583 1517.6265

1518.7810	1519.6350	1523.3053
1523.5778	1528.6300	1533.6722
1536.4800	1539.5740	1548.8772
1555.3906	1557.7279	1566.7419
1611.5924	1671.8043	1679.4416
1684.6589	1688.3283	1692.6279
1693.0675	1695.4596	1696.6533
1700.2004	1776.6230	3063.7803
3065.8778	3070.0973	3075.0806
3077.2085	3082.6757	3083.4542
3084.5513	3088.7214	3091.7983
3096.5461	3097.5469	3100.1016
3113.9297	3115.2813	3117.8092
3132.0504	3133.2423	3140.6284
3142.0436	3147.3050	3151.7958
3163.9378	3164.4782	3164.9932
3167.0154	3168.4032	3169.3862
3170.8616	3171.7298	3172.2333
3173.0898	3175.0746	3179.7670
3180.6457	3181.1027	3181.6407
3183.3911	3184.0522	3190.4863
3192.1260	3193.2945	3196.0046
3198.3736	3199.9723	3200.7513
3201.8110	3203.0834	3203.8560
3205.5910	3213.6838	3214.4281
3218.3977	3223.7492	3224.1896
3225.6393	3235.3922	3350.6412

TS7a4

Zero-point correction= 1.018049

Thermal correction to Energy= 1.072557

Thermal correction to Enthalpy= 1.073502

Thermal correction to Gibbs Free Energy= 0.930258

Sum of electronic and zero-point Energies= -2568.059813

Sum of electronic and thermal Energies= -2568.005305

Sum of electronic and thermal Enthalpies= -2568.004360

Sum of electronic and thermal Free Energies= -2568.147604

Cartesian coordinates

C	-4.725492	-1.615203	1.285144
C	-3.358155	-1.370330	1.381602
C	-2.759278	-1.014625	2.586985
C	-3.573992	-0.907635	3.713439
C	-4.947882	-1.144279	3.625387
C	-5.535818	-1.495073	2.411111

C	-5.120683	-1.954631	-0.133607
H	-1.694294	-0.809765	2.620632
H	-3.135401	-0.637099	4.669738
H	-5.566965	-1.058972	4.512936
H	-6.602938	-1.680921	2.346129
H	-5.649278	-1.115462	-0.602083
C	-1.515738	-3.641667	0.081905
C	-2.867829	-4.269277	-0.000178
C	-3.786020	-2.213524	-0.862826
C	-2.709297	-1.499860	0.023204
C	-0.192200	-1.907384	-0.091864
H	-2.786873	-5.321073	-0.264953
H	-2.454249	-0.524060	-0.387935
N	-0.318887	-4.147699	0.029414
N	0.498275	-3.049750	-0.067203
N	-1.475018	-2.281090	0.034546
C	1.922007	-3.269683	-0.046072
C	2.615070	-3.314089	-1.263359
C	2.525165	-3.482856	1.190706
C	3.989902	-3.513436	-1.201433
C	3.906553	-3.690109	1.196281
C	4.651820	-3.696068	0.016985
H	4.557361	-3.542472	-2.128487
H	4.409315	-3.843846	2.146898
O	-3.536375	-3.599386	-1.056386
H	-3.403577	-4.175176	0.954008
H	-3.782613	-1.794672	-1.873383
H	-5.768499	-2.832274	-0.209235
C	1.898791	-3.116873	-2.570150
H	1.566009	-2.079249	-2.690932
H	1.007645	-3.748651	-2.632878
H	2.555667	-3.359227	-3.407651
C	6.143700	-3.902466	0.039111
H	6.658036	-3.036741	-0.389383
H	6.425080	-4.774787	-0.558178
H	6.511720	-4.050178	1.056124
C	1.726811	-3.505765	2.467112
H	1.237210	-4.479891	2.587754
H	0.942871	-2.745326	2.475511
H	2.373503	-3.341179	3.327337
C	0.219135	-0.410985	0.012194
O	-0.316061	0.075004	1.073746
C	1.750702	-0.147572	-0.185504
C	2.490920	-0.166571	1.177631

H	2.162975	-0.959730	-0.783127
H	1.899632	-0.797353	1.848481
H	3.450529	-0.673354	1.035527
C	2.753201	1.155335	1.871581
C	4.068679	1.526896	2.174367
C	1.714354	2.016567	2.236722
C	4.344869	2.741869	2.791014
H	4.885905	0.868603	1.893447
C	1.990385	3.235625	2.853432
H	0.694507	1.708113	2.020028
C	3.304300	3.608082	3.124786
H	5.373907	3.017411	3.000466
H	1.168039	3.894392	3.120397
H	3.513694	4.560405	3.600859
N	-0.331373	1.671280	-1.144277
N	-0.452549	0.300238	-1.294687
C	-0.827437	-0.114601	-2.549610
O	-1.057005	0.616985	-3.487126
O	-0.961494	-1.452402	-2.586308
C	-1.344811	-1.982753	-3.860710
H	-0.585414	-1.727596	-4.628590
H	-1.407256	-3.074506	-3.715826
H	-2.327178	-1.566865	-4.154963
C	0.872970	2.123021	-0.942975
C	1.985671	1.130096	-1.072566
C	1.112942	3.512748	-0.679665
C	3.369221	1.714452	-0.967358
H	1.870780	0.767796	-2.106557
C	2.388578	3.948377	-0.568268
H	0.271516	4.189226	-0.588073
C	4.486871	0.899411	-1.134656
C	3.545409	3.085242	-0.713509
H	2.573666	5.001103	-0.373367
C	5.766931	1.431728	-1.019393
H	4.356624	-0.160327	-1.344484
C	4.838705	3.610506	-0.595390
C	5.945307	2.788310	-0.740027
H	6.630156	0.786240	-1.146378
H	4.963288	4.669038	-0.385596
H	6.945185	3.198559	-0.643613
N	-2.683935	2.743820	-0.644366
C	-2.846422	2.184374	0.733972
C	-4.285602	2.010557	1.221995
C	-1.986127	2.934276	1.746028

H	-2.400900	1.184555	0.677828
H	-4.851135	1.326476	0.583243
H	-4.263263	1.565264	2.221930
H	-4.830712	2.956756	1.281719
H	-0.958042	3.043824	1.384094
H	-2.384701	3.922956	1.993934
H	-1.946085	2.339796	2.665348
C	-2.599923	4.220608	-0.785777
C	-3.815264	5.031800	-0.323282
C	-2.190163	4.584567	-2.213501
H	-1.773745	4.519606	-0.131001
H	-4.032356	4.865203	0.733251
H	-3.587912	6.094930	-0.448329
H	-4.714352	4.813012	-0.901200
H	-1.336535	3.986974	-2.552369
H	-3.006439	4.438948	-2.926107
H	-1.904714	5.638349	-2.249260
C	-3.459635	2.021819	-1.675293
C	-4.893814	2.467151	-1.985562
H	-3.481762	0.975390	-1.355012
H	-2.878221	2.037336	-2.602752
H	-5.358007	1.709536	-2.622715
H	-5.505015	2.577173	-1.088166
H	-4.917749	3.410665	-2.533188
H	-1.321103	2.247313	-0.958213

Vibrational frequencies

-336.3246	4.5252	21.2079
33.1018	34.2658	35.7766
43.3347	51.4016	53.9304
56.4025	59.7008	63.3719
69.2097	71.3825	75.5319
78.1408	82.7624	85.0276
88.8144	95.0636	97.1148
103.0446	116.6711	120.4040
124.3153	128.9490	130.8494
141.1070	150.5333	153.0005
168.9806	177.5458	180.9922
191.7501	193.8886	202.5097
203.2634	206.5263	212.7479
224.3646	225.9539	240.2550
240.8295	241.7166	253.6887
262.5625	264.4090	273.5787
277.9892	280.2768	284.7005
290.5000	293.9881	301.7236

312.0170 318.4133 321.3733
336.7160 346.6426 348.2573
352.6732 359.7143 364.7135
372.8832 382.8275 387.4243
389.0772 395.1239 408.1371
416.9786 421.6378 423.1272
428.7495 437.5977 441.2984
446.1666 468.4625 483.7777
485.0815 493.0060 495.2824
502.9298 510.5492 513.2224
525.7391 529.6652 531.3327
536.8483 538.5798 547.6170
562.5913 588.2898 590.6375
602.2250 606.6496 611.9510
618.8603 623.6440 630.4042
641.1536 671.3279 675.5335
684.0375 700.8286 719.3470
721.9181 730.4195 734.1191
739.8463 748.6048 756.9016
758.1199 766.7279 770.4733
778.0824 780.5745 787.5506
794.0251 805.0476 812.7711
823.9192 831.0179 840.9716
851.4524 863.0866 865.1581
874.3744 880.7929 885.0139
891.6005 893.8128 903.0630
913.2082 916.2201 920.2962
928.5168 931.9059 935.4551
940.7131 953.0341 955.5772
960.0903 961.9754 964.5407
970.8095 973.4314 980.6256
989.4365 997.3077 1008.8638
1010.8973 1011.3461 1019.9189
1022.0567 1022.6284 1026.7579
1029.7526 1033.9251 1042.0377
1042.6721 1046.2432 1049.5917
1052.1565 1054.1831 1057.1454
1066.5140 1067.4963 1067.7306
1071.9881 1073.6228 1083.6583
1086.6927 1089.5580 1102.9968
1114.1437 1117.5507 1118.2555
1126.8001 1132.1747 1147.0976
1151.4951 1154.9922 1168.8399
1173.3077 1178.7572 1179.0937

1184.0377	1188.1402	1192.6526
1196.1139	1204.3302	1207.0968
1210.6747	1219.8152	1221.9755
1228.5037	1232.6392	1239.4297
1241.6416	1247.7045	1248.2159
1251.7397	1254.2870	1257.3422
1257.6614	1269.2848	1276.4883
1276.8793	1284.4983	1293.4162
1298.8431	1312.9751	1316.5939
1327.3752	1328.9287	1339.2766
1342.9454	1349.4415	1353.9964
1356.6148	1358.8200	1359.6133
1368.5908	1368.9536	1374.2758
1376.4756	1381.1749	1383.5471
1390.4661	1395.7308	1398.1594
1401.4645	1408.8429	1412.0655
1415.1191	1417.7016	1418.5887
1422.5717	1424.7960	1433.0751
1435.5885	1437.1658	1439.0683
1441.7864	1458.3406	1464.0920
1468.9898	1477.1034	1481.9008
1484.6827	1484.7752	1486.8067
1489.4533	1491.3827	1491.9174
1493.2470	1494.6146	1495.9854
1496.2597	1496.8434	1500.9275
1502.6488	1507.8224	1508.6197
1510.2441	1513.7522	1515.0360
1516.7556	1518.8233	1521.2100
1522.6363	1528.4098	1530.2842
1533.5083	1534.2143	1537.2579
1541.5536	1549.6107	1552.2452
1580.1395	1640.4764	1657.2430
1670.8743	1683.4817	1686.6053
1694.6532	1695.3915	1697.2077
1697.6048	1698.6604	1704.7580
1767.5008	1834.1931	2979.0439
3023.3859	3057.6355	3059.7557
3059.9100	3069.1095	3069.5761
3071.2750	3072.0589	3076.7796
3078.6872	3082.2066	3084.9070
3088.8641	3090.9952	3094.1874
3096.8051	3117.0907	3128.0836
3128.7772	3136.6618	3137.5417
3138.1969	3141.0624	3141.7851

3142.9939	3144.7609	3146.8217
3147.3446	3154.3440	3160.4103
3163.3062	3167.2811	3168.0005
3168.1864	3168.5929	3183.1628
3185.3594	3186.4753	3189.7225
3190.1249	3191.3037	3198.2841
3198.5637	3199.2681	3203.2607
3207.6201	3210.8544	3211.1110
3213.0686	3213.6678	3218.9061
3219.7081	3224.1293	3227.9503
3231.3501	3234.5847	3240.8630

M7a4

Zero-point correction= 1.022817
Thermal correction to Energy= 1.078253
Thermal correction to Enthalpy= 1.079197
Thermal correction to Gibbs Free Energy= 0.934834
Sum of electronic and zero-point Energies= -2568.070394
Sum of electronic and thermal Energies= -2568.014958
Sum of electronic and thermal Enthalpies= -2568.014014
Sum of electronic and thermal Free Energies= -2568.158378
Cartesian coordinates

C	-2.955014	-4.385105	0.561850
C	-1.964882	-3.425640	0.751333
C	-1.049345	-3.516838	1.795784
C	-1.139916	-4.603532	2.660717
C	-2.131571	-5.571750	2.478485
C	-3.045233	-5.469002	1.432294
C	-3.823154	-4.057087	-0.625117
H	-0.285058	-2.758403	1.947801
H	-0.435344	-4.693081	3.481407
H	-2.188671	-6.414574	3.159627
H	-3.811900	-6.225009	1.293817
H	-4.834501	-3.784214	-0.309102
C	-0.388729	-2.943174	-2.012173
C	-1.397116	-3.892922	-2.564075
C	-3.137970	-2.855738	-1.321634
C	-2.054335	-2.342623	-0.298589
C	0.288688	-1.342894	-0.700969
H	-1.131517	-4.171838	-3.583276
H	-2.345843	-1.382545	0.120274
N	0.813706	-2.662023	-2.422284
N	1.229727	-1.670024	-1.591033
N	-0.749524	-2.157994	-0.958540

C	2.587112	-1.206365	-1.758559
C	2.873051	-0.297880	-2.780154
C	3.570872	-1.834895	-0.982397
C	4.217818	0.032905	-2.965516
C	4.893374	-1.463067	-1.208105
C	5.233054	-0.528906	-2.192727
H	4.473583	0.739873	-3.751025
H	5.678001	-1.928941	-0.618237
O	-2.621802	-3.191394	-2.597998
H	-1.454517	-4.798083	-1.944116
H	-3.843465	-2.049693	-1.525234
H	-3.921204	-4.889070	-1.329687
C	1.817389	0.293875	-3.677671
H	1.673644	1.356170	-3.456515
H	0.849550	-0.195982	-3.569066
H	2.140867	0.213863	-4.718217
C	6.664992	-0.115436	-2.403745
H	6.851702	0.854855	-1.931586
H	6.889100	-0.008434	-3.467470
H	7.357165	-0.839963	-1.971414
C	3.205618	-2.892080	0.026154
H	2.675831	-3.720720	-0.454473
H	2.556239	-2.502244	0.818430
H	4.102266	-3.288740	0.504226
C	0.291055	-0.331444	0.427905
O	-0.702225	-0.289084	1.121514
C	1.528611	0.481248	0.774181
C	1.503286	0.785598	2.285294
H	2.412777	-0.123102	0.546162
H	2.374374	1.406611	2.512062
H	0.607965	1.367096	2.523711
C	1.552597	-0.468094	3.127246
C	0.445244	-0.889210	3.866771
C	2.720772	-1.237194	3.166750
C	0.500009	-2.056957	4.624911
H	-0.467751	-0.301456	3.836641
C	2.775359	-2.411747	3.912976
H	3.598122	-0.909129	2.610413
C	1.662910	-2.824614	4.644600
H	-0.369644	-2.370649	5.194093
H	3.687999	-2.999028	3.929804
H	1.704397	-3.736182	5.232387
N	-0.586335	2.228565	-0.745144
N	-0.504530	1.109426	-1.495527

C	-1.535099	1.023671	-2.378703
O	-2.368629	1.880054	-2.644198
O	-1.517435	-0.194442	-2.971111
C	-2.507452	-0.376654	-3.986537
H	-2.394635	0.377809	-4.767096
H	-2.345705	-1.376722	-4.381203
H	-3.509116	-0.299330	-3.556718
C	0.438254	2.622096	-0.041332
C	1.687293	1.791398	-0.094846
C	0.372671	3.827611	0.744004
C	2.920248	2.534352	0.366077
H	1.819765	1.462629	-1.131601
C	1.499933	4.350602	1.265865
H	-0.581906	4.328779	0.844332
C	4.176328	1.970279	0.161263
C	2.811956	3.749975	1.061031
H	1.451477	5.278158	1.828707
C	5.321945	2.604336	0.635195
H	4.257379	1.025894	-0.370953
C	3.969480	4.381717	1.533373
C	5.218781	3.813240	1.323202
H	6.295264	2.153617	0.470257
H	3.877490	5.323657	2.066335
H	6.110026	4.307904	1.693696
H	-1.512376	2.717414	-0.644439
N	-3.199881	3.234480	0.393872
C	-3.361691	4.670418	0.074684
C	-4.317652	5.472126	0.969166
C	-3.683404	4.875219	-1.404427
H	-2.367127	5.112893	0.236308
H	-3.983595	5.475255	2.009757
H	-4.336806	6.512117	0.629196
H	-5.339529	5.087757	0.936190
H	-3.028871	4.266905	-2.035302
H	-4.721412	4.617044	-1.635428
H	-3.541488	5.928418	-1.659301
C	-4.184425	2.301970	-0.197285
C	-5.664451	2.504086	0.165857
C	-3.759299	0.855903	0.061729
H	-4.101298	2.443805	-1.276653
H	-6.042205	3.459888	-0.203288
H	-6.253455	1.717079	-0.316595
H	-5.853005	2.451988	1.239455
H	-2.689505	0.723871	-0.124455

H	-3.962556	0.530890	1.087205
H	-4.313848	0.196961	-0.613908
C	-2.798315	2.971936	1.783914
C	-3.869465	2.769526	2.864708
H	-2.173293	3.817668	2.090886
H	-2.140775	2.090004	1.787845
H	-3.376122	2.735952	3.840844
H	-4.601706	3.578851	2.882646
H	-4.407736	1.827929	2.740244

Vibrational frequencies

21.1011	24.6662	27.3106
30.7314	34.2462	38.7450
45.5035	49.4597	53.6234
54.7370	65.2969	69.3991
71.9374	73.1885	76.3040
81.7017	89.4492	92.0522
92.7322	101.6242	103.2392
108.8967	111.8557	118.4554
123.5188	134.2405	143.6924
144.7598	151.0338	160.4783
167.5601	170.8610	174.2518
182.7763	189.6820	200.5595
203.9537	205.4429	216.7604
220.6056	231.7463	234.5191
237.4897	242.7550	243.9707
252.0839	257.5831	267.3110
274.0548	279.9053	283.7573
286.4960	288.2270	299.2777
302.6854	308.0747	318.3440
323.1483	333.9466	338.5309
351.4043	352.2239	354.0672
360.5413	365.2736	378.3238
389.3455	393.5512	405.0445
410.2802	419.3303	421.0789
425.8124	434.3021	443.3171
447.6213	456.7540	487.1428
489.3893	498.0206	502.6593
507.1380	516.5973	520.3322
525.3242	530.3448	537.4852
549.9380	557.4861	567.1604
567.6576	588.2497	595.4277
598.4683	602.8856	611.0288
613.5334	625.5643	631.4449
634.4878	639.2203	660.6697

690.2828 699.3329 714.8183
719.3603 722.7289 723.7476
735.8575 748.8079 755.5054
765.4176 775.3052 776.4737
777.1015 779.9536 791.3124
795.6989 796.8635 807.3439
815.9994 835.4877 836.4209
863.4682 865.9222 866.5789
876.0474 879.5230 884.4229
886.6664 889.2351 896.4880
913.1670 922.8334 925.2701
926.1355 929.3473 938.8226
941.3340 957.1551 962.4495
963.3009 963.6043 969.5902
971.3609 981.3729 986.2657
988.5322 996.6366 998.4716
1006.6798 1017.4089 1017.7780
1020.8728 1027.2938 1027.9927
1028.8666 1031.4534 1033.7771
1035.6146 1038.1939 1053.0189
1054.9450 1060.6094 1063.0926
1065.0008 1068.3611 1068.9676
1069.8374 1076.9716 1079.0861
1084.6530 1084.8471 1112.9480
1115.6688 1123.3032 1123.5719
1129.8118 1130.0555 1146.0282
1155.4724 1157.4158 1163.3453
1166.6282 1177.8002 1181.7225
1190.4013 1190.7344 1193.3179
1194.6108 1198.6166 1202.8369
1206.1204 1206.8946 1209.0998
1214.3351 1219.0838 1226.9378
1233.8995 1243.1410 1248.1489
1251.2229 1254.1702 1254.2998
1263.2461 1266.0810 1268.5578
1283.1894 1284.9224 1285.2126
1305.9937 1309.7120 1316.4044
1327.9139 1329.6748 1338.9577
1344.2459 1349.0149 1349.7146
1352.4694 1354.7501 1359.2109
1361.2094 1364.7437 1368.8600
1373.2688 1375.5951 1379.5539
1382.8572 1385.1067 1395.7530
1404.3174 1406.6117 1410.6613

1413.5963	1418.3293	1423.1664
1425.7727	1431.3317	1433.8431
1438.2613	1441.3174	1443.1892
1463.6038	1465.0404	1467.4422
1478.4582	1480.6167	1483.4742
1483.9306	1489.3644	1490.8540
1491.5769	1493.2157	1494.0893
1495.8036	1497.4129	1498.9019
1502.0175	1502.6940	1506.3639
1506.8805	1507.8525	1512.6364
1513.9024	1515.7033	1516.8270
1520.2594	1524.5761	1524.8804
1526.8030	1532.6052	1538.5746
1539.6929	1541.5690	1550.4030
1552.1243	1553.9101	1583.8169
1653.6551	1674.3547	1681.9806
1686.0479	1689.0617	1689.9903
1693.5538	1698.6590	1704.3765
1707.4884	1727.7002	1769.3446
1824.4562	3011.2678	3036.4997
3043.9935	3066.6451	3067.9767
3072.6118	3075.0489	3075.9181
3076.7832	3077.1360	3080.6217
3081.2164	3087.8503	3094.3676
3098.8600	3109.3038	3112.6702
3128.3576	3131.9185	3134.3444
3135.2210	3147.3788	3147.9074
3148.4053	3148.5634	3153.0255
3153.2502	3154.2956	3157.6584
3158.6600	3162.9722	3164.8859
3170.8254	3171.1501	3176.2157
3176.8881	3177.7519	3178.6868
3188.5499	3194.2355	3195.3646
3200.2568	3202.2058	3205.3437
3206.0763	3210.1078	3211.5334
3213.8738	3218.2381	3218.6784
3220.1179	3221.4288	3222.8133
3227.7964	3229.8735	3236.3042
3236.9542	3240.4511	3261.4139

TS8a4

Zero-point correction= 1.020265

Thermal correction to Energy= 1.075576

Thermal correction to Enthalpy= 1.076520

Thermal correction to Gibbs Free Energy= 0.929442
Sum of electronic and zero-point Energies= -2568.032529
Sum of electronic and thermal Energies= -2567.977219
Sum of electronic and thermal Enthalpies= -2567.976274
Sum of electronic and thermal Free Energies= -2568.123353
Cartesian coordinates

C	-6.307954	0.501000	0.766182
C	-5.087100	0.690243	0.112249
C	-4.394531	1.892964	0.218666
C	-4.937772	2.902059	1.013819
C	-6.154089	2.713948	1.672860
C	-6.851805	1.514411	1.547589
C	-6.868060	-0.872537	0.502179
H	-3.468074	2.050228	-0.327094
H	-4.413535	3.847352	1.105052
H	-6.565459	3.514005	2.280315
H	-7.804663	1.373638	2.049025
H	-7.938517	-0.871080	0.285537
C	-3.928271	-2.636562	0.505747
C	-5.221247	-3.343645	0.242922
C	-6.042162	-1.340072	-0.715012
C	-4.703931	-0.553631	-0.658095
C	-2.407772	-1.027767	0.324765
H	-5.012177	-4.378171	-0.033763
H	-4.288576	-0.353514	-1.645873
N	-2.873287	-3.127508	1.087526
N	-1.958757	-2.117815	0.969099
N	-3.699034	-1.359645	0.064678
C	-0.659018	-2.235843	1.558342
C	0.342467	-2.949041	0.897507
C	-0.423402	-1.511217	2.739187
C	1.648529	-2.818223	1.384388
C	0.886800	-1.434917	3.197371
C	1.940936	-2.047225	2.508254
H	2.455081	-3.327348	0.860933
H	1.102135	-0.850592	4.088760
O	-5.872715	-2.738058	-0.853985
H	-5.851275	-3.352532	1.139457
H	-6.552056	-1.024075	-1.627654
H	-6.715685	-1.517119	1.374905
C	0.062887	-3.816976	-0.300599
H	0.705770	-3.547461	-1.143582
H	-0.980369	-3.754268	-0.615014
H	0.272199	-4.861791	-0.054310

C	3.356205	-1.861473	2.985934
H	3.573205	-0.796773	3.123356
H	4.075034	-2.270470	2.272702
H	3.511351	-2.354655	3.950296
C	-1.547646	-0.799733	3.446272
H	-2.378140	-1.484008	3.643280
H	-1.949305	0.020481	2.841011
H	-1.200193	-0.389032	4.395358
C	-1.442464	0.178814	-1.067565
O	-2.316872	0.569329	-1.821676
C	-0.561092	1.155998	-0.271962
C	-0.192440	2.366910	-1.164197
H	-1.160608	1.500184	0.574588
H	0.690614	2.840015	-0.717734
H	0.098934	2.018618	-2.161130
C	-1.289717	3.396968	-1.280099
C	-2.062883	3.509872	-2.436454
C	-1.545226	4.259716	-0.210181
C	-3.077765	4.459102	-2.520775
H	-1.878659	2.832922	-3.264974
C	-2.553818	5.216298	-0.294594
H	-0.941580	4.186483	0.692590
C	-3.326607	5.314622	-1.450104
H	-3.674602	4.530494	-3.424464
H	-2.735342	5.885985	0.540743
H	-4.115944	6.056398	-1.516647
N	0.754530	-0.765301	-1.761594
N	-0.589694	-1.005561	-1.564439
C	-1.087303	-1.920395	-2.496279
O	-0.388254	-2.436285	-3.342356
O	-2.359634	-2.175095	-2.261621
C	-2.983525	-3.148814	-3.115328
H	-2.482228	-4.111746	-3.005491
H	-4.013294	-3.202126	-2.764459
H	-2.938944	-2.819006	-4.153416
C	1.466428	-0.104390	-0.891628
C	0.710852	0.459470	0.264012
C	2.869891	0.074489	-1.072735
C	1.546525	1.281653	1.209644
H	0.363662	-0.421460	0.820413
C	3.558158	0.793089	-0.151677
H	3.362955	-0.380382	-1.926208
C	0.971339	1.865146	2.336725
C	2.930610	1.416940	0.998438

H	4.643383	0.878782	-0.264836
C	1.754736	2.582929	3.236476
H	-0.092822	1.753317	2.526160
C	3.710620	2.145874	1.909119
C	3.126910	2.727736	3.023834
H	1.291590	3.031116	4.109068
H	4.777029	2.246576	1.726361
H	3.731793	3.290705	3.725656
N	6.747473	0.212857	-0.623431
C	6.952457	-0.899058	0.323155
C	6.073008	-2.107663	-0.002533
C	6.635243	-0.436890	1.747589
H	8.001907	-1.241990	0.303455
H	6.360802	-2.608322	-0.929605
H	6.161915	-2.840884	0.803731
H	5.020473	-1.807164	-0.077691
H	7.284253	0.372693	2.088384
H	5.596150	-0.092007	1.804091
H	6.753564	-1.270835	2.444782
C	6.719219	-0.177356	-2.045900
C	8.023208	-0.764208	-2.602206
C	6.225409	0.961393	-2.939818
H	5.954780	-0.958443	-2.112120
H	8.429681	-1.540374	-1.946258
H	7.843277	-1.212141	-3.584221
H	8.782606	0.013088	-2.728769
H	5.343504	1.447170	-2.510311
H	6.991388	1.723734	-3.107461
H	5.953368	0.558745	-3.919483
C	7.564002	1.393390	-0.307584
C	9.052821	1.174804	-0.010791
H	7.113866	1.897185	0.557069
H	7.464676	2.097735	-1.135837
H	9.533816	2.144814	0.142577
H	9.207253	0.585254	0.897239
H	9.568443	0.668188	-0.828874
H	1.132810	-1.197645	-2.608063

Vibrational frequencies

-180.0431	14.0475	16.3523
21.2112	24.3926	30.6969
33.3722	36.1606	40.1797
42.2646	48.4060	51.1905
54.3128	58.5101	62.3113
67.6637	72.4053	80.3454

84.2906	92.8934	99.3866
100.7247	107.4514	111.3712
118.8357	123.9769	130.0048
132.6607	148.2418	159.4597
161.1661	163.4838	177.3046
181.2731	194.3501	196.1647
200.6589	207.4332	216.8522
220.6437	221.6029	229.5001
233.1733	238.6104	240.4793
253.1842	254.5656	257.3425
271.5498	275.9807	280.9815
287.7441	296.9466	298.6146
301.7232	320.1953	324.3604
327.4978	338.8402	339.1061
346.4682	353.7972	358.0216
364.1248	367.7452	381.4131
400.3064	407.9972	411.1467
413.3079	422.1535	432.1029
438.6008	440.6638	455.6091
456.2471	467.6625	479.0956
479.2658	494.2732	503.0304
506.9811	510.5924	516.6209
519.6840	528.7909	530.6097
534.7335	537.9138	544.1044
569.4461	582.1603	591.0552
596.3162	598.8809	605.2098
606.7670	622.2367	625.2526
630.1176	631.8257	642.8915
655.6234	679.6987	709.9363
710.7381	715.8838	718.0044
730.9219	736.7111	748.0831
757.2703	760.4544	766.3433
771.6101	777.3897	781.1449
785.1444	797.7083	804.7553
810.8517	818.6994	830.7658
849.9565	853.1771	865.9267
867.3391	868.9548	883.9832
886.7682	900.6127	901.5792
903.7827	907.6350	918.9608
921.6177	930.3852	936.1587
938.0042	940.4127	943.8562
953.3815	962.4264	969.6202
970.4224	974.2816	981.0128
994.4871	996.1282	1006.4813

1008.2277	1011.9579	1018.4355
1020.4154	1021.7281	1025.2009
1030.3504	1031.7307	1040.4604
1044.8233	1046.6390	1056.7989
1057.7304	1062.3882	1065.3120
1066.5598	1068.3434	1070.4405
1075.4710	1076.2197	1085.9060
1089.8389	1098.9214	1106.7038
1112.2401	1115.4398	1120.7233
1135.8948	1138.5029	1140.4181
1146.4064	1160.0413	1166.5901
1169.3064	1176.6334	1179.0132
1187.0919	1188.3591	1189.6696
1190.1311	1193.6204	1198.8941
1203.1731	1205.0558	1207.7733
1208.2122	1224.3527	1231.0593
1240.9001	1241.3018	1247.3026
1248.0936	1253.4339	1260.9423
1262.9651	1268.0158	1276.5645
1277.9117	1278.8261	1285.0883
1302.5626	1314.9558	1317.8777
1323.1659	1327.5296	1333.0995
1335.7934	1342.6226	1351.4405
1355.1721	1360.4913	1360.9735
1366.7878	1369.2987	1370.0118
1371.7266	1372.8674	1374.1506
1380.8403	1383.1427	1385.6021
1391.5719	1394.6238	1397.3643
1409.4849	1411.0190	1420.0715
1420.3670	1422.4440	1423.3990
1425.6781	1427.6908	1433.7018
1434.3150	1458.1948	1467.0976
1478.1613	1478.3562	1485.0473
1485.5752	1486.2198	1488.2686
1488.6505	1489.7963	1490.4335
1492.0100	1495.6384	1497.8546
1500.5314	1502.3079	1503.5776
1503.9056	1506.3848	1506.6101
1508.6948	1511.1495	1511.4736
1513.4757	1518.0820	1518.1465
1521.5547	1522.6640	1523.0217
1526.6627	1536.4767	1539.4638
1550.3947	1555.3046	1560.9487
1635.9229	1676.3438	1679.1575

1679.6724	1680.1220	1686.2579
1693.3326	1696.8770	1700.2963
1703.8253	1727.8667	1744.2927
1840.7687	2999.0486	3057.1053
3060.0062	3063.9300	3065.1823
3065.3146	3067.1727	3068.5014
3069.7128	3074.9190	3080.1905
3082.3155	3084.2702	3094.9652
3095.9347	3097.5355	3116.2442
3130.8716	3137.1039	3138.0956
3138.5930	3138.7850	3139.1879
3139.2310	3142.6812	3144.2410
3145.1687	3150.0752	3150.7125
3151.0840	3151.1437	3153.4660
3158.8763	3160.7676	3171.1078
3174.8381	3178.9157	3179.6982
3180.4571	3181.3888	3181.4724
3195.0345	3202.5623	3203.0153
3203.3273	3206.4237	3206.9441
3209.3252	3209.4174	3210.3492
3216.9770	3217.9601	3221.1117
3222.1306	3222.5420	3229.3817
3231.6871	3235.7692	3476.2648

TS8a5

Zero-point correction= 1.018954

Thermal correction to Energy= 1.072968

Thermal correction to Enthalpy= 1.073913

Thermal correction to Gibbs Free Energy= 0.934894

Sum of electronic and zero-point Energies= -2568.035779

Sum of electronic and thermal Energies= -2567.981765

Sum of electronic and thermal Enthalpies= -2567.980820

Sum of electronic and thermal Free Energies= -2568.119839

Cartesian coordinates

C	-5.876386	1.172210	-1.188044
C	-4.588653	1.282930	-0.670497
C	-4.196990	2.379358	0.092103
C	-5.138023	3.376280	0.338507
C	-6.433759	3.273481	-0.175610
C	-6.811751	2.174548	-0.944335
C	-6.038473	-0.094186	-1.989191
H	-3.177193	2.446361	0.459782
H	-4.862673	4.242369	0.931256
H	-7.154581	4.059384	0.026326

H	-7.819388	2.098199	-1.341413
H	-6.091361	0.126738	-3.060016
C	-3.802882	-1.307516	0.964647
C	-5.178197	-1.707452	0.542218
C	-4.776854	-0.932378	-1.679983
C	-3.750244	0.085469	-1.059674
C	-1.832605	-0.454791	0.559367
H	-5.493629	-2.599991	1.081188
H	-2.965975	0.362699	-1.763799
N	-3.055290	-1.729152	1.941924
N	-1.831480	-1.176133	1.683710
N	-3.100881	-0.503246	0.118266
C	-0.797968	-1.361850	2.668355
C	-0.033357	-2.535510	2.609219
C	-0.672622	-0.418823	3.688443
C	0.953874	-2.700464	3.573377
C	0.349112	-0.621954	4.620898
C	1.174676	-1.741951	4.571666
H	1.569824	-3.595800	3.548532
H	0.482210	0.107997	5.413208
O	-5.060938	-2.037385	-0.832001
H	-5.902578	-0.901416	0.713194
H	-4.357065	-1.381841	-2.581560
H	-6.936681	-0.663142	-1.731046
C	-0.303716	-3.579332	1.559630
H	-0.260178	-3.160036	0.550042
H	-1.310640	-3.992046	1.682501
H	0.414406	-4.397443	1.636164
C	2.278610	-1.945630	5.575793
H	3.252227	-2.014564	5.070066
H	2.127908	-2.883709	6.129177
H	2.318761	-1.118985	6.295748
C	-1.628879	0.734468	3.861507
H	-2.350166	0.491870	4.646113
H	-2.194312	0.966573	2.956669
H	-1.091962	1.634196	4.170183
C	-0.784650	0.372922	-0.224500
O	-1.328674	1.448043	-0.638770
C	0.626033	0.500670	0.428545
C	0.575254	1.697182	1.431362
H	0.819463	-0.408233	1.007111
H	-0.464713	1.783008	1.764097
H	1.155746	1.427305	2.319507
C	1.034556	3.072099	0.972721

C	1.973009	3.762120	1.749297
C	0.558301	3.687097	-0.189341
C	2.447250	5.013077	1.367440
H	2.359263	3.296906	2.653169
C	1.037448	4.936981	-0.577093
H	-0.178969	3.166094	-0.789205
C	1.985953	5.603762	0.192838
H	3.185690	5.519910	1.981321
H	0.664955	5.390188	-1.489392
H	2.360123	6.575128	-0.113369
N	0.205530	0.193494	-2.436259
N	-0.428378	-0.618642	-1.525735
C	-1.082525	-1.664562	-2.125610
O	-1.067998	-1.889339	-3.321861
O	-1.700827	-2.436953	-1.218388
C	-2.348820	-3.608841	-1.732049
H	-1.599304	-4.347017	-2.024237
H	-2.963818	-3.979397	-0.914675
H	-2.969113	-3.357479	-2.592350
C	1.230257	0.917321	-2.002649
C	1.736304	0.639778	-0.674014
C	1.832704	1.880016	-2.876633
C	2.954318	1.390453	-0.290071
H	2.336725	-0.557034	-0.913479
C	2.916216	2.572070	-2.448629
H	1.395812	2.054856	-3.854159
C	3.616781	1.108578	0.916536
C	3.531670	2.331812	-1.169049
H	3.363331	3.320095	-3.097783
C	4.797444	1.753379	1.245124
H	3.196135	0.376434	1.601979
C	4.718431	2.996860	-0.811009
C	5.350284	2.712068	0.383748
H	5.295646	1.516918	2.180036
H	5.139240	3.724808	-1.499003
H	6.270835	3.219110	0.651181
N	3.068177	-1.765059	-1.321859
C	3.779712	-1.273500	-2.548301
C	4.044414	-2.322335	-3.631189
C	5.069663	-0.514541	-2.229060
H	3.075304	-0.549205	-2.982729
H	3.124841	-2.781927	-3.998181
H	4.520065	-1.821195	-4.478457
H	4.719703	-3.112347	-3.289653

H	4.959159	0.194746	-1.407939
H	5.893895	-1.193177	-1.996518
H	5.354319	0.052610	-3.119096
C	3.929998	-2.188982	-0.178522
C	4.901622	-3.345319	-0.443331
C	3.072840	-2.478755	1.048100
H	4.532044	-1.305794	0.051944
H	5.533462	-3.165478	-1.313929
H	5.559709	-3.436631	0.425690
H	4.392523	-4.300619	-0.573859
H	2.353512	-1.677460	1.237783
H	2.518296	-3.416022	0.949436
H	3.715117	-2.565189	1.929470
C	1.914962	-2.643654	-1.637470
C	2.121992	-4.149570	-1.800320
H	1.471681	-2.231362	-2.551194
H	1.174922	-2.482068	-0.848814
H	1.206158	-4.562085	-2.232510
H	2.950233	-4.404814	-2.461232
H	2.280828	-4.646638	-0.841182
H	-0.254030	0.361299	-3.325854

Vibrational frequencies

-1372.0229	20.0246	25.3226
31.1109	33.5659	39.1443
46.1274	48.8605	57.1825
59.0403	64.0729	71.7836
81.9962	83.1369	88.7694
95.7936	96.5607	99.0474
103.3953	112.5325	113.7045
120.0473	124.5150	129.4260
133.7107	148.6822	152.3668
158.3948	167.3357	171.9312
181.5739	189.2759	197.0048
198.7719	201.9162	208.3687
218.4081	219.8882	225.7443
227.0090	231.0300	238.0388
246.4664	247.7726	253.1896
263.0933	265.7098	271.0820
272.4669	284.6646	286.1279
288.9477	291.3310	296.9532
301.3319	313.7218	322.1808
329.6667	333.7607	336.1945
348.9379	355.1280	357.5622
359.8378	369.4252	373.4246

391.5890 403.5048 411.6503
414.9193 425.7272 428.2977
429.3162 438.8243 449.1353
451.4600 473.6703 482.8205
489.2877 491.4374 496.1444
499.2947 511.1043 514.7645
518.0466 527.0848 534.7788
538.8316 547.3061 558.3964
567.2354 571.0984 583.8340
594.3729 597.8544 601.8448
608.4048 621.3825 625.9243
631.0099 644.0838 665.6285
684.5758 689.6523 703.7249
710.6530 719.5371 724.8502
729.5463 740.4026 744.1868
751.2412 755.0334 763.8818
773.7545 775.9433 780.2161
781.7550 786.8090 803.4551
815.4519 821.5312 826.7547
837.9237 845.3232 856.3262
859.3328 873.1495 878.7753
879.1322 881.8085 889.5608
899.8639 901.7370 914.4623
921.9875 927.1512 934.4410
936.5692 944.2859 953.7070
959.7920 961.3528 966.6197
970.2347 971.7852 972.7713
979.3037 991.1645 999.4790
1002.2992 1004.9375 1006.2797
1008.5722 1018.5223 1019.4225
1024.6132 1024.8995 1027.4824
1034.7505 1042.1130 1044.2052
1050.4707 1052.0375 1052.4569
1058.1942 1062.4575 1065.2639
1065.9836 1072.6814 1077.4589
1079.9775 1089.8865 1091.9560
1105.2355 1117.3306 1118.3050
1119.7982 1127.0061 1135.2209
1145.9861 1150.4510 1151.1288
1169.3131 1172.7823 1174.1861
1178.8038 1181.9070 1187.8199
1190.0490 1193.3403 1197.0984
1203.4701 1204.0382 1206.8454
1211.4731 1225.7695 1227.6130

1233.7712	1238.1229	1241.3935
1242.2804	1246.5966	1247.8811
1259.7897	1264.2491	1276.7256
1277.0816	1289.3365	1291.8487
1296.0523	1309.1036	1311.7844
1324.7017	1331.3424	1335.7328
1336.6313	1345.2015	1353.2008
1356.4807	1358.9337	1362.4918
1370.6838	1373.4539	1376.3615
1377.0490	1380.1468	1384.9595
1389.4162	1396.3967	1405.9079
1410.9030	1414.9181	1417.3154
1419.9986	1421.6262	1422.5183
1424.1715	1432.6993	1435.5419
1441.3225	1447.4914	1455.8214
1465.7929	1468.5871	1471.5103
1471.7223	1478.0827	1485.3071
1487.5430	1489.1044	1490.8231
1493.7551	1494.8490	1495.0722
1496.4692	1497.0178	1498.2807
1498.5926	1502.7212	1505.8288
1506.3911	1507.3570	1508.7630
1511.0607	1511.3195	1515.4341
1517.6819	1518.8628	1521.4680
1522.7402	1525.6542	1526.3832
1529.8887	1531.6294	1537.8111
1540.0969	1541.2520	1548.9575
1560.6148	1580.6584	1629.7497
1649.8984	1672.8540	1683.1294
1686.2132	1692.4123	1693.4735
1696.2386	1696.8754	1697.1788
1705.7274	1805.5348	3026.6250
3063.6301	3074.3693	3077.0943
3078.7254	3081.5603	3083.1771
3085.7472	3087.7824	3088.5741
3090.2634	3092.3138	3095.7631
3096.5543	3102.1745	3108.6085
3119.8172	3129.4697	3132.9549
3137.4595	3141.3246	3146.5181
3147.2227	3153.2298	3155.0959
3157.0671	3160.3787	3162.8881
3167.4129	3170.0805	3171.2436
3171.4290	3174.4515	3183.1426
3185.9823	3190.6736	3191.0359

3194.2964	3194.5899	3197.2246
3201.3146	3202.3259	3208.5364
3211.1570	3211.9166	3211.9778
3213.5365	3215.5182	3220.2245
3221.8136	3221.8935	3223.2067
3224.9689	3231.7375	3232.4221
3241.5837	3242.3454	3584.4745

M8a5

Zero-point correction= 0.742005
Thermal correction to Energy= 0.784044
Thermal correction to Enthalpy= 0.784988
Thermal correction to Gibbs Free Energy= 0.666703
Sum of electronic and zero-point Energies= -2197.024109
Sum of electronic and thermal Energies= -2196.982070
Sum of electronic and thermal Enthalpies= -2196.981126
Sum of electronic and thermal Free Energies= -2197.099411
Cartesian coordinates

C	5.685697	0.332262	-0.327736
C	4.330711	0.655806	-0.312877
C	3.863358	1.869811	-0.805739
C	4.792764	2.764438	-1.333560
C	6.153526	2.447886	-1.355082
C	6.610972	1.232012	-0.849266
C	5.921982	-1.029132	0.277224
H	2.802190	2.095182	-0.748089
H	4.457375	3.718370	-1.727704
H	6.862857	3.156557	-1.770903
H	7.669069	0.988334	-0.868894
H	6.337411	-0.937320	1.286549
C	2.579021	-1.453151	-1.745469
C	3.935328	-2.040276	-1.970915
C	4.523085	-1.677471	0.334532
C	3.520201	-0.472113	0.292740
C	1.071022	-0.504889	-0.470186
H	3.880578	-2.846065	-2.702645
H	3.134504	-0.215240	1.279632
N	1.479212	-1.532721	-2.431485
N	0.548681	-0.920609	-1.626140
N	2.376487	-0.819281	-0.554386
C	-0.788852	-0.763301	-2.132309
C	-1.633619	-1.871720	-2.142237
C	-1.157135	0.493741	-2.623240
C	-2.930175	-1.677721	-2.620191

C	-2.461400	0.634548	-3.089135
C	-3.360886	-0.436116	-3.084603
H	-3.625285	-2.513679	-2.602084
H	-2.787888	1.605676	-3.452677
O	4.327003	-2.604078	-0.730986
H	4.643367	-1.279364	-2.322856
H	4.375705	-2.269404	1.238745
H	6.603323	-1.657887	-0.302868
C	-1.162208	-3.220387	-1.670180
H	-0.470520	-3.130981	-0.828082
H	-0.639572	-3.742826	-2.478146
H	-2.011011	-3.829482	-1.353923
C	-4.771038	-0.247313	-3.578232
H	-5.137170	0.753749	-3.337157
H	-5.444650	-0.977695	-3.124277
H	-4.822116	-0.367253	-4.665518
C	-0.177305	1.638847	-2.625419
H	0.701208	1.392877	-3.231829
H	0.179549	1.869495	-1.614051
H	-0.640317	2.537760	-3.035605
C	0.552952	0.346005	0.744927
O	1.242864	1.436928	0.768183
C	-0.998027	0.522822	0.774577
C	-1.360669	1.602384	1.842159
H	-1.280568	0.923772	-0.202414
H	-2.149553	1.212143	2.492785
H	-0.474855	1.781870	2.457942
C	-1.814360	2.920753	1.255200
C	-0.955966	3.666252	0.437896
C	-3.095830	3.417154	1.508323
C	-1.377178	4.871745	-0.116869
H	0.043889	3.274666	0.264862
C	-3.518253	4.625609	0.956091
H	-3.773096	2.843123	2.136743
C	-2.659841	5.356043	0.138961
H	-0.700191	5.440588	-0.747866
H	-4.518551	4.993797	1.163474
H	-2.986782	6.296466	-0.293924
N	0.270934	-1.914160	1.620770
N	0.861755	-0.669350	1.899572
C	0.946577	-0.267782	3.216971
O	1.413334	0.778867	3.614789
O	0.526267	-1.247926	4.051964
C	0.687965	-0.950132	5.439459

H	0.098653	-0.072934	5.711327
H	0.331274	-1.829343	5.972684
H	1.737703	-0.760780	5.670790
C	-1.129040	-1.901026	1.466779
C	-1.762075	-0.769501	0.996529
C	-1.831590	-3.118469	1.675200
C	-3.159703	-0.846022	0.693369
H	0.610684	-2.620325	2.262991
C	-3.161376	-3.201373	1.382309
H	-1.289697	-3.981424	2.053037
C	-3.881729	0.263032	0.175561
C	-3.859602	-2.074136	0.867631
H	-3.701526	-4.131413	1.536104
C	-5.211815	0.153538	-0.153037
H	-3.376003	1.209948	0.022030
C	-5.230904	-2.158528	0.518189
C	-5.898832	-1.069774	0.014643
H	-5.738158	1.015831	-0.551831
H	-5.743217	-3.107041	0.657630
H	-6.948370	-1.143362	-0.251825

Vibrational frequencies

10.4750	16.5126	26.2665
27.9544	34.3606	42.2463
43.4651	55.0949	59.0294
64.1084	75.2360	82.2409
91.5885	100.4059	109.9457
115.8354	132.3938	138.7730
143.5158	153.1364	155.7614
161.8538	170.3056	174.6482
180.7892	188.3972	200.7373
206.7194	212.4358	225.7482
231.6476	237.4886	245.1740
258.7507	260.5414	273.2104
280.5903	286.1943	304.0782
307.4108	325.1278	334.0309
348.7993	364.2096	375.0490
392.5142	394.5037	402.2918
410.4604	417.2039	420.9312
424.9363	438.6508	445.3418
464.0614	481.8643	493.4657
497.0204	505.9284	509.1830
513.4347	521.6662	529.6791
534.4429	536.4657	554.3115
565.3525	581.8743	586.5999

589.7236 597.7778 608.2262
617.1785 621.2092 628.1668
633.9744 641.1008 661.2945
690.6312 712.8182 718.8376
725.0165 733.3195 738.7583
745.8916 754.1802 759.8287
768.6831 771.4286 778.6648
779.3934 792.1240 796.6848
802.6223 813.1451 827.7411
833.4894 841.0620 848.5786
863.7257 875.4809 879.3688
889.4359 894.2755 895.5719
905.0272 914.0011 924.0631
935.4004 952.2325 958.1380
966.4599 969.2340 969.7351
984.0480 987.7681 988.2001
999.1316 1012.1552 1014.3660
1016.8337 1018.9330 1031.0186
1034.3882 1039.6901 1044.1916
1045.7395 1050.0411 1055.0805
1060.5022 1064.3759 1065.0541
1067.5268 1068.1482 1071.1878
1071.6562 1072.9513 1097.3557
1112.8670 1113.2645 1118.4452
1129.1758 1146.8403 1159.4130
1169.8501 1170.4941 1179.0637
1188.3552 1191.3236 1193.2769
1198.1202 1201.6556 1204.0112
1210.1274 1214.6345 1222.1467
1231.1168 1232.3952 1240.2347
1246.1729 1246.6416 1263.2577
1273.4549 1275.1643 1282.8159
1283.5393 1290.7046 1299.5128
1306.1379 1318.1377 1318.6129
1329.7071 1338.8497 1341.8462
1351.6654 1353.1130 1356.1078
1367.8050 1370.7167 1375.1310
1376.9306 1397.6593 1412.0145
1416.6788 1421.0295 1427.2254
1427.8993 1436.6777 1456.9464
1466.6305 1468.6265 1471.8215
1475.6031 1476.8384 1485.3675
1488.0157 1494.5381 1499.5345
1500.3754 1502.2268 1503.1238

1505.8806	1507.2206	1514.2373
1516.6560	1518.2789	1521.8185
1523.9278	1529.9130	1535.4822
1540.5972	1544.9553	1578.1229
1584.1676	1672.5559	1674.6282
1679.9836	1689.3974	1692.2671
1695.2533	1695.9112	1698.6578
1699.7772	1717.6661	1829.1267
3057.2917	3069.0116	3076.9505
3080.9366	3085.7273	3085.9508
3097.4162	3124.1539	3126.1015
3139.6635	3141.5162	3144.6087
3149.5515	3157.0602	3164.6868
3165.5829	3175.7885	3183.5846
3184.6884	3184.8912	3188.8253
3189.4471	3192.0492	3194.2763
3197.9943	3199.8065	3202.6268
3205.5124	3205.9361	3206.8019
3211.3715	3212.2490	3216.0183
3220.1498	3222.0822	3225.4205
3238.1161	3240.0544	3611.9109

TS6b

Zero-point correction= 0.740531
Thermal correction to Energy= 0.782601
Thermal correction to Enthalpy= 0.783545
Thermal correction to Gibbs Free Energy= 0.665150
Sum of electronic and zero-point Energies= -2196.992009
Sum of electronic and thermal Energies= -2196.949939
Sum of electronic and thermal Enthalpies= -2196.948995
Sum of electronic and thermal Free Energies= -2197.067390
Cartesian coordinates

C	-5.183672	0.908171	-0.664584
C	-3.795981	1.020243	-0.673382
C	-3.168534	2.255852	-0.809194
C	-3.964217	3.391631	-0.936156
C	-5.357620	3.286238	-0.932205
C	-5.976388	2.045350	-0.799002
C	-5.615318	-0.527085	-0.508760
H	-2.084518	2.328583	-0.824053
H	-3.497814	4.366271	-1.038848
H	-5.963551	4.181568	-1.029329
H	-7.059407	1.966820	-0.791125
H	-6.030931	-0.911942	-1.445576

C	-2.506628	-0.452995	1.873472
C	-3.936683	-0.765122	2.162478
C	-4.330680	-1.303575	-0.134531
C	-3.146363	-0.336681	-0.502728
C	-0.814637	-0.109949	0.549497
H	-4.034073	-1.198137	3.157459
H	-2.637939	-0.679876	-1.403075
N	-1.483955	-0.346585	2.671057
N	-0.437096	-0.117824	1.827256
N	-2.143547	-0.295548	0.569722
C	0.864294	0.175368	2.358065
C	1.677734	-0.891961	2.743567
C	1.252096	1.516266	2.427832
C	2.966262	-0.576755	3.172884
C	2.552693	1.776121	2.857640
C	3.422456	0.743497	3.219778
H	3.634371	-1.383723	3.463286
H	2.894832	2.806908	2.904469
O	-4.347171	-1.731048	1.219480
H	-4.544622	0.149047	2.105334
H	-4.225565	-2.224917	-0.708094
H	-6.374863	-0.669342	0.265964
C	1.175732	-2.309714	2.672582
H	0.574656	-2.487530	1.772759
H	0.529277	-2.524715	3.529880
H	2.012650	-3.010104	2.693627
C	4.841937	1.037375	3.628941
H	5.533149	0.757530	2.826720
H	5.121925	0.463380	4.515623
H	4.983392	2.098445	3.842279
C	0.324043	2.619003	1.988801
H	-0.680304	2.480040	2.399635
H	0.239567	2.657435	0.893575
H	0.703444	3.588647	2.314486
C	-0.039674	0.105907	-0.735460
O	-0.732060	0.488860	-1.674956
C	1.494981	0.322417	-0.736937
C	1.851427	1.192219	-1.958953
H	1.755875	0.904203	0.151336
H	2.925668	1.112882	-2.140962
H	1.328538	0.821866	-2.843670
C	1.504230	2.638814	-1.681869
C	0.331727	3.228391	-2.160900
C	2.345837	3.397786	-0.859929

C	0.001965	4.538657	-1.814976
H	-0.331818	2.644627	-2.791009
C	2.020584	4.706035	-0.512657
H	3.264797	2.951067	-0.483611
C	0.841704	5.279571	-0.986482
H	-0.913579	4.979860	-2.197929
H	2.685990	5.278007	0.126924
H	0.583149	6.298459	-0.716340
N	0.160203	-1.998802	-1.008326
N	-0.793215	-2.830325	-1.511198
C	-1.605610	-3.241131	-0.526662
O	-1.535658	-3.052223	0.696410
O	-2.622720	-4.007279	-1.047081
C	-3.392347	-4.703556	-0.076200
H	-3.823960	-4.016464	0.655080
H	-4.179524	-5.217179	-0.629507
H	-2.778068	-5.437141	0.455380
C	1.398500	-2.088374	-1.327924
C	2.241818	-1.034908	-0.643777
C	1.999988	-3.078834	-2.202071
C	3.696252	-1.013426	-1.050791
H	2.245770	-1.311467	0.418665
C	3.309355	-3.003414	-2.499960
H	1.348780	-3.840258	-2.615659
C	4.569509	-0.087608	-0.481104
C	4.196399	-1.974666	-1.946542
H	3.757196	-3.730207	-3.173019
C	5.921303	-0.080430	-0.816210
H	4.183396	0.632459	0.239477
C	5.557220	-1.958788	-2.277618
C	6.415229	-1.016162	-1.724264
H	6.587169	0.649615	-0.367342
H	5.938740	-2.700387	-2.974148
H	7.466801	-1.015908	-1.991317

Vibrational frequencies

-47.1717	10.5554	18.6910
27.4055	35.2473	42.7977
47.8687	50.5877	59.1215
63.9143	66.2098	71.2390
73.0651	77.3804	86.8737
95.7908	102.6152	119.2127
123.9547	131.9888	137.8948
146.3906	157.3638	162.7180
169.4308	178.5303	182.9451

188.7260 201.1012 216.6431
221.3222 225.3314 234.1855
239.6085 243.5337 254.2573
270.8239 285.0587 286.4579
297.3082 306.5262 326.7874
330.7103 337.6309 357.2952
377.5006 397.0591 398.0075
412.4334 415.7955 418.1112
424.0194 426.5668 439.8386
450.3569 460.5378 484.8756
493.9812 497.0160 509.6709
514.5765 516.7476 526.4746
529.1083 537.4111 539.4173
556.6205 569.8726 587.7218
588.4303 599.7333 609.5939
611.2442 624.0092 630.8961
631.9190 651.3517 668.6760
690.6007 711.1490 716.2869
719.3093 724.4754 735.8161
741.6067 748.4302 757.4702
763.4022 771.9636 775.6949
780.6699 788.3118 805.4827
814.1285 819.6267 836.5703
844.6201 856.0901 860.7400
874.0678 876.5457 880.9483
885.0986 890.6454 915.4780
918.0774 918.7404 924.6698
939.6593 958.1158 962.8588
967.2701 980.9019 985.9123
990.5347 991.6502 1003.7116
1004.4259 1016.9167 1021.6646
1022.2457 1024.1757 1028.5124
1031.7780 1034.9794 1036.9221
1046.2346 1052.1702 1058.6467
1064.1866 1064.6532 1065.6598
1066.8588 1067.3413 1071.2171
1083.8875 1087.8765 1106.9819
1108.8631 1119.8965 1129.2385
1150.5759 1156.0222 1160.1184
1162.9471 1176.0333 1178.6302
1182.4621 1194.8397 1196.9670
1199.0465 1201.6126 1203.0115
1209.8011 1223.7134 1234.2535
1236.5099 1238.8350 1243.3611

1246.0980	1249.8937	1255.2243
1270.7050	1279.6105	1285.3173
1297.7638	1299.2110	1304.9761
1315.9375	1325.9899	1333.8315
1336.4991	1341.0871	1343.2974
1348.8664	1351.1217	1353.2508
1356.7093	1361.7083	1375.2290
1377.1499	1387.1140	1389.6997
1392.5140	1421.5207	1423.6822
1431.8735	1439.9308	1441.3289
1460.0744	1465.4761	1479.0221
1482.8602	1487.2810	1489.8160
1492.5367	1494.8386	1499.0274
1499.6000	1500.2679	1504.5688
1507.2647	1508.0822	1517.1721
1521.1888	1528.0057	1536.3502
1541.1195	1546.2845	1548.3591
1551.6083	1597.8287	1654.1112
1673.9101	1682.5467	1684.3937
1687.8863	1690.5253	1693.8713
1694.2141	1697.2302	1701.5867
1709.0518	1715.9112	1735.3355
3050.3724	3057.2302	3061.4723
3067.9587	3072.4383	3084.1880
3094.3643	3105.1754	3128.1074
3128.4719	3139.9413	3140.3038
3142.1856	3155.8963	3161.2063
3163.2570	3171.7776	3175.6179
3176.3747	3182.0099	3188.3740
3188.6562	3189.8125	3190.4344
3192.9900	3200.5253	3202.9029
3204.1607	3207.2196	3211.1389
3213.5608	3214.1847	3217.1232
3221.6355	3230.9937	3232.7855
3237.1398	3239.3080	3243.6752

M6b

Zero-point correction= 0.740944
Thermal correction to Energy= 0.783285
Thermal correction to Enthalpy= 0.784229
Thermal correction to Gibbs Free Energy= 0.665935
Sum of electronic and zero-point Energies= -2196.996399
Sum of electronic and thermal Energies= -2196.954059
Sum of electronic and thermal Enthalpies= -2196.953114

Sum of electronic and thermal Free Energies= -2197.071408

Cartesian coordinates

C	-5.239455	0.686075	-0.569604
C	-3.856943	0.832539	-0.648176
C	-3.263127	2.083184	-0.798057
C	-4.090473	3.202600	-0.851228
C	-5.478874	3.065561	-0.766495
C	-6.063257	1.807771	-0.631202
C	-5.626135	-0.765722	-0.437725
H	-2.182769	2.160281	-0.893612
H	-3.652896	4.189813	-0.963042
H	-6.108914	3.948615	-0.806592
H	-7.142573	1.704896	-0.567623
H	-6.067830	-1.135022	-1.368964
C	-2.481282	-0.549931	1.820669
C	-3.884365	-0.947098	2.138540
C	-4.304793	-1.513075	-0.143291
C	-3.165248	-0.508800	-0.544295
C	-0.811361	-0.203914	0.456246
H	-3.937723	-1.373685	3.139938
H	-2.667278	-0.807517	-1.465078
N	-1.466199	-0.328188	2.601730
N	-0.434846	-0.101511	1.734109
N	-2.130253	-0.465360	0.504750
C	0.819528	0.369011	2.256036
C	1.731938	-0.558052	2.763221
C	1.056336	1.746466	2.210619
C	2.968908	-0.062993	3.176433
C	2.309686	2.188368	2.632943
C	3.278799	1.297458	3.102304
H	3.710164	-0.759697	3.559138
H	2.534770	3.250716	2.584594
O	-4.234111	-1.953400	1.209493
H	-4.557519	-0.080814	2.079055
H	-4.201065	-2.428564	-0.725893
H	-6.350551	-0.953884	0.360815
C	1.386832	-2.021390	2.847618
H	0.824785	-2.363938	1.971680
H	0.754771	-2.208237	3.722193
H	2.293844	-2.620078	2.951384
C	4.646659	1.784647	3.501582
H	5.378473	1.545176	2.720934
H	4.983021	1.301138	4.423741
H	4.654970	2.866583	3.651960

C	0.026449	2.693490	1.653155
H	-0.962563	2.500648	2.080383
H	-0.053080	2.592800	0.561538
H	0.303945	3.727355	1.863522
C	-0.063485	-0.087425	-0.909265
O	-0.819246	0.474349	-1.769740
C	1.450130	0.363166	-0.818815
C	1.790330	1.206924	-2.061643
H	1.612776	0.996266	0.051021
H	2.864089	1.143792	-2.260088
H	1.255004	0.816887	-2.929801
C	1.416077	2.652306	-1.807520
C	0.211385	3.195451	-2.261535
C	2.253351	3.452529	-1.021964
C	-0.151723	4.498904	-1.925518
H	-0.453398	2.569322	-2.845423
C	1.893378	4.754344	-0.681900
H	3.198196	3.046886	-0.664588
C	0.683546	5.281073	-1.130051
H	-1.093407	4.902505	-2.286447
H	2.556333	5.356430	-0.067578
H	0.397055	6.293943	-0.864904
N	0.163069	-1.663762	-1.237840
N	-0.892552	-2.462464	-1.593034
C	-1.268584	-3.207389	-0.537859
O	-0.802135	-3.239382	0.608197
O	-2.331776	-3.993208	-0.881280
C	-2.843926	-4.797184	0.175202
H	-3.214592	-4.170897	0.990153
H	-3.662314	-5.370863	-0.260869
H	-2.077312	-5.473657	0.560737
C	1.400672	-2.009845	-1.218219
C	2.260164	-0.940026	-0.626695
C	1.951741	-3.261827	-1.677022
C	3.712801	-1.024244	-1.007072
H	2.246293	-1.158924	0.453465
C	3.286310	-3.325250	-1.860592
H	1.281958	-4.071654	-1.938602
C	4.605039	-0.005850	-0.681639
C	4.198757	-2.215268	-1.578310
H	3.728587	-4.234474	-2.260033
C	5.962980	-0.138292	-0.960840
H	4.231333	0.893659	-0.197195
C	5.566399	-2.339113	-1.852874

C	6.444206	-1.304555	-1.555015
H	6.645901	0.666883	-0.710223
H	5.935505	-3.258822	-2.298157
H	7.501399	-1.409485	-1.773673

Vibrational frequencies

17.2346	22.8172	27.6190
34.0855	43.0407	45.9854
53.2480	56.0084	60.5859
69.7497	77.2801	81.3224
84.6041	87.3146	94.0095
103.1285	106.3120	120.1760
129.4515	134.4887	138.6169
146.1252	161.1900	167.3004
176.1596	183.6357	186.2562
190.4914	208.4290	217.1773
226.0076	228.4024	241.5480
245.0316	251.2224	270.2594
281.1655	284.6271	291.0392
299.4329	322.3669	328.8725
337.6205	344.9691	362.2273
385.5820	393.7809	405.1923
411.5857	417.5325	426.7976
432.9663	437.2078	446.6462
450.9328	490.2214	497.3356
500.3358	504.2526	511.5000
517.5895	528.1743	530.4637
536.7425	548.0951	550.3544
569.9503	579.4924	588.8621
595.4047	606.8487	617.2895
620.2265	628.1387	630.3102
631.3926	648.6813	690.9916
703.6529	712.1060	718.2127
724.7755	731.6551	743.9135
751.0148	757.7964	767.5234
776.3541	780.1149	782.7997
785.4648	801.6193	816.1453
817.5098	835.7170	838.9679
852.3227	853.4840	859.3890
875.9359	880.0925	883.6825
884.9183	887.9743	907.8609
921.6358	923.5011	924.7873
940.0484	955.9590	960.5872
965.8866	979.7666	982.6256
988.5359	997.9847	1002.7937

1009.1286	1011.8886	1016.4353
1019.7696	1023.5999	1027.0147
1032.6950	1033.2057	1035.8790
1045.4950	1053.2460	1058.3446
1062.9650	1065.4568	1066.3844
1068.7413	1069.2062	1071.5436
1078.8565	1082.5448	1093.0006
1111.7468	1117.6028	1131.1524
1134.6503	1152.2220	1161.8027
1165.1325	1177.5839	1179.0356
1180.4072	1189.5004	1194.6425
1198.3785	1203.3730	1204.6211
1208.5243	1213.2207	1219.3659
1224.4861	1233.7053	1238.9355
1244.7718	1245.3734	1251.4273
1261.8811	1278.2957	1282.3485
1290.8639	1297.5484	1300.6951
1309.3715	1319.5241	1324.5341
1338.7115	1340.7414	1341.9050
1342.6751	1355.1996	1356.1931
1357.9863	1360.3628	1367.3953
1371.3993	1380.2690	1389.0305
1401.5197	1419.8944	1425.1271
1429.9930	1435.1284	1450.0148
1458.6194	1460.9023	1465.0072
1477.0553	1483.1359	1484.7806
1487.0100	1490.9430	1492.1085
1493.3653	1496.1768	1497.3160
1504.9520	1508.1771	1509.6573
1513.9286	1517.3053	1521.5103
1523.8897	1535.0897	1539.5453
1547.3336	1550.6212	1573.9385
1647.6409	1672.4287	1681.2547
1684.6529	1690.1197	1690.4485
1694.7784	1695.2439	1695.7220
1706.0659	1716.1619	1754.2168
3038.4760	3056.5985	3059.0189
3064.0749	3067.5893	3079.1070
3087.8851	3096.1486	3127.5659
3127.9632	3133.1796	3135.8895
3154.3415	3156.9238	3162.8680
3164.8118	3175.9024	3178.0826
3181.8229	3182.1837	3185.3031
3185.7246	3189.9309	3191.9787

3200.3638	3206.2177	3206.9121
3209.0381	3209.4086	3213.5699
3214.0937	3216.7683	3219.7696
3224.5486	3228.4837	3230.8086
3236.1675	3245.5722	3250.2218

TS7b

Zero-point correction= 0.739300
Thermal correction to Energy= 0.781688
Thermal correction to Enthalpy= 0.782632
Thermal correction to Gibbs Free Energy= 0.663619
Sum of electronic and zero-point Energies= -2196.983594
Sum of electronic and thermal Energies= -2196.941207
Sum of electronic and thermal Enthalpies= -2196.940263
Sum of electronic and thermal Free Energies= -2197.059275
Cartesian coordinates

C	-5.252912	0.544419	0.133886
C	-3.880199	0.761208	0.052512
C	-3.321723	2.005044	0.331109
C	-4.171359	3.041833	0.708752
C	-5.550258	2.830774	0.799274
C	-6.100950	1.584383	0.508405
C	-5.603048	-0.873817	-0.240316
H	-2.250419	2.157232	0.226124
H	-3.760934	4.022391	0.928235
H	-6.199064	3.648582	1.096885
H	-7.173217	1.425778	0.577610
H	-6.123909	-0.905616	-1.202676
C	-2.359458	-1.416841	1.783962
C	-3.724033	-1.996199	1.956184
C	-4.249320	-1.618402	-0.339314
C	-3.147682	-0.496170	-0.357543
C	-0.776018	-0.413052	0.591734
H	-3.712076	-2.791350	2.701676
H	-2.689431	-0.408711	-1.343952
N	-1.319677	-1.447461	2.560274
N	-0.361956	-0.810461	1.805013
N	-2.075022	-0.802414	0.594161
C	0.934176	-0.555690	2.358353
C	1.861446	-1.603576	2.408555
C	1.235576	0.747306	2.760260
C	3.151443	-1.296901	2.834720
C	2.543933	1.004885	3.177015
C	3.513223	0.002275	3.204442

H	3.898979	-2.086347	2.860463
H	2.808742	2.013760	3.484276
O	-4.082905	-2.565268	0.710592
H	-4.440067	-1.223090	2.269629
H	-4.173507	-2.212342	-1.250251
H	-6.250717	-1.367801	0.491329
C	1.475710	-2.985236	1.952057
H	1.027592	-2.963869	0.950557
H	0.726069	-3.416706	2.622191
H	2.348497	-3.640222	1.938604
C	4.935902	0.309334	3.590801
H	5.577068	0.296671	2.702380
H	5.326676	-0.437430	4.286593
H	5.019731	1.293871	4.055204
C	0.193839	1.836712	2.725306
H	-0.756781	1.484731	3.136085
H	-0.004242	2.175557	1.701285
H	0.526472	2.700112	3.304173
C	-0.057557	0.496708	-1.192000
O	-0.966441	1.201141	-1.584261
C	1.354838	0.950506	-0.786490
C	1.849283	1.997765	-1.802321
H	1.334716	1.394114	0.209765
H	2.935202	2.094737	-1.700569
H	1.654336	1.649120	-2.822306
C	1.202265	3.344052	-1.571699
C	0.302480	3.888436	-2.488550
C	1.493857	4.064786	-0.409320
C	-0.292730	5.124990	-2.252613
H	0.054249	3.326974	-3.384292
C	0.897816	5.299333	-0.166204
H	2.196977	3.654683	0.314552
C	0.001568	5.833681	-1.090042
H	-0.993240	5.532028	-2.975008
H	1.136165	5.845719	0.741048
H	-0.464272	6.796318	-0.904891
N	0.164524	-0.848423	-1.846931
N	-0.881956	-1.500644	-2.430776
C	-1.113350	-2.668827	-1.791958
O	-0.501301	-3.189793	-0.855936
O	-2.217223	-3.263923	-2.327047
C	-2.604828	-4.477879	-1.692151
H	-2.904386	-4.290749	-0.657182
H	-3.452500	-4.853893	-2.265487

H	-1.789256	-5.204261	-1.705368
C	1.392103	-1.248607	-1.719275
C	2.143383	-0.370485	-0.776065
C	2.002790	-2.385305	-2.347665
C	3.635644	-0.416507	-0.922567
H	1.942805	-0.834111	0.202871
C	3.351056	-2.461883	-2.312673
H	1.391291	-3.096650	-2.887385
C	4.462294	0.482033	-0.252209
C	4.206216	-1.481041	-1.645963
H	3.850872	-3.279877	-2.824908
C	5.847437	0.357927	-0.330987
H	4.017329	1.277111	0.342681
C	5.600677	-1.599542	-1.711527
C	6.418166	-0.682371	-1.065268
H	6.482237	1.072557	0.183205
H	6.036678	-2.421154	-2.272812
H	7.496759	-0.779640	-1.124941

Vibrational frequencies

-125.4621	14.8824	25.0846
30.2250	35.4780	38.8593
47.6458	49.6950	50.4075
58.0020	61.3888	68.8121
74.8995	83.9511	85.7429
92.7827	104.7074	112.9419
118.9820	121.7989	124.1744
136.7072	143.3632	155.5436
165.0196	166.8081	173.3639
181.6795	185.1534	209.2496
216.6632	221.5723	226.4030
235.2888	243.9834	246.2640
273.4134	279.3326	280.6740
287.5987	306.4503	320.9212
328.7731	336.3913	348.4607
357.5281	374.1539	381.9957
403.1772	417.6380	418.0793
429.8265	433.6439	443.9179
448.7182	481.1333	489.3304
498.0187	504.4680	508.4044
510.1822	515.3396	531.3781
533.8469	543.1602	551.3344
571.9283	575.9862	588.5572
592.1748	599.7452	607.8325
618.0019	627.3614	630.2090

633.0953 642.8572 680.8798
705.6590 706.9895 711.1397
712.8700 721.3125 722.7097
744.7422 751.2926 753.7615
761.8771 768.5763 774.6823
776.5124 787.2609 805.5310
813.6102 829.5395 834.9907
857.0069 858.3397 875.1555
877.8153 878.9524 880.3021
883.3091 887.5459 908.8594
911.8127 913.1955 924.3519
946.9739 955.1380 958.6643
964.7314 979.5595 983.1874
985.1801 1000.0986 1003.5702
1010.4279 1018.6088 1018.8565
1020.9344 1025.0342 1027.9383
1030.5758 1032.2092 1035.5003
1043.7929 1051.4486 1054.6325
1059.7874 1063.8140 1065.4079
1066.2278 1069.2748 1072.1070
1074.1795 1076.8317 1096.5652
1100.7162 1119.1363 1121.1243
1139.0645 1148.1635 1169.9280
1172.5028 1174.7262 1178.8910
1181.9698 1187.3101 1194.5380
1197.4496 1199.3029 1210.2153
1211.5533 1213.6153 1214.1330
1226.9375 1231.0992 1242.4234
1244.0667 1248.4280 1249.4574
1263.8105 1278.2773 1278.8656
1281.5115 1299.5883 1305.8713
1309.9045 1311.0183 1322.8010
1333.7565 1335.6349 1338.3585
1349.5129 1352.2339 1352.9603
1360.3428 1360.9814 1365.5000
1371.7213 1381.6796 1383.3003
1402.9512 1421.2371 1425.0633
1425.7317 1428.2796 1437.3325
1459.1721 1465.3081 1468.2079
1476.5480 1485.3384 1486.5842
1488.0192 1490.4294 1490.8774
1494.4383 1497.7124 1500.0445
1501.7311 1505.7619 1511.3197
1511.9407 1515.5712 1519.2495

1523.8602	1540.7422	1544.3646
1559.8171	1565.1111	1642.2483
1679.9795	1682.5735	1683.0883
1683.2941	1692.4278	1698.0545
1700.3432	1701.4857	1702.3731
1716.2081	1728.8081	1783.7164
3061.8945	3063.0677	3064.0886
3065.1456	3072.6360	3079.5254
3079.7907	3081.7972	3124.1127
3131.4622	3133.7046	3134.3129
3143.5995	3158.9960	3164.2335
3165.3639	3169.1187	3172.0260
3173.5463	3175.3263	3179.4808
3184.7911	3186.1707	3189.4469
3189.9416	3196.6427	3199.1933
3205.2914	3207.9102	3211.4302
3212.8898	3217.5668	3217.7594
3225.2321	3225.7336	3225.8060
3235.1318	3239.6208	3255.3172

M7b

Zero-point correction= 0.352956
Thermal correction to Energy= 0.374191
Thermal correction to Enthalpy= 0.375135
Thermal correction to Gibbs Free Energy= 0.301023
Sum of electronic and zero-point Energies= -1145.427376
Sum of electronic and thermal Energies= -1145.406140
Sum of electronic and thermal Enthalpies= -1145.405196
Sum of electronic and thermal Free Energies= -1145.479308
Cartesian coordinates

C	-0.132706	-1.266094	0.763088
O	-0.478865	-2.373321	1.042599
C	-0.873382	0.049976	0.855066
C	-1.792159	0.192248	-0.385216
H	-1.470024	0.071529	1.768638
H	-2.204633	1.204821	-0.378936
H	-1.182328	0.101244	-1.292119
C	-2.911299	-0.818117	-0.389598
C	-2.796534	-2.023968	-1.084174
C	-4.079105	-0.563415	0.334511
C	-3.830089	-2.957018	-1.056895
H	-1.890953	-2.234493	-1.647570
C	-5.113111	-1.493676	0.364957
H	-4.177451	0.376310	0.873651

C	-4.990004	-2.694171	-0.332344
H	-3.728255	-3.890105	-1.601667
H	-6.015859	-1.280359	0.928385
H	-5.795836	-3.420809	-0.311674
N	1.163544	-0.975889	0.159408
N	1.915009	-2.007821	-0.303492
C	3.203814	-1.910684	0.095517
O	3.743617	-1.047298	0.787131
O	3.899077	-2.974339	-0.386018
C	5.273699	-2.994745	-0.026440
H	5.395146	-3.050575	1.057970
H	5.692113	-3.884535	-0.495673
H	5.787488	-2.100924	-0.389178
C	1.358559	0.324104	0.090905
C	0.295104	1.062126	0.851826
C	2.369772	1.000073	-0.657451
C	0.069070	2.475682	0.389116
H	0.669755	1.130667	1.885654
C	2.178433	2.316475	-0.910825
H	3.214003	0.452950	-1.051358
C	-1.009977	3.223841	0.850399
C	1.027780	3.079785	-0.444715
H	2.901983	2.844596	-1.526506
C	-1.160478	4.553421	0.463600
H	-1.737780	2.767164	1.516398
C	0.870175	4.419764	-0.821733
C	-0.220802	5.152404	-0.375362
H	-2.011820	5.123605	0.820091
H	1.612269	4.878273	-1.468704
H	-0.338867	6.188201	-0.673915

Vibrational frequencies

23.8453	39.3315	44.8870
51.0682	66.7423	67.9216
91.8331	95.5227	117.5731
129.5799	156.4677	171.1166
177.7229	215.3502	224.3092
267.8995	282.5559	303.5889
323.3295	354.6383	372.5020
396.7682	418.7931	424.1537
456.1065	482.6062	500.6895
509.5029	532.0278	557.6274
584.2885	593.4958	622.9995
629.2320	650.1624	699.7694
719.4561	722.4842	734.1092

746.4426	764.2860	773.1720
779.4872	781.6989	812.3153
820.0691	861.3678	878.2344
881.0119	884.5940	912.0299
923.4587	948.8022	972.1062
985.1863	995.6969	1004.0631
1015.1283	1018.9122	1025.9489
1027.7076	1042.8586	1069.3676
1072.6327	1081.7881	1101.6196
1118.6787	1148.8240	1150.1204
1172.5159	1176.3967	1179.8356
1186.3353	1187.0029	1205.5743
1213.0165	1219.2839	1243.1303
1248.4124	1249.7234	1252.0365
1292.6086	1303.2819	1320.4215
1346.6910	1351.0286	1357.3398
1361.0453	1366.9558	1369.7453
1401.1234	1464.2066	1492.0636
1494.3689	1494.9364	1507.8538
1508.5508	1515.2819	1548.9078
1555.2058	1636.5582	1644.6588
1680.1481	1688.2581	1700.5443
1702.9408	1738.0031	1943.2984
3034.6016	3077.1231	3078.7648
3136.5001	3154.7461	3158.1420
3185.8666	3186.1242	3196.1961
3202.4321	3205.2944	3207.0789
3209.0252	3217.8313	3220.6451
3226.7793	3232.3136	3271.1756

M7b1

Zero-point correction= 1.020941
Thermal correction to Energy= 1.076135
Thermal correction to Enthalpy= 1.077079
Thermal correction to Gibbs Free Energy= 0.932835
Sum of electronic and zero-point Energies= -2568.074293
Sum of electronic and thermal Energies= -2568.019100
Sum of electronic and thermal Enthalpies= -2568.018155
Sum of electronic and thermal Free Energies= -2568.162400
Cartesian coordinates

C	-3.752609	-3.414534	0.140364
C	-2.560204	-2.749066	0.411375
C	-1.665606	-3.213998	1.372695
C	-1.986110	-4.382889	2.057729

C	-3.179431	-5.059877	1.789555
C	-4.072045	-4.579484	0.834264
C	-4.553642	-2.702436	-0.918776
H	-0.754887	-2.659758	1.584487
H	-1.302778	-4.771297	2.806116
H	-3.413241	-5.970339	2.331972
H	-4.998215	-5.107686	0.629127
H	-5.445337	-2.236875	-0.487020
C	-0.976526	-2.341654	-2.299160
C	-2.211999	-2.908359	-2.915258
C	-3.608900	-1.617726	-1.486617
C	-2.411537	-1.527257	-0.467009
C	0.100654	-1.083649	-0.876324
H	-2.042902	-3.122418	-3.969965
H	-2.433825	-0.600705	0.102108
N	0.261412	-2.389025	-2.692496
N	0.921390	-1.608664	-1.788550
N	-1.118767	-1.566591	-1.182598
C	2.360651	-1.590301	-1.798302
C	3.024270	-0.721123	-2.665066
C	3.012502	-2.454954	-0.912686
C	4.415300	-0.676633	-2.566718
C	4.402297	-2.371477	-0.855657
C	5.114758	-1.477294	-1.660244
H	4.964989	0.002842	-3.213276
H	4.937387	-3.013879	-0.160854
O	-3.197535	-1.898501	-2.817096
H	-2.516683	-3.830445	-2.402234
H	-4.097924	-0.645216	-1.558251
H	-4.893698	-3.361624	-1.723818
C	2.269533	0.121330	-3.659785
H	1.332184	0.509524	-3.248744
H	2.006360	-0.479031	-4.536542
H	2.885275	0.957715	-3.995267
C	6.611503	-1.359390	-1.543246
H	6.877996	-0.478834	-0.949070
H	7.074405	-1.243244	-2.525818
H	7.042352	-2.236141	-1.056445
C	2.233372	-3.376092	-0.010949
H	1.464322	-3.921303	-0.566686
H	1.736542	-2.816559	0.794152
H	2.900300	-4.097440	0.462920
C	0.313226	-0.095399	0.307801
O	-0.491219	-0.364255	1.255251

C	1.813082	0.266175	0.654575
C	1.958689	0.428972	2.178165
H	2.476891	-0.542416	0.355649
H	2.827440	1.059620	2.386900
H	1.076036	0.919927	2.592653
C	2.166067	-0.925761	2.820842
C	1.122817	-1.617107	3.441315
C	3.420023	-1.540671	2.735404
C	1.327391	-2.898593	3.951399
H	0.143375	-1.152422	3.492345
C	3.627263	-2.821122	3.241151
H	4.244199	-1.011466	2.259936
C	2.576568	-3.507165	3.847742
H	0.506684	-3.421082	4.434036
H	4.607124	-3.282187	3.161618
H	2.731855	-4.506101	4.242496
N	-0.101603	1.328556	-0.400322
N	-1.402149	1.601189	-0.733668
C	-1.735886	1.311417	-2.032556
O	-0.960184	0.932806	-2.889538
O	-3.045908	1.505288	-2.224707
C	-3.501108	1.288392	-3.570903
H	-3.328893	0.249402	-3.855053
H	-4.564932	1.515858	-3.552551
H	-2.977810	1.957654	-4.255123
C	0.859984	2.193038	-0.457421
C	2.162442	1.514017	-0.198819
C	0.760133	3.594272	-0.726810
C	3.285372	2.430982	0.189295
H	2.443558	1.135558	-1.196951
C	1.850355	4.352207	-0.453284
H	-0.179876	4.016553	-1.062585
C	4.524590	1.929868	0.577265
C	3.114873	3.819797	0.034009
H	1.791169	5.429133	-0.590346
C	5.575293	2.798923	0.859429
H	4.668740	0.854355	0.652213
C	4.180987	4.685237	0.317871
C	5.402526	4.178668	0.737200
H	6.533664	2.398574	1.173148
H	4.041008	5.755754	0.199945
H	6.223209	4.851776	0.958532
N	-3.205123	2.590004	1.065168
C	-2.923298	2.204620	2.476675

C	-1.458106	2.478146	2.816618
C	-3.217748	0.728533	2.743505
H	-3.560584	2.800313	3.145677
H	-1.179969	3.530965	2.735473
H	-1.261950	2.164320	3.845651
H	-0.822803	1.875618	2.159759
H	-4.272886	0.472466	2.624114
H	-2.601597	0.092827	2.100166
H	-2.945934	0.505602	3.778749
C	-2.919769	4.035740	0.805086
C	-3.446143	5.020491	1.856586
C	-3.370536	4.467698	-0.588550
H	-1.824173	4.110372	0.811763
H	-3.007501	4.857225	2.843150
H	-3.184504	6.035881	1.546264
H	-4.533000	4.970811	1.953756
H	-3.048184	3.762404	-1.358545
H	-4.458222	4.574291	-0.650306
H	-2.931754	5.444178	-0.809409
C	-4.512246	2.106212	0.573306
C	-5.762019	2.592239	1.306418
H	-4.472636	1.012852	0.604595
H	-4.581066	2.359930	-0.485433
H	-6.628136	2.020074	0.962990
H	-5.682593	2.458613	2.389100
H	-5.964823	3.646984	1.106310
H	-2.117418	1.909755	0.037413

Vibrational frequencies

17.1956	23.0407	28.4940
29.4334	33.7727	38.3037
38.6687	46.4735	49.1837
60.0163	63.8992	73.1856
74.1216	78.5059	81.1513
86.1044	87.3798	91.2175
97.5591	104.4022	107.1680
109.3898	111.3783	112.5118
128.7296	133.9228	138.0675
139.0509	153.5501	156.8279
158.8515	168.1195	173.6028
178.7064	185.0985	197.6482
200.6532	209.3875	211.1561
217.8470	224.4849	229.1263
236.5413	240.0431	242.9779
246.3221	252.1313	265.2962

269.6624	276.6869	280.8133
282.1553	288.7307	294.2492
303.4323	315.4661	326.8067
340.0585	342.6664	346.2288
355.6169	359.0406	371.5226
383.4567	391.9374	398.3120
408.2701	417.5520	421.5449
425.5521	432.6376	433.9064
442.3591	446.4758	451.9483
461.0643	473.4829	482.9471
496.5458	498.1216	499.9983
502.6790	511.3742	518.9216
527.0692	528.3078	531.9332
543.6903	547.3615	567.0249
577.9291	588.4110	595.2006
606.0909	609.1220	619.3319
627.7633	628.6472	632.3899
641.2486	647.2345	682.7892
708.1045	711.7274	713.6309
722.4360	724.8510	730.7716
744.7181	749.2057	755.4088
764.7874	775.3772	778.1175
780.6877	784.5980	792.1593
797.3426	811.9674	818.8490
835.6392	840.8800	850.3126
857.8590	860.6088	863.0110
876.9923	882.2985	884.4677
885.9778	889.6104	903.0322
916.7319	918.0955	918.9421
928.1359	933.1658	944.2719
949.9434	958.0910	960.1528
962.7166	967.4653	968.2457
975.5757	982.6182	986.2569
993.5102	994.0341	995.1316
996.9636	1007.4542	1011.4548
1018.2625	1025.2827	1029.8173
1030.9438	1031.5064	1037.5105
1044.7630	1046.3555	1055.1018
1056.9782	1060.9172	1064.0513
1066.1075	1069.7096	1073.0519
1073.8973	1079.6434	1081.6932
1082.8105	1093.5082	1097.4539
1111.4424	1112.9293	1123.5525
1127.4499	1138.4933	1141.5873

1150.6822 1155.2320 1158.4233
1170.1155 1177.2417 1182.2295
1183.9478 1184.5097 1193.9129
1194.2131 1199.6558 1200.2853
1202.2432 1205.2834 1209.1730
1215.0778 1217.5426 1225.4746
1228.7363 1237.8002 1238.3507
1242.9471 1248.4909 1250.6346
1252.8295 1257.0432 1265.7579
1278.2088 1280.4885 1296.5014
1300.3869 1305.9980 1317.4024
1323.6804 1328.6447 1341.7995
1343.6282 1344.2483 1345.5865
1355.3494 1356.4299 1357.9718
1359.4013 1360.7736 1367.0250
1373.8925 1375.8851 1382.5606
1383.9932 1385.0263 1390.2652
1392.5191 1405.1747 1409.9724
1412.3453 1421.8859 1425.2297
1425.7781 1428.4821 1430.0696
1433.1042 1434.7060 1435.8458
1458.4349 1459.5664 1466.5579
1467.1454 1477.2505 1480.4457
1481.9857 1487.4102 1488.7841
1489.0433 1491.0567 1492.8861
1495.1684 1496.2257 1498.3488
1499.7490 1502.0342 1503.3051
1505.2584 1506.5572 1508.2653
1511.0720 1513.1970 1516.5309
1520.6964 1521.8023 1522.7225
1523.6257 1524.0771 1528.0225
1536.3977 1542.2438 1543.7661
1546.4576 1552.5664 1574.8763
1631.6081 1662.2286 1673.5138
1680.6577 1686.1061 1686.7599
1688.6682 1692.3269 1695.0671
1696.9905 1699.1955 1724.3622
1818.7386 2174.2864 3030.2308
3054.4570 3055.3302 3060.9597
3074.1493 3074.8900 3076.1812
3076.7578 3077.5284 3078.7335
3082.2964 3083.2232 3085.0273
3101.2380 3103.7526 3103.8445
3126.4604 3128.2411 3148.0948

3149.2913	3149.4738	3150.2020
3152.3521	3154.9738	3156.7002
3160.0701	3160.4837	3168.1837
3169.2849	3170.4048	3172.4753
3172.7348	3173.9268	3174.1333
3177.6561	3178.0300	3186.7514
3188.7515	3190.3806	3196.3779
3197.8663	3198.1627	3200.3431
3206.3372	3210.9518	3211.6118
3214.2536	3214.4355	3215.6424
3218.5904	3220.4773	3221.0455
3224.6082	3227.5315	3232.5159
3235.5529	3236.3019	3255.3041

TS8b1

Zero-point correction= 1.020237

Thermal correction to Energy= 1.075360

Thermal correction to Enthalpy= 1.076304

Thermal correction to Gibbs Free Energy= 0.931809

Sum of electronic and zero-point Energies= -2568.040262

Sum of electronic and thermal Energies= -2567.985139

Sum of electronic and thermal Enthalpies= -2567.984195

Sum of electronic and thermal Free Energies= -2568.128689

Cartesian coordinates

C	-6.145332	-1.286058	-0.082605
C	-4.914991	-0.640821	-0.177815
C	-4.804905	0.738354	-0.011008
C	-5.958833	1.465462	0.268556
C	-7.195807	0.822606	0.371482
C	-7.299042	-0.554264	0.191513
C	-6.011552	-2.768755	-0.317155
H	-3.845061	1.239551	-0.116725
H	-5.892992	2.540548	0.401311
H	-8.085439	1.403231	0.593894
H	-8.261738	-1.050350	0.271647
H	-6.476274	-3.059410	-1.264248
C	-2.902069	-2.087379	1.803298
C	-3.985852	-3.102037	1.961763
C	-4.489439	-3.041888	-0.361087
C	-3.798766	-1.629568	-0.442816
C	-1.665739	-0.678535	0.591898
H	-3.743047	-3.805295	2.757890
H	-3.339781	-1.474908	-1.418888
N	-1.981863	-1.690257	2.626865

N	-1.243546	-0.820458	1.857910
N	-2.746575	-1.505391	0.570756
C	-0.147039	-0.100167	2.433009
C	1.094754	-0.731870	2.529923
C	-0.359466	1.223477	2.835333
C	2.172731	0.033677	2.976248
C	0.753020	1.952380	3.256191
C	2.028430	1.381385	3.310336
H	3.147502	-0.439956	3.065237
H	0.619297	2.987884	3.560702
O	-4.043823	-3.820009	0.740428
H	-4.945930	-2.619433	2.191356
H	-4.215858	-3.632904	-1.236256
H	-6.479354	-3.373612	0.466349
C	1.265247	-2.169578	2.125438
H	1.279846	-2.268662	1.034430
H	0.440963	-2.784748	2.494588
H	2.201833	-2.562019	2.524273
C	3.222756	2.207574	3.706693
H	3.656229	2.687820	2.821246
H	4.001217	1.589079	4.159513
H	2.945477	2.994258	4.411879
C	-1.744917	1.817837	2.846716
H	-2.386550	1.264835	3.539827
H	-2.229997	1.770196	1.865461
H	-1.714019	2.861503	3.164391
C	-1.222228	0.531007	-1.288938
O	-2.300884	0.550282	-1.837250
C	-0.405914	1.676273	-0.689145
C	-0.554107	2.915980	-1.593630
H	-0.780251	1.915330	0.305194
H	0.205722	3.647473	-1.302453
H	-0.359539	2.651838	-2.638934
C	-1.932304	3.520164	-1.440472
C	-2.851171	3.516888	-2.489628
C	-2.314162	4.067703	-0.211730
C	-4.126499	4.049000	-2.317709
H	-2.568564	3.080197	-3.443305
C	-3.590179	4.595707	-0.032915
H	-1.603812	4.087237	0.613558
C	-4.499734	4.588736	-1.089167
H	-4.830898	4.037030	-3.143186
H	-3.871268	5.018467	0.926706
H	-5.494094	5.002643	-0.954448

N	-0.209095	-0.406748	-1.815610
N	-0.611027	-1.510490	-2.523777
C	-0.614579	-2.693600	-1.762855
O	0.174845	-2.908448	-0.877925
O	-1.560541	-3.510099	-2.202453
C	-1.628693	-4.778741	-1.520228
H	-2.021541	-4.623602	-0.512520
H	-2.310060	-5.387131	-2.110177
H	-0.638972	-5.232747	-1.477668
C	1.028780	-0.041002	-1.587241
C	1.019051	1.071013	-0.591402
C	2.202401	-0.531129	-2.200096
C	2.234167	1.948151	-0.641512
H	1.063244	0.535131	0.376200
C	3.293170	0.290054	-2.147744
H	2.177336	-1.431443	-2.801211
C	2.330639	3.095182	0.142473
C	3.330244	1.549942	-1.429291
H	4.171757	0.027196	-2.727223
C	3.484804	3.873427	0.103248
H	1.500545	3.381730	0.783641
C	4.479700	2.354076	-1.475067
C	4.556134	3.511677	-0.717438
H	3.545031	4.770963	0.709936
H	5.313450	2.052486	-2.101604
H	5.447870	4.127336	-0.751321
N	5.312699	-1.014560	-0.488403
C	5.903176	-1.705646	-1.644576
C	6.589598	-3.054617	-1.369610
C	6.834896	-0.797639	-2.446834
H	5.048710	-1.942087	-2.300471
H	5.881583	-3.787078	-0.975171
H	6.986335	-3.455594	-2.307465
H	7.419132	-2.960384	-0.663977
H	6.368228	0.164056	-2.678444
H	7.771093	-0.597798	-1.918439
H	7.085206	-1.285795	-3.391630
C	6.146874	-0.076623	0.273401
C	7.410233	-0.660568	0.929902
C	5.329662	0.668875	1.332233
H	6.485598	0.682681	-0.443936
H	8.090918	-1.096910	0.196023
H	7.951683	0.138198	1.447185
H	7.162165	-1.429360	1.666260

H	4.366827	1.016254	0.946025
H	5.143667	0.040547	2.208916
H	5.894850	1.541820	1.671489
C	4.330487	-1.805052	0.242298
C	4.821698	-2.714827	1.381178
H	3.809228	-2.417796	-0.504506
H	3.564185	-1.127044	0.648655
H	4.044835	-3.441465	1.636163
H	5.718597	-3.270635	1.103803
H	5.052002	-2.144948	2.286454
H	-1.464039	-1.310341	-3.043074

Vibrational frequencies

-109.0163	6.5253	19.9519
30.9427	35.7560	43.0244
44.5960	47.4653	50.6649
52.9590	57.8018	63.5626
68.0647	69.5784	73.6268
78.2952	82.2671	86.9548
89.0759	94.2485	100.4621
106.6469	110.2706	114.2184
117.9621	123.4385	126.8517
137.9389	141.2436	159.8427
161.0520	174.7856	180.1124
183.3164	185.7062	190.1723
200.6526	208.8980	213.4308
221.4692	225.2538	228.5127
231.3930	237.9226	240.1277
244.0483	245.3772	259.0081
260.9296	265.2730	271.9436
283.7166	285.9354	292.2469
297.3194	301.2779	321.4026
333.1425	334.9386	341.9904
342.1793	350.2425	357.9553
363.5196	366.6917	374.6415
377.1887	388.2713	403.5904
407.3571	415.3359	423.4853
426.6119	434.9310	446.1668
452.0675	482.2014	492.4975
494.7897	495.4080	500.2462
509.0721	509.7698	511.8620
527.2651	530.6881	536.2758
543.4194	570.0470	571.9329
575.2679	577.2750	588.8838
591.0501	599.4234	601.4095

611.8465	617.7288	628.3399
629.5626	636.3934	649.4691
669.9792	701.8676	702.3031
704.9892	709.8647	713.6368
720.1391	722.7449	745.0937
752.0868	757.6183	773.2048
774.6642	786.7857	791.0914
799.3242	800.1968	805.8361
815.8957	834.2561	843.1803
850.4293	860.6443	862.3238
871.6634	877.0721	879.5933
883.1116	884.0818	889.6553
890.4907	916.3321	917.1123
926.8687	928.1696	931.6557
937.9608	953.1054	957.0768
960.7709	960.9135	964.0875
965.5677	977.4650	980.9865
991.0744	992.2810	997.8881
1004.4391	1007.3888	1016.5166
1017.3315	1022.1591	1023.6043
1026.2306	1032.0953	1035.7336
1040.0837	1040.4543	1041.4658
1054.2397	1060.0450	1061.4586
1062.3594	1067.0156	1067.8121
1068.6342	1071.8362	1072.5556
1076.5518	1082.4773	1083.2905
1095.7466	1115.8735	1122.1375
1122.9597	1130.9405	1131.3511
1147.6204	1149.2531	1154.8508
1158.5720	1173.3076	1175.7884
1176.1120	1180.8052	1190.3767
1192.8517	1195.2218	1199.5850
1201.8085	1203.0611	1205.6319
1207.8253	1211.2057	1211.9170
1227.6472	1228.8472	1234.3039
1242.2015	1243.5743	1254.4137
1255.6181	1260.1167	1272.7252
1278.0142	1280.7925	1288.0784
1299.4982	1301.9300	1305.2999
1311.9601	1315.6008	1323.5082
1329.4862	1342.1217	1345.1399
1349.3383	1351.1980	1356.3767
1360.9692	1361.2854	1366.3295
1368.7485	1370.5649	1375.5374

1376.4672	1379.4317	1395.5123
1406.1919	1407.7612	1409.6916
1410.3731	1414.1907	1415.8507
1418.6792	1424.7198	1425.7840
1428.0752	1433.4015	1434.1215
1436.1686	1456.3681	1464.5547
1475.0405	1477.4055	1483.7174
1484.1269	1484.5703	1486.2126
1488.5805	1490.2096	1492.0116
1493.5469	1494.7875	1495.9647
1497.6850	1499.2094	1502.1644
1503.3792	1504.0380	1506.6275
1507.4988	1510.4135	1510.6783
1512.0756	1514.4366	1515.0523
1520.6182	1523.0508	1528.5517
1529.1813	1533.3966	1539.0258
1548.6793	1552.7109	1566.0073
1607.8218	1668.5509	1679.7663
1681.1060	1682.9193	1687.2645
1691.3793	1696.3196	1698.2478
1700.0090	1712.1833	1820.9893
1880.5095	2997.8885	3004.0214
3037.1302	3059.9314	3064.7462
3066.4417	3071.4155	3072.2301
3074.9935	3075.3285	3077.3426
3078.2683	3078.8017	3080.8013
3086.0021	3086.3437	3098.0270
3130.1644	3130.9697	3132.4128
3133.7752	3143.7450	3147.8184
3148.5818	3151.2136	3154.3112
3154.9288	3157.9830	3159.3471
3163.1111	3166.3537	3167.1517
3171.0453	3172.8472	3174.3574
3180.1117	3181.1829	3182.4960
3186.0554	3186.4649	3188.1544
3194.4038	3197.2981	3206.5969
3206.9589	3207.3299	3207.3776
3210.5758	3213.8239	3221.5002
3224.8442	3227.4478	3231.7215
3232.6214	3233.3013	3250.8748
3259.9458	3270.7232	3552.7165

M8b1

Zero-point correction= 0.632311

Thermal correction to Energy= 0.666544
Thermal correction to Enthalpy= 0.667488
Thermal correction to Gibbs Free Energy= 0.566176
Sum of electronic and zero-point Energies= -1516.495012
Sum of electronic and thermal Energies= -1516.460779
Sum of electronic and thermal Enthalpies= -1516.459834
Sum of electronic and thermal Free Energies= -1516.561147
Cartesian coordinates

C	-0.121533	1.061537	-1.742974
O	-0.837269	1.046908	-2.698926
C	1.378194	0.861135	-1.607910
C	1.579496	-0.678594	-1.710789
H	1.913040	1.376374	-2.406148
H	0.857833	-1.175910	-1.052461
H	1.312109	-0.953009	-2.736937
C	2.964929	-1.155963	-1.368142
C	4.029204	-0.953512	-2.248976
C	3.205425	-1.772552	-0.137826
C	5.319423	-1.334457	-1.891748
H	3.848059	-0.485660	-3.213726
C	4.494034	-2.155796	0.221648
H	2.376450	-1.932747	0.549193
C	5.554896	-1.930092	-0.653118
H	6.141192	-1.169291	-2.581036
H	4.670405	-2.623499	1.184939
H	6.561779	-2.224059	-0.374867
N	-0.627951	1.131216	-0.393276
N	-1.965513	1.129403	-0.095133
C	-2.612272	2.282238	-0.505321
O	-2.055211	3.286680	-0.885015
O	-3.930895	2.118937	-0.386787
C	-4.716484	3.262856	-0.749540
H	-4.551868	3.511746	-1.798587
H	-5.750291	2.970410	-0.581095
H	-4.450871	4.116339	-0.124525
C	0.350346	1.243252	0.503215
C	1.637388	1.481292	-0.209053
C	0.240608	1.123520	1.892219
C	2.872055	1.228103	0.602051
H	1.618760	2.576823	-0.361814
C	1.418539	0.961158	2.582183
H	-0.729934	1.062052	2.369056
C	4.145270	1.356271	0.058007
C	2.725064	0.974695	1.983843

H	1.366731	0.790601	3.655015
C	5.262643	1.139450	0.855144
H	4.265275	1.588232	-0.995081
C	3.867851	0.764963	2.779861
C	5.126858	0.830249	2.214352
H	6.251536	1.208970	0.414258
H	3.746242	0.562169	3.839429
H	6.007771	0.659839	2.822720
N	-3.263013	-1.242081	0.249126
C	-2.355448	-2.340899	-0.172899
C	-1.077096	-2.340091	0.669100
C	-2.002331	-2.212914	-1.655341
H	-2.851270	-3.311684	-0.028249
H	-1.249068	-2.627461	1.707983
H	-0.359074	-3.047266	0.246106
H	-0.615704	-1.344935	0.670848
H	-2.851407	-2.428830	-2.306932
H	-1.648826	-1.202819	-1.891889
H	-1.209307	-2.922293	-1.904558
C	-3.541525	-1.243479	1.715679
C	-4.009377	-2.578739	2.305386
C	-4.505615	-0.126901	2.107743
H	-2.578251	-0.999920	2.181067
H	-3.328444	-3.403421	2.082778
H	-4.062627	-2.481296	3.393471
H	-5.004764	-2.852281	1.949427
H	-4.224960	0.826313	1.652018
H	-5.535014	-0.361531	1.819667
H	-4.487233	-0.011038	3.194159
C	-4.442338	-1.087521	-0.632034
C	-5.367795	-2.292938	-0.790452
H	-4.061581	-0.788317	-1.613159
H	-5.008290	-0.227414	-0.272276
H	-6.086667	-2.087987	-1.588130
H	-4.821245	-3.200289	-1.063167
H	-5.935656	-2.496890	0.119347
H	-2.474966	0.162397	-0.001895

Vibrational frequencies

17.2732	25.4967	25.8851
42.1488	53.7370	60.0626
70.2662	74.5105	76.4299
85.2221	93.1207	95.7956
102.1426	109.6742	113.7226
129.2845	131.4792	138.6588

152.5638	155.2270	161.9195
185.0445	205.1685	218.8831
223.0337	248.0315	250.0223
258.0622	259.6077	273.0557
279.8804	301.6506	319.0892
321.9885	339.0454	348.2461
354.2246	361.0865	370.0612
397.3207	413.9147	418.9287
420.7262	439.2886	451.3122
462.6688	478.6051	484.3163
497.6461	501.4094	504.1528
524.9143	552.8695	573.3609
590.3261	627.3687	633.4154
637.6835	652.0860	707.2027
707.6428	715.9128	721.9287
726.9983	733.8251	767.7134
775.4704	778.0802	781.7256
794.3294	814.5485	846.7506
863.8027	867.2577	872.7186
876.5213	893.9643	902.8129
906.3961	916.3961	931.8470
944.2042	954.5883	956.2439
967.4557	977.1304	982.0499
985.7096	990.6906	1001.6047
1003.1233	1017.4623	1018.4655
1026.1619	1027.3032	1045.4291
1068.7029	1078.7571	1079.7278
1089.4834	1090.4018	1099.3022
1114.2681	1121.5931	1134.7165
1143.5636	1150.1648	1155.8949
1166.7125	1173.4618	1177.6125
1181.5564	1189.6198	1190.4537
1192.4602	1205.2514	1207.4744
1224.6205	1228.8221	1235.6577
1243.0296	1252.8807	1255.9319
1256.3597	1263.8534	1278.2150
1309.4286	1335.0988	1340.8334
1350.3099	1359.8473	1362.2297
1366.7670	1369.5920	1374.8808
1385.2420	1385.6332	1389.9115
1392.9777	1408.0769	1411.0972
1414.1134	1427.3812	1429.6506
1435.2070	1436.2499	1476.5761
1477.3569	1488.3735	1491.7243

1495.3075	1496.1022	1499.4891
1500.6901	1505.5719	1506.7145
1507.6435	1507.9575	1510.3973
1512.8531	1516.6073	1518.9102
1528.4096	1544.8928	1551.0412
1554.9472	1592.0096	1639.3514
1664.5192	1675.9099	1677.5648
1697.1235	1699.2905	1852.4111
1938.8607	2179.4343	3000.5860
3048.6589	3067.1603	3073.0160
3074.5890	3077.3976	3078.8306
3083.4772	3083.8370	3101.8088
3106.0677	3134.5145	3146.5668
3149.2282	3151.8609	3153.7562
3156.4758	3159.6130	3164.7077
3168.4441	3169.0645	3169.9955
3172.5528	3178.4663	3182.4731
3192.7762	3199.2388	3213.1521
3215.1991	3216.2915	3218.2786
3220.7161	3222.8734	3230.0658
3235.1241	3240.7123	3257.1524

TS8b2

Zero-point correction= 1.017644

Thermal correction to Energy= 1.072310

Thermal correction to Enthalpy= 1.073254

Thermal correction to Gibbs Free Energy= 0.931850

Sum of electronic and zero-point Energies= -2568.037417

Sum of electronic and thermal Energies= -2567.982751

Sum of electronic and thermal Enthalpies= -2567.981807

Sum of electronic and thermal Free Energies= -2568.123211

Cartesian coordinates

C	-5.855618	-0.971736	-1.075105
C	-4.599911	-0.372167	-1.094106
C	-4.403420	0.899092	-1.616701
C	-5.501965	1.572901	-2.145223
C	-6.763788	0.973233	-2.147026
C	-6.950916	-0.300750	-1.611851
C	-5.792102	-2.328698	-0.419696
H	-3.416488	1.353031	-1.600909
H	-5.380211	2.571697	-2.551744
H	-7.611470	1.510596	-2.559938
H	-7.937431	-0.754221	-1.600944
H	-5.872621	-3.127232	-1.164477

C	-3.312631	-0.169859	1.701724
C	-4.600623	-0.827085	2.077369
C	-4.405640	-2.377010	0.261823
C	-3.562597	-1.271625	-0.463556
C	-1.533706	0.071542	0.443928
H	-4.723670	-0.811455	3.159786
H	-2.879640	-1.692257	-1.197370
N	-2.531559	0.610491	2.383920
N	-1.434001	0.758027	1.587070
N	-2.753225	-0.508324	0.502545
C	-0.451271	1.729660	1.989905
C	0.563766	1.344263	2.862760
C	-0.666054	3.050803	1.588367
C	1.492290	2.323526	3.218869
C	0.296750	3.987258	1.956301
C	1.396114	3.633801	2.744428
H	2.297926	2.058644	3.899186
H	0.174194	5.018981	1.635128
O	-4.487104	-2.178736	1.668096
H	-5.456190	-0.326012	1.607129
H	-3.927646	-3.351494	0.156267
H	-6.579436	-2.493004	0.321643
C	0.596377	-0.048430	3.425891
H	0.642977	-0.804378	2.637394
H	-0.323599	-0.253177	3.981026
H	1.443702	-0.169799	4.102049
C	2.442843	4.659153	3.092571
H	3.028097	4.923542	2.205880
H	3.131664	4.281690	3.851054
H	1.984716	5.578380	3.466658
C	-1.930070	3.433817	0.869135
H	-2.800898	3.137764	1.462873
H	-2.006064	2.946473	-0.108344
H	-1.968116	4.510947	0.709650
C	-0.544589	-0.322739	-0.703494
O	-1.156697	-0.615461	-1.764996
C	0.851874	0.390824	-0.857282
C	0.810947	1.332714	-2.068756
H	1.078269	0.949562	0.060010
H	1.800275	1.764084	-2.202422
H	0.602823	0.715878	-2.947017
C	-0.138660	2.506704	-2.050009
C	-1.384255	2.437811	-2.680365
C	0.287942	3.738723	-1.542362

C	-2.183574	3.574516	-2.801135
H	-1.709876	1.484874	-3.088824
C	-0.505503	4.875614	-1.664194
H	1.264707	3.810380	-1.067419
C	-1.745069	4.796981	-2.297283
H	-3.140938	3.506564	-3.309959
H	-0.153008	5.825037	-1.272022
H	-2.361508	5.684114	-2.401693
N	0.076595	-1.725834	0.056347
N	-0.793857	-2.775202	0.236782
C	-1.327855	-3.028887	1.475442
O	-1.216277	-2.305916	2.440839
O	-2.005603	-4.181321	1.438223
C	-2.637294	-4.551042	2.674183
H	-3.378097	-3.799168	2.946827
H	-3.112029	-5.510007	2.478112
H	-1.887451	-4.649616	3.460248
C	1.220061	-1.978322	-0.577792
C	1.887991	-0.780675	-1.044639
C	1.651682	-3.301804	-0.915667
C	2.737872	-0.991341	-2.259986
H	2.925033	-0.601426	-0.250809
C	2.463956	-3.440552	-1.991372
H	1.241144	-4.158072	-0.394651
C	3.467658	0.039596	-2.880271
C	2.994181	-2.312213	-2.711364
H	2.740283	-4.434859	-2.332700
C	4.295204	-0.205384	-3.965576
H	3.418973	1.051306	-2.502155
C	3.845551	-2.548068	-3.807978
C	4.475828	-1.504347	-4.453460
H	4.819754	0.624684	-4.427420
H	4.012107	-3.573618	-4.124871
H	5.127074	-1.690077	-5.300017
N	4.154681	-0.472667	0.605673
C	4.837516	-1.791622	0.383016
C	5.580979	-2.379822	1.587537
C	5.762029	-1.799656	-0.834574
H	4.003400	-2.475594	0.172079
H	4.933263	-2.515647	2.455585
H	5.954270	-3.366839	1.301463
H	6.441603	-1.773924	1.881658
H	5.306283	-1.362588	-1.722573
H	6.702297	-1.279006	-0.632832

H	6.005478	-2.840010	-1.065625
C	4.899918	0.755141	0.208523
C	6.220263	1.027468	0.942036
C	3.987525	1.978155	0.286467
H	5.146028	0.598420	-0.845177
H	6.862047	0.146586	0.987559
H	6.761966	1.800633	0.389428
H	6.067464	1.395979	1.956829
H	3.054697	1.823779	-0.264595
H	3.729600	2.235072	1.319154
H	4.501228	2.837075	-0.152906
C	3.436585	-0.408221	1.896380
C	4.210212	0.021258	3.146479
H	2.994988	-1.400388	2.044652
H	2.598571	0.281545	1.757191
H	3.641873	-0.265317	4.035416
H	5.193950	-0.441398	3.219555
H	4.344541	1.105172	3.177762
H	-0.956685	-3.420870	-0.527363

Vibrational frequencies

-1296.5248	18.6763	23.2054
26.8103	29.6774	39.0714
46.3438	47.3081	51.6789
56.8938	63.5893	72.6445
75.3088	80.0397	82.6547
89.7191	94.1982	97.0642
97.8023	105.0398	107.8060
110.9992	120.2352	123.8943
129.9359	133.2021	139.4690
145.5834	156.5353	160.2706
167.7108	175.6144	184.0326
188.8442	190.9455	195.5550
199.6098	209.7786	219.4283
230.6676	233.8842	238.1914
242.4859	249.1865	255.6425
256.6251	258.3473	266.3629
276.1803	283.3790	286.2585
291.5631	299.5657	304.4947
307.8738	313.7524	319.8377
327.7797	332.0782	341.0308
348.5000	349.9716	358.8761
360.2025	375.3845	376.6001
379.2006	381.8487	403.3932
408.8840	416.4500	418.2167

425.6944 427.8077 431.4986
445.5911 450.2146 462.5070
485.7505 490.3203 495.3883
496.2223 501.4040 510.0316
513.7409 526.1669 533.8651
537.7290 542.7250 558.7064
565.4192 566.5175 573.4522
581.9080 591.9571 597.2045
610.9493 622.2757 630.0652
630.8074 637.9780 650.4954
678.1631 689.2538 706.5863
713.0689 720.8559 723.2380
735.8471 738.1469 744.7282
748.8896 752.4123 757.3743
765.3528 774.1148 781.8666
787.2276 792.9186 803.6155
813.0828 815.2333 827.4659
840.6177 853.9043 857.6244
860.1042 866.5608 873.9042
878.0383 883.3885 889.5246
893.9493 900.6356 909.2539
911.4464 912.5694 934.1280
937.7011 948.0277 950.3546
955.1802 959.0029 960.5532
965.7349 966.3523 967.5160
979.7832 983.1143 990.7228
999.7344 1005.2636 1010.9427
1018.0836 1019.6286 1023.0045
1024.7411 1026.4483 1027.6663
1031.6216 1035.7492 1036.8217
1042.5482 1049.6422 1053.8588
1058.2334 1061.5976 1063.2543
1064.5746 1071.9049 1072.6447
1082.7816 1085.2346 1089.5042
1097.3571 1105.4494 1117.3315
1120.6821 1122.3926 1133.1671
1135.6305 1149.4360 1149.5894
1158.0142 1171.9658 1174.4755
1175.5370 1177.4805 1189.0711
1191.4229 1193.5069 1194.4046
1198.5893 1201.4792 1209.4764
1216.5595 1224.2826 1226.0462
1234.8849 1235.1320 1243.1811
1246.0266 1247.5571 1249.4302

1261.1467 1263.2467 1274.7011
1278.2606 1278.7399 1286.5989
1292.3884 1298.4130 1310.7337
1311.1627 1324.8575 1335.5152
1340.8243 1344.7992 1351.7169
1354.4682 1359.6923 1361.0466
1368.1663 1371.9951 1374.8689
1377.2358 1378.5532 1380.8155
1382.2681 1386.3103 1405.0533
1408.3883 1414.7766 1416.1441
1419.4092 1423.6926 1424.2979
1426.2094 1431.6806 1433.3068
1440.6802 1443.6017 1446.9997
1454.5958 1465.1115 1467.3015
1477.8204 1478.4029 1479.4561
1481.6305 1483.2042 1486.1886
1488.4406 1489.4856 1490.4469
1490.7373 1493.9873 1495.4817
1495.9834 1496.2412 1499.3058
1500.5771 1501.7579 1504.1122
1505.2139 1508.0616 1511.3533
1514.1684 1519.4046 1519.6723
1523.9051 1528.0716 1530.3857
1534.1389 1535.8954 1538.7134
1542.8704 1547.2678 1553.4961
1555.1487 1574.8090 1588.0467
1626.0774 1671.7647 1680.7247
1686.4613 1687.5668 1691.4410
1695.2799 1696.8530 1697.5675
1701.2191 1849.4145 3070.0628
3073.7188 3076.5919 3078.8597
3080.8763 3081.4651 3082.6863
3086.1901 3089.0763 3089.9689
3090.0118 3092.3151 3094.4745
3104.1552 3120.9147 3126.5901
3137.8366 3141.7956 3143.8905
3151.6558 3152.1168 3154.5401
3157.8991 3159.4211 3160.4185
3161.8314 3167.9901 3168.5515
3174.4160 3174.6825 3182.9186
3184.9417 3187.3273 3188.5078
3189.9674 3194.4363 3197.8465
3198.7529 3198.9481 3199.4504
3200.0872 3201.3219 3201.8603

3204.3223	3205.4612	3206.2972
3209.9919	3211.0055	3214.6779
3218.1877	3218.5605	3224.0746
3228.7078	3232.6366	3236.8349
3239.6491	3268.6253	3597.2926

M8b2

Zero-point correction= 1.025189
Thermal correction to Energy= 1.079757
Thermal correction to Enthalpy= 1.080701
Thermal correction to Gibbs Free Energy= 0.938821
Sum of electronic and zero-point Energies= -2568.087704
Sum of electronic and thermal Energies= -2568.033137
Sum of electronic and thermal Enthalpies= -2568.032193
Sum of electronic and thermal Free Energies= -2568.174073
Cartesian coordinates

C	6.513324	-0.673461	0.401180
C	5.250188	-0.093738	0.482670
C	5.080018	1.284416	0.490543
C	6.214030	2.091842	0.428143
C	7.486642	1.518719	0.364232
C	7.645943	0.133879	0.349009
C	6.409306	-2.177177	0.364400
H	4.083857	1.716376	0.535676
H	6.108263	3.172009	0.418245
H	8.360880	2.159705	0.313716
H	8.636106	-0.306345	0.280380
H	6.699642	-2.613102	1.326233
C	3.376694	-0.951264	-1.793309
C	4.592354	-1.730919	-2.179012
C	4.916863	-2.461195	0.084762
C	4.169683	-1.152449	0.511778
C	1.918459	-0.205598	-0.336257
H	4.470647	-2.140392	-3.181310
H	3.686141	-1.230435	1.485833
N	2.427544	-0.439100	-2.516876
N	1.533712	0.026784	-1.593337
N	3.115658	-0.815006	-0.457490
C	0.408055	0.800821	-2.035475
C	-0.799694	0.170104	-2.318737
C	0.607173	2.183783	-2.146855
C	-1.858883	0.993998	-2.714653
C	-0.485125	2.957364	-2.522669
C	-1.727062	2.378236	-2.808144

H	-2.804747	0.528674	-2.985174
H	-0.363059	4.034304	-2.608766
O	4.680195	-2.816990	-1.273049
H	5.490300	-1.100524	-2.151144
H	4.550368	-3.313429	0.657118
H	7.031540	-2.640430	-0.406816
C	-0.974449	-1.321189	-2.212363
H	-1.657929	-1.562852	-1.389708
H	-0.039666	-1.841715	-2.002139
H	-1.401816	-1.713534	-3.139789
C	-2.893739	3.242846	-3.209614
H	-3.420365	3.617343	-2.324897
H	-3.611311	2.684055	-3.815325
H	-2.560852	4.110329	-3.783660
C	1.949651	2.790807	-1.840767
H	2.741520	2.302703	-2.417364
H	2.191803	2.682901	-0.776118
H	1.951552	3.856550	-2.071337
C	1.136623	-0.174884	1.019710
O	1.948458	-0.209046	2.024533
C	-0.080088	0.863081	1.113624
C	0.209943	1.897402	2.217272
H	-0.244584	1.385873	0.167011
H	-0.733514	2.300062	2.594128
H	0.700621	1.365788	3.034621
C	1.075465	3.036981	1.743778
C	2.447300	3.052455	2.003030
C	0.517696	4.100721	1.025048
C	3.242031	4.112160	1.564355
H	2.881701	2.213649	2.540458
C	1.308032	5.156332	0.579988
H	-0.550651	4.103158	0.817140
C	2.676267	5.165614	0.850202
H	4.304952	4.114449	1.789193
H	0.856736	5.974161	0.026062
H	3.294468	5.990749	0.511331
N	0.347215	-1.515306	0.823300
N	1.057904	-2.630277	1.209152
C	1.587235	-3.430276	0.225477
O	1.351435	-3.355892	-0.962053
O	2.385308	-4.355106	0.784180
C	2.920893	-5.317206	-0.134616
H	3.490968	-4.811551	-0.915603
H	3.562617	-5.962182	0.462553

H	2.111934	-5.896422	-0.583635
C	-0.915632	-1.351671	1.384667
C	-1.263251	-0.019558	1.452685
C	-1.770749	-2.386678	1.829375
C	-2.562593	0.341863	1.885554
H	-5.239639	-0.117729	0.676222
C	-2.983523	-2.041698	2.370186
H	-1.438829	-3.417993	1.781916
C	-3.076088	1.669963	1.815978
C	-3.412959	-0.684797	2.410037
H	-3.638470	-2.808135	2.777222
C	-4.317283	1.979738	2.316971
H	-2.477902	2.440299	1.338499
C	-4.670925	-0.321254	2.964918
C	-5.115499	0.980366	2.929086
H	-4.690155	2.996632	2.249432
H	-5.281464	-1.097230	3.421937
H	-6.073428	1.245925	3.364960
N	-5.647810	-0.582469	-0.148620
C	-6.442237	-1.724466	0.497474
C	-6.827382	-2.852367	-0.450806
C	-7.631108	-1.182794	1.280266
H	-5.715392	-2.127172	1.210969
H	-5.955754	-3.381230	-0.838409
H	-7.407897	-3.571666	0.131492
H	-7.450325	-2.521000	-1.282447
H	-7.348063	-0.353422	1.932727
H	-8.447699	-0.862923	0.629503
H	-8.007485	-1.989047	1.913272
C	-6.448660	0.548659	-0.793371
C	-7.418032	0.116383	-1.885495
C	-5.489364	1.642247	-1.247825
H	-7.034078	0.943303	0.041412
H	-8.198318	-0.546288	-1.511758
H	-7.910116	1.021699	-2.249070
H	-6.927893	-0.356579	-2.735581
H	-4.779254	1.910502	-0.458947
H	-4.931085	1.356432	-2.141989
H	-6.074056	2.531327	-1.492488
C	-4.430256	-1.070604	-0.908243
C	-4.635374	-1.462306	-2.364045
H	-4.049811	-1.912374	-0.321462
H	-3.687157	-0.269954	-0.831446
H	-3.710106	-1.933392	-2.702757

H	-5.442059	-2.178590	-2.511776
H	-4.818376	-0.599987	-3.006940
H	1.574481	-2.536817	2.081966

Vibrational frequencies

16.3360	19.2468	27.8579
31.6505	34.8305	40.2974
43.8932	50.9693	52.7438
60.3786	66.1898	71.6151
76.4350	81.7242	88.8058
92.1551	101.6828	103.8596
106.0171	111.6960	114.6259
119.2721	125.6861	130.2451
132.0104	141.7551	144.4025
149.1321	172.6605	176.4435
179.6956	186.3726	188.0672
200.7220	208.6228	216.9864
221.7243	225.5604	227.5372
232.6887	234.7130	239.2443
246.4080	247.1975	248.0816
259.8836	261.1881	264.4391
267.7585	280.6744	284.9733
295.8817	303.0314	307.0439
309.7955	317.8590	329.6221
334.2790	337.1189	342.9670
348.7150	355.1531	358.9078
363.1333	382.4530	384.9685
400.1945	409.8316	412.0150
421.1669	421.4009	428.7318
432.2254	443.9332	448.4108
457.2835	477.3027	491.1478
496.2031	497.5687	501.8662
514.3695	518.6574	526.1290
528.3760	540.6622	551.7958
554.8840	555.2714	565.1645
577.0509	582.9545	588.6740
592.0614	601.6016	613.1439
626.3068	631.8926	632.8254
638.7351	652.2410	674.5828
688.1795	710.1234	714.5606
715.8772	719.9790	732.6329
741.3136	751.8957	755.9468
759.5062	766.3429	773.5481
783.5955	784.5934	787.9331
790.5986	794.6768	810.9338

822.2850 843.3486 846.5540
851.4731 853.3128 856.3885
875.9315 878.8024 881.4578
882.5247 884.8654 890.4920
896.6699 913.5102 916.3947
917.5762 938.9770 941.6810
947.5038 952.7706 953.5971
957.5767 958.2070 960.0937
969.4089 976.0526 978.6977
983.6470 985.1025 988.4141
998.3630 1000.3549 1004.7554
1017.5544 1018.7885 1020.0377
1020.6954 1026.0548 1029.5125
1036.4694 1044.1896 1049.3279
1055.2312 1056.9065 1059.4883
1063.0385 1064.7753 1067.0022
1068.2614 1068.6836 1069.8324
1075.5279 1077.8266 1087.4862
1096.4074 1113.4446 1117.3405
1125.0230 1126.4114 1131.5390
1134.5425 1147.6992 1161.1294
1166.9093 1175.6269 1177.2998
1180.4204 1183.8643 1186.1708
1194.2113 1200.8021 1201.7698
1203.6783 1205.5094 1207.1784
1216.9811 1219.2539 1226.7195
1231.8630 1232.7595 1234.6294
1243.7452 1245.8911 1252.4001
1257.4133 1268.6732 1278.1156
1282.6194 1286.1113 1288.3882
1291.8538 1310.7575 1311.7376
1327.2193 1332.5889 1340.4128
1342.3287 1351.4441 1354.7775
1361.0520 1361.9488 1366.5514
1367.3534 1373.9632 1376.1569
1382.6284 1385.4945 1392.8159
1399.6451 1405.9351 1412.6492
1415.0374 1416.7069 1419.2063
1421.4195 1423.6512 1426.9811
1428.7607 1431.1086 1436.3069
1438.8379 1440.5132 1452.6666
1458.3320 1461.7814 1465.4990
1474.7163 1475.2370 1478.5067
1481.7981 1483.2033 1488.5025

1489.0910	1490.7996	1491.0121
1493.6475	1496.3039	1496.7997
1499.9373	1500.8155	1503.8030
1505.8622	1506.6776	1508.1246
1510.2059	1515.5565	1517.9002
1518.6843	1520.4322	1523.4218
1523.5005	1524.6147	1527.7037
1533.1781	1534.5621	1536.6685
1537.6688	1541.2274	1551.9516
1576.7273	1577.9130	1658.9587
1675.0259	1678.9807	1682.6613
1687.0001	1692.3489	1697.5694
1698.0647	1703.9380	1704.5328
1843.2445	3066.0564	3066.3723
3066.7411	3082.3589	3084.0220
3084.5524	3088.1935	3094.0561
3103.0716	3104.8878	3105.7333
3106.6791	3110.7068	3117.4262
3122.7697	3132.5764	3133.4147
3135.8822	3136.0111	3139.7930
3155.2411	3164.5396	3166.4869
3169.7452	3170.8561	3173.6913
3175.4589	3177.5553	3179.4407
3180.9350	3181.0967	3182.6646
3184.6994	3185.0150	3188.5638
3188.6030	3190.2946	3192.4519
3192.6098	3194.7004	3195.1911
3200.2061	3202.8629	3203.5494
3204.6994	3207.2560	3207.7043
3212.0004	3212.6452	3213.3158
3214.3279	3219.3809	3224.6033
3225.2765	3225.8879	3233.1637
3236.4567	3370.0235	3523.4182

TS7b3

Zero-point correction= 1.005983

Thermal correction to Energy= 1.059311

Thermal correction to Enthalpy= 1.060256

Thermal correction to Gibbs Free Energy= 0.923280

Sum of electronic and zero-point Energies= -2567.570832

Sum of electronic and thermal Energies= -2567.517504

Sum of electronic and thermal Enthalpies= -2567.516560

Sum of electronic and thermal Free Energies= -2567.653535

Cartesian coordinates

C	-5.809863	-0.741504	-1.184012
C	-4.552476	-0.153728	-1.065993
C	-4.373311	1.218554	-1.204243
C	-5.493161	2.008052	-1.457757
C	-6.758668	1.426813	-1.578321
C	-6.925729	0.049120	-1.446183
C	-5.722960	-2.237406	-1.001239
H	-3.373738	1.639025	-1.130787
H	-5.382253	3.082781	-1.565439
H	-7.621284	2.055580	-1.776238
H	-7.911496	-0.397495	-1.538665
H	-5.836227	-2.750735	-1.962116
C	-3.173103	-0.869322	1.607698
C	-4.444311	-1.630924	1.795430
C	-4.309442	-2.490131	-0.427152
C	-3.498107	-1.199397	-0.784164
C	-1.449165	-0.176699	0.435478
H	-4.527653	-1.964662	2.830042
H	-2.839462	-1.371132	-1.629804
N	-2.390729	-0.316345	2.481102
N	-1.325146	0.114918	1.738488
N	-2.655520	-0.785416	0.350215
C	-0.380109	0.951903	2.422490
C	0.385300	0.403974	3.455528
C	-0.450035	2.323366	2.168481
C	1.238935	1.273546	4.134260
C	0.450290	3.146084	2.844759
C	1.316011	2.632581	3.812921
H	1.852711	0.880405	4.942202
H	0.439616	4.214128	2.641099
O	-4.349848	-2.773469	0.969097
H	-5.315701	-1.011250	1.544939
H	-3.819293	-3.361293	-0.860100
H	-6.482713	-2.640566	-0.324787
C	0.201563	-1.027872	3.879297
H	0.187553	-1.708216	3.021228
H	-0.764756	-1.131613	4.381937
H	0.983080	-1.321794	4.580513
C	2.310112	3.521991	4.511445
H	3.296982	3.427149	4.045029
H	2.417029	3.245850	5.563279
H	2.013981	4.571461	4.454816
C	-1.562650	2.869333	1.316771
H	-2.524048	2.614875	1.779063

H	-1.562903	2.451196	0.308309
H	-1.492227	3.952754	1.227083
C	-0.617773	-0.022336	-0.906355
O	-1.456526	0.291710	-1.831654
C	0.763090	0.805296	-0.934952
C	0.630773	1.935434	-1.981499
H	0.983275	1.216200	0.057082
H	1.629012	2.249389	-2.280495
H	0.155565	1.486705	-2.855690
C	-0.109201	3.191808	-1.600176
C	-1.405740	3.435628	-2.062281
C	0.526310	4.181538	-0.843144
C	-2.053104	4.634028	-1.769263
H	-1.900429	2.659717	-2.638852
C	-0.113573	5.385150	-0.553876
H	1.540480	4.009528	-0.485820
C	-1.408158	5.614901	-1.016761
H	-3.059343	4.807902	-2.139761
H	0.399346	6.145390	0.028193
H	-1.908620	6.552684	-0.796562
N	-0.056128	-1.484822	-1.079414
N	-0.884447	-2.601426	-1.124714
C	-0.935626	-3.155451	0.092734
O	-0.374891	-2.814840	1.146521
O	-1.770575	-4.243754	0.079734
C	-1.984374	-4.841871	1.347697
H	-2.403593	-4.120676	2.053264
H	-2.698242	-5.649364	1.180961
H	-1.054225	-5.244502	1.757689
C	1.129173	-1.459045	-1.626322
C	1.846237	-0.220968	-1.414689
C	1.638332	-2.527275	-2.455367
C	2.912376	0.066810	-2.397963
H	2.763147	-0.534735	-0.404593
C	2.638448	-2.228659	-3.312156
H	1.114105	-3.474575	-2.461394
C	3.706043	1.230932	-2.345636
C	3.297914	-0.938135	-3.323649
H	2.986436	-2.974956	-4.022451
C	4.760969	1.432205	-3.222619
H	3.497312	1.985491	-1.592063
C	4.368390	-0.717323	-4.207554
C	5.090107	0.461506	-4.176460
H	5.339996	2.348316	-3.159522

H	4.631408	-1.503627	-4.910440
H	5.913056	0.622707	-4.864093
N	3.673367	-0.944122	0.546718
C	4.395223	-2.070001	-0.146056
C	4.837092	-3.244882	0.732953
C	5.574830	-1.598643	-0.996311
H	3.632623	-2.470084	-0.824892
H	4.008811	-3.690682	1.286312
H	5.239285	-4.016088	0.070157
H	5.627380	-2.972618	1.437322
H	5.332481	-0.742475	-1.625859
H	6.445142	-1.350371	-0.381652
H	5.861862	-2.421608	-1.656460
C	4.502015	0.231918	0.945486
C	5.608475	-0.031306	1.974340
C	3.615567	1.381419	1.411164
H	4.984476	0.548724	0.016800
H	6.185236	-0.930042	1.750685
H	6.298875	0.817001	1.955835
H	5.215208	-0.114243	2.988646
H	2.861686	1.642035	0.663882
H	3.100968	1.146965	2.347249
H	4.239149	2.263201	1.583649
C	2.675839	-1.430154	1.533495
C	3.181337	-1.766646	2.938709
H	2.185758	-2.294904	1.074353
H	1.891142	-0.666977	1.598220
H	2.506986	-2.492867	3.396517
H	4.181669	-2.197501	2.935680
H	3.199639	-0.877428	3.576231

Vibrational frequencies

-1328.8801	26.6554	31.2033
33.2016	35.2411	45.3362
49.4667	53.2056	58.9116
62.4556	68.2563	69.7694
74.7429	90.8343	92.7914
94.0131	97.7721	101.2367
106.9824	110.4264	115.4058
121.4393	123.6534	125.8855
135.0210	141.7895	146.2649
152.9834	162.6750	173.0158
175.3038	180.4198	189.9723
195.8377	198.4476	209.5465
214.8014	220.4228	229.0031

239.8158 244.1144 250.0101
256.3511 258.5249 262.9846
268.7477 275.0904 276.9101
285.9103 296.9530 306.0852
306.2709 315.0053 319.3638
324.7099 326.8088 331.1083
343.6891 344.8503 347.5877
351.1055 357.3606 369.6967
378.0055 381.4291 387.3693
397.6383 404.0885 415.1759
419.7932 424.9723 425.5015
432.9603 438.8686 451.0874
456.9632 464.1942 485.5599
492.6566 495.7892 503.2555
508.5687 516.9526 517.6864
524.8354 538.4742 541.8916
553.5817 566.6020 568.1069
576.4394 588.7751 593.3425
597.8167 600.4936 610.1977
627.5954 629.6344 633.5363
635.6727 650.4436 685.6770
693.3403 702.5245 713.7041
720.1504 721.4036 733.1813
742.0596 746.8965 750.2242
754.9549 760.9026 771.8618
775.3519 784.1606 788.7879
805.1636 808.4109 817.7198
823.3998 839.1025 851.2421
855.9227 857.7712 871.0406
872.8870 876.7030 879.1106
883.0233 889.1168 899.3879
906.1459 909.4040 913.3589
918.2426 926.5244 940.2679
941.3108 945.2223 952.1564
957.4281 963.1026 968.6352
972.8970 974.8829 982.5614
984.8161 990.8751 993.1145
1002.8035 1006.4223 1007.3594
1016.6502 1018.2456 1022.2143
1022.7936 1025.7766 1029.2865
1031.1781 1036.7869 1044.4774
1049.6617 1060.1637 1064.5410
1065.0826 1066.4883 1068.6261
1069.3810 1071.0515 1075.3492

1076.4245	1080.2272	1087.7668
1109.2490	1114.8594	1116.0475
1121.0026	1125.9044	1132.2305
1148.8864	1149.4015	1153.1155
1162.9690	1173.0591	1174.0433
1175.2612	1179.0442	1188.3228
1191.1139	1192.3496	1197.8809
1200.8360	1202.2846	1207.0803
1207.7717	1211.0507	1216.8565
1228.3982	1232.4906	1238.3112
1243.0160	1243.6574	1255.3672
1257.4380	1260.2613	1278.1496
1279.2980	1288.0352	1295.7355
1301.7426	1305.6158	1320.2897
1333.2367	1335.3226	1337.8809
1341.3158	1351.8608	1356.2854
1359.3621	1362.5356	1366.0171
1366.2670	1368.1990	1369.8109
1371.4615	1375.2056	1383.4213
1386.0913	1401.1671	1409.3150
1412.9640	1416.2597	1421.3380
1424.0220	1425.3910	1425.7895
1428.7177	1434.4419	1436.5591
1449.2306	1449.5947	1452.9591
1456.4659	1464.4706	1476.2944
1478.3983	1479.9757	1481.9936
1487.7159	1491.2611	1492.4360
1493.1014	1494.5587	1495.2146
1495.9571	1498.3103	1499.3182
1501.9037	1504.5003	1507.1336
1507.4827	1507.8145	1511.2468
1513.5248	1514.3726	1516.6354
1519.4829	1521.0637	1523.7183
1529.0706	1532.2829	1534.5373
1536.7701	1538.3761	1549.4450
1550.9372	1564.4349	1567.9981
1624.9435	1662.5017	1673.9636
1678.7541	1682.2699	1690.7351
1695.5646	1697.4530	1699.1330
1700.8899	1708.6117	1718.3144
3066.2016	3068.7119	3071.9775
3075.5955	3076.0861	3077.1125
3080.4040	3082.9440	3084.4651
3087.2982	3091.6857	3096.9890

3099.1153	3099.6427	3125.1110
3129.1194	3132.2048	3133.6188
3138.5172	3149.1376	3150.2498
3152.3720	3153.5953	3156.5780
3161.0684	3162.3499	3165.8009
3168.2461	3170.6714	3172.8206
3173.2286	3173.6588	3177.6462
3177.7500	3180.7340	3181.6262
3185.5740	3190.9033	3191.3561
3195.5634	3195.9797	3196.0533
3201.3273	3202.8305	3203.3172
3204.8724	3206.0384	3210.4321
3214.2813	3214.5682	3217.3843
3218.1905	3222.3140	3227.4811
3227.7938	3232.6152	3246.0514

M7b3

Zero-point correction= 1.010092
Thermal correction to Energy= 1.064829
Thermal correction to Enthalpy= 1.065773
Thermal correction to Gibbs Free Energy= 0.923027
Sum of electronic and zero-point Energies= -2567.604960
Sum of electronic and thermal Energies= -2567.550224
Sum of electronic and thermal Enthalpies= -2567.549279
Sum of electronic and thermal Free Energies= -2567.692026
Cartesian coordinates

C	-5.910325	-1.121632	-1.362487
C	-4.676528	-0.475435	-1.372364
C	-4.513116	0.777057	-1.955460
C	-5.629337	1.391917	-2.519013
C	-6.873322	0.755181	-2.506355
C	-7.021934	-0.507795	-1.934622
C	-5.803291	-2.474421	-0.702411
H	-3.520467	1.219314	-1.980560
H	-5.532196	2.370591	-2.978598
H	-7.733091	1.247750	-2.950078
H	-7.989840	-1.000871	-1.930710
H	-5.843963	-3.272919	-1.451036
C	-3.489189	-0.243346	1.500173
C	-4.745224	-0.975973	1.838728
C	-4.425477	-2.471021	-0.001228
C	-3.619854	-1.318579	-0.695487
C	-1.719888	0.135942	0.263262
H	-4.897190	-0.983060	2.918070

H	-2.876518	-1.709838	-1.387499
N	-2.785809	0.596265	2.196005
N	-1.691236	0.836780	1.402420
N	-2.893205	-0.529952	0.309733
C	-0.807171	1.881329	1.847612
C	0.216326	1.556880	2.738093
C	-1.123955	3.194080	1.489855
C	0.997162	2.605491	3.221692
C	-0.336312	4.210398	2.025684
C	0.730871	3.933588	2.880529
H	1.813125	2.380944	3.905291
H	-0.545057	5.240014	1.746208
O	-4.558017	-2.310663	1.410535
H	-5.614261	-0.508226	1.355825
H	-3.885991	-3.411698	-0.113370
H	-6.595898	-2.671446	0.026047
C	0.394811	0.138692	3.198752
H	0.396662	-0.571916	2.364843
H	-0.451773	-0.156437	3.828615
H	1.305608	0.040753	3.793704
C	1.560302	5.052315	3.454341
H	2.594700	4.736064	3.611394
H	1.161609	5.371361	4.423103
H	1.560485	5.918486	2.788709
C	-2.298035	3.491598	0.596549
H	-3.232512	3.163928	1.064828
H	-2.216965	2.968306	-0.361585
H	-2.363741	4.561880	0.395055
C	-0.795431	-0.026805	-0.985777
O	-1.541125	0.036106	-2.045515
C	0.508858	0.882000	-1.022088
C	0.229769	2.206155	-1.742030
H	0.834085	1.059321	0.016251
H	0.585270	2.127421	-2.777570
H	-0.856016	2.306775	-1.844389
C	0.802931	3.467295	-1.131598
C	0.192358	4.694790	-1.417071
C	1.943222	3.477777	-0.322750
C	0.707063	5.890470	-0.926330
H	-0.702912	4.706414	-2.034697
C	2.471484	4.673004	0.162123
H	2.431400	2.541783	-0.064252
C	1.857156	5.884897	-0.137188
H	0.212032	6.828006	-1.161257

H	3.359600	4.652933	0.787490
H	2.265736	6.816122	0.243425
N	-0.100753	-1.377711	-0.705796
N	-0.843088	-2.574587	-0.668150
C	-1.059057	-2.936172	0.594503
O	-0.772532	-2.382327	1.673436
O	-1.738418	-4.141929	0.621668
C	-2.134385	-4.573520	1.911944
H	-2.827831	-3.861027	2.366799
H	-2.632124	-5.534184	1.767590
H	-1.272699	-4.700940	2.573668
C	1.029622	-1.365104	-1.469445
C	1.492736	-0.068173	-1.691064
C	1.695343	-2.503572	-1.990038
C	2.694223	0.136440	-2.406876
H	3.257828	-1.919410	-0.329646
C	2.856235	-2.313458	-2.703301
H	1.256783	-3.483032	-1.832048
C	3.279304	1.416308	-2.663248
C	3.393431	-1.015662	-2.914915
H	3.384684	-3.167194	-3.123447
C	4.458783	1.538908	-3.350247
H	2.783655	2.309468	-2.305234
C	4.613308	-0.845183	-3.624311
C	5.144628	0.398902	-3.839863
H	4.874138	2.527250	-3.523221
H	5.116580	-1.734147	-3.998675
H	6.076921	0.515824	-4.382036
N	3.582590	-2.281121	0.579143
C	4.314799	-3.555684	0.162039
C	4.543313	-4.551697	1.291179
C	5.583913	-3.219698	-0.609647
H	3.604845	-4.004305	-0.540540
H	3.604384	-4.952836	1.674464
H	5.107968	-5.389141	0.874351
H	5.120866	-4.138907	2.119268
H	5.395850	-2.478302	-1.392082
H	6.385128	-2.858805	0.039821
H	5.934513	-4.133564	-1.093880
C	4.433490	-1.133252	1.111034
C	5.277543	-1.470944	2.333124
C	3.548101	0.091206	1.313142
H	5.110034	-0.915111	0.279765
H	6.040281	-2.218909	2.114519

H	5.796444	-0.555763	2.629094
H	4.685384	-1.807861	3.183814
H	2.932408	0.277527	0.427012
H	2.894555	-0.004669	2.182799
H	4.192209	0.960078	1.467644
C	2.268114	-2.554252	1.291875
C	2.292144	-2.741306	2.797548
H	1.856999	-3.437882	0.793950
H	1.596652	-1.733311	1.032379
H	1.256809	-2.966377	3.067678
H	2.934824	-3.554266	3.135491
H	2.574151	-1.828782	3.323567

Vibrational frequencies

19.1980	20.1538	27.2677
29.3009	34.5510	38.9050
42.6347	49.7818	52.4295
57.4000	61.8881	68.1034
70.3718	76.8656	80.9963
87.0437	90.2245	98.7961
102.7515	103.9018	115.8998
125.2644	129.2838	130.0743
138.0004	144.3760	146.6789
151.5399	156.5942	166.4673
171.6572	178.8675	187.0095
191.9490	194.3238	204.4062
211.8589	216.5674	228.9137
234.1559	238.0847	243.2115
245.8415	248.2549	250.9394
256.1318	264.2366	270.9937
274.9280	277.3939	278.7690
287.9169	293.7416	295.7416
300.0075	305.8029	308.1212
327.4658	333.7327	339.1395
348.5169	351.4937	353.9029
366.5399	372.4680	374.2622
384.2400	408.3301	411.3227
418.7367	419.1090	433.6095
439.9302	445.8002	449.8336
470.4558	471.3097	490.1766
495.7004	502.4489	510.0719
515.2706	519.9832	529.9549
534.8222	542.4455	545.6721
551.4929	563.6579	573.4753
587.7229	591.2856	592.4924

602.7755 608.9690 616.3318
624.5366 630.1658 640.1460
653.2825 685.7321 691.4005
708.6655 713.5867 717.0293
719.5954 727.6077 733.9152
741.5079 748.4022 758.9213
762.6620 772.6868 774.1473
781.4506 787.7881 792.5652
795.9873 812.6747 817.6783
840.5967 852.5782 854.4209
858.4270 867.6254 875.0648
879.3090 881.8650 882.4756
883.3969 890.1865 892.9567
916.2348 919.9262 923.4612
927.4879 936.1468 948.7382
952.4620 952.9838 957.2724
961.3290 967.4635 970.3317
979.9776 983.8158 985.7047
987.5002 990.8901 1001.5590
1002.0942 1003.7905 1011.7655
1014.4680 1017.2177 1023.4636
1025.3253 1025.9889 1039.5595
1043.1622 1049.6784 1052.4923
1053.2261 1056.2014 1059.3438
1060.0409 1061.9015 1063.1983
1070.7112 1073.8927 1076.3665
1083.9070 1087.8041 1104.8236
1113.0777 1122.8607 1125.6652
1127.0664 1129.9068 1143.0925
1150.6372 1157.9988 1169.3768
1172.2667 1172.9876 1177.2700
1186.5750 1186.9790 1191.1072
1192.9932 1202.5584 1203.9104
1206.4142 1207.2093 1208.7787
1218.9669 1219.8398 1223.4025
1224.6396 1225.5337 1232.7166
1238.2517 1242.3212 1252.9230
1257.7229 1280.3465 1282.6896
1284.8715 1294.2430 1299.4881
1307.2077 1322.5384 1328.8304
1336.4440 1339.3327 1343.5698
1348.2340 1354.9505 1357.3974
1361.7149 1362.8020 1365.6738
1371.3761 1373.9936 1386.0068

1389.5870	1393.8597	1398.1367
1401.0485	1403.0087	1406.5326
1415.2276	1416.0811	1416.7109
1420.3553	1423.6567	1426.6697
1427.8962	1431.4929	1439.8159
1440.4403	1447.2930	1451.8182
1463.7576	1466.4209	1469.9399
1477.0474	1481.1248	1483.7306
1485.1168	1485.7689	1488.9916
1491.5250	1492.5654	1494.9807
1495.4856	1496.0700	1496.6911
1498.2159	1500.1725	1501.7605
1503.5765	1504.6021	1508.3749
1511.0290	1512.6148	1514.9083
1515.2149	1519.9327	1523.2121
1525.7121	1530.7641	1532.0537
1534.9740	1539.2914	1541.3571
1552.5481	1575.0884	1580.3937
1644.1250	1669.0264	1671.1554
1681.4847	1688.7772	1696.0567
1696.4851	1698.5466	1704.4137
1707.5040	1712.0800	3030.8569
3060.1751	3064.9206	3066.9437
3067.6022	3067.8790	3069.9605
3078.1081	3078.6849	3081.6848
3095.6708	3097.5440	3100.7313
3115.2018	3116.1287	3118.8748
3125.3479	3128.7905	3131.1615
3134.0489	3137.1953	3149.2058
3159.6011	3162.1173	3162.5341
3163.1111	3167.8235	3168.2439
3169.4470	3170.6010	3170.6718
3173.6367	3174.9425	3175.7393
3176.9076	3181.5006	3182.0228
3182.9918	3183.9002	3188.4007
3192.5727	3193.6184	3194.2814
3196.3184	3201.4805	3201.5938
3205.0967	3209.0118	3209.2883
3210.3059	3210.6074	3215.9045
3222.7262	3227.9357	3231.9756
3249.8971	3256.2050	3372.2972

TS6c

Zero-point correction= 1.017722

Thermal correction to Energy= 1.073177
Thermal correction to Enthalpy= 1.074122
Thermal correction to Gibbs Free Energy= 0.927627
Sum of electronic and zero-point Energies= -2568.069535
Sum of electronic and thermal Energies= -2568.014079
Sum of electronic and thermal Enthalpies= -2568.013135
Sum of electronic and thermal Free Energies= -2568.159630
Cartesian coordinates

C	0.393185	5.061680	-1.487999
C	0.996782	3.818218	-1.314252
C	2.349280	3.624835	-1.582350
C	3.096794	4.710784	-2.030679
C	2.496521	5.959920	-2.209553
C	1.142117	6.143452	-1.942478
C	-1.071943	5.012250	-1.140664
H	2.812701	2.651421	-1.452632
H	4.153299	4.584895	-2.242479
H	3.094026	6.796877	-2.556030
H	0.679471	7.116222	-2.077404
H	-1.685574	5.039901	-2.046845
C	0.501061	2.652421	1.604729
C	-0.241515	3.938482	1.764535
C	-1.264349	3.667880	-0.407903
C	-0.012279	2.808449	-0.805248
C	1.165022	0.919239	0.478526
H	-0.536873	4.066793	2.805702
H	-0.281805	2.063490	-1.555184
N	1.122642	1.902612	2.474217
N	1.524938	0.826813	1.755414
N	0.516363	2.089469	0.364267
C	2.326364	-0.210357	2.351235
C	1.694533	-1.138543	3.185373
C	3.686424	-0.240705	2.032803
C	2.488175	-2.174709	3.672799
C	4.431413	-1.296512	2.556463
C	3.847718	-2.275310	3.362088
H	2.032710	-2.921529	4.318335
H	5.491349	-1.353070	2.323010
O	-1.419422	3.840747	0.992166
H	0.387843	4.784145	1.455490
H	-2.176857	3.151205	-0.710469
H	-1.396966	5.836098	-0.499234
C	0.242092	-1.003744	3.555295
H	-0.378072	-0.700149	2.705816

H	0.122443	-0.234129	4.324795
H	-0.130988	-1.947188	3.958357
C	4.661872	-3.430120	3.882778
H	4.421654	-3.640040	4.927734
H	5.731575	-3.227423	3.805664
H	4.448309	-4.337420	3.308778
C	4.316008	0.795219	1.138975
H	3.927289	1.796375	1.347922
H	4.139097	0.568961	0.078741
H	5.397704	0.806054	1.279585
C	1.476284	0.019198	-0.695475
O	1.524259	0.579545	-1.767876
C	1.647245	-1.479710	-0.533675
C	2.437366	-2.014482	-1.742116
H	2.244492	-1.669140	0.362994
H	2.445391	-3.105592	-1.686873
H	1.933647	-1.732228	-2.670877
C	3.859070	-1.498720	-1.716484
C	4.272151	-0.441978	-2.532657
C	4.779331	-2.055146	-0.821238
C	5.572693	0.053319	-2.450046
H	3.563731	-0.001389	-3.228241
C	6.079223	-1.563997	-0.737791
H	4.471389	-2.881068	-0.182767
C	6.478506	-0.504371	-1.550781
H	5.877427	0.875110	-3.090358
H	6.781801	-2.009319	-0.039843
H	7.490675	-0.118566	-1.485555
N	-1.350833	-0.486401	0.442800
N	-2.382845	0.400288	0.224959
C	-2.541247	1.217890	1.324749
O	-1.843094	1.286582	2.320899
O	-3.646350	1.976896	1.150799
C	-4.011206	2.784564	2.269534
H	-3.217208	3.496659	2.494564
H	-4.919712	3.305987	1.970478
H	-4.206365	2.159569	3.144966
C	-0.906310	-1.160171	-0.560613
C	0.217309	-2.131935	-0.259793
C	-1.287969	-1.025554	-1.967306
C	0.039040	-3.409169	-1.049201
H	0.176472	-2.351579	0.810600
C	-1.058620	-2.047896	-2.811415
H	-1.765009	-0.105662	-2.291662

C	0.488181	-4.633331	-0.566484
C	-0.526905	-3.331584	-2.335545
H	-1.330343	-1.970884	-3.861110
C	0.391101	-5.781779	-1.352787
H	0.925654	-4.688110	0.427359
C	-0.609467	-4.484427	-3.120678
C	-0.151586	-5.705337	-2.633020
H	0.744239	-6.732107	-0.966455
H	-1.043713	-4.420021	-4.114511
H	-0.220505	-6.595416	-3.249290
N	-4.604857	-0.901004	-0.192891
C	-4.391681	-1.913463	0.900166
C	-5.178653	-3.217268	0.760141
C	-4.575430	-1.305161	2.288683
H	-3.328256	-2.170743	0.803024
H	-4.907322	-3.762835	-0.145759
H	-4.929827	-3.857084	1.610881
H	-6.259081	-3.060288	0.764129
H	-3.987666	-0.394645	2.428380
H	-5.623009	-1.085198	2.509978
H	-4.227125	-2.031936	3.026070
C	-5.736180	0.066918	-0.011284
C	-7.138313	-0.529647	0.128244
C	-5.674083	1.130332	-1.105582
H	-5.505839	0.574958	0.927255
H	-7.223500	-1.179940	1.000628
H	-7.838918	0.297985	0.272598
H	-7.460792	-1.085779	-0.752005
H	-4.662082	1.533439	-1.197555
H	-5.998182	0.746442	-2.076621
H	-6.340310	1.953227	-0.835001
C	-4.452427	-1.484070	-1.553828
C	-5.663088	-2.102579	-2.251337
H	-3.655487	-2.228376	-1.466834
H	-4.055491	-0.689424	-2.192992
H	-5.300711	-2.620081	-3.143941
H	-6.192813	-2.828771	-1.634374
H	-6.375902	-1.345895	-2.582998
H	-3.510759	-0.175040	-0.068328

Vibrational frequencies

-972.9146	9.6330	15.7577
23.3606	25.9698	28.3976
36.7788	43.5662	44.9483
49.4946	56.7857	59.5464

64.1037 71.8012 72.8329
77.8936 81.0523 81.6439
83.9653 91.7855 95.7065
98.7667 105.6237 110.0810
115.3674 118.0352 126.2630
130.3348 142.9137 151.7116
161.2636 171.5992 177.1207
188.2346 191.2201 194.9702
205.1023 210.3653 213.8285
220.3139 230.5193 231.1867
233.6167 236.6139 239.9658
243.2181 253.1190 255.0459
266.1572 270.5869 274.9029
285.6394 289.6301 294.0185
298.7971 302.6048 306.9354
315.3743 333.0962 336.1928
340.3904 347.8133 353.8013
358.9574 363.2689 366.0590
386.1335 393.7625 395.0702
396.9838 405.8539 412.5218
419.8274 423.9213 425.2177
445.3075 446.9464 460.3393
486.5062 487.5606 497.6689
503.2170 509.5199 518.8606
521.4948 526.7915 530.9377
534.5467 547.4777 561.6190
565.1637 575.8065 589.1016
596.0095 600.6083 607.6760
610.9279 622.6822 631.4288
644.6124 654.1726 668.4948
682.3843 686.9781 712.2692
715.5939 721.0780 725.1993
733.0826 744.3355 754.3669
755.5927 766.0784 773.1046
775.3371 781.4861 789.0229
804.4211 809.3159 810.9133
819.4529 826.3303 836.1076
844.8831 855.7191 868.9026
869.8823 874.7712 881.1374
884.8904 887.8861 893.2557
900.9425 904.1441 919.7268
920.1935 923.3263 935.2134
940.8503 944.6344 956.9987
958.3483 963.6242 966.6966

970.8085 974.2614 976.2077
985.4669 988.0082 994.1297
999.5489 1007.2649 1018.4171
1019.3098 1020.9777 1026.9164
1027.1623 1027.5673 1028.5854
1038.5204 1040.0464 1045.3992
1049.6617 1057.9761 1061.6961
1063.2850 1067.4410 1070.3310
1070.7568 1075.2746 1077.7272
1080.7776 1090.4023 1099.0553
1112.5702 1114.0195 1119.4380
1128.5947 1133.9025 1135.9600
1156.1587 1157.1241 1159.3994
1162.1964 1178.9583 1181.9151
1184.3339 1187.1200 1189.6781
1191.4832 1191.6438 1197.1975
1199.6558 1205.2620 1207.4170
1209.7179 1210.7440 1222.6096
1232.2673 1233.9677 1239.2510
1242.0257 1243.9804 1245.7994
1251.2427 1258.6667 1267.8095
1282.5826 1285.0774 1286.5657
1304.0516 1306.7297 1308.9546
1322.1370 1329.9574 1332.2075
1339.8833 1341.1702 1343.6536
1345.8074 1353.7462 1355.2195
1359.8908 1364.9862 1372.6251
1373.6805 1376.8303 1379.3135
1380.6278 1383.1000 1392.1994
1399.6754 1416.4581 1417.9727
1420.5401 1420.9845 1422.0035
1424.2007 1426.0080 1432.6991
1434.5637 1441.2362 1447.1304
1457.9467 1464.7134 1467.1153
1477.2079 1478.7259 1482.9350
1488.2525 1488.9108 1490.6045
1490.7926 1492.4235 1494.5174
1495.0691 1495.4859 1496.1751
1499.1273 1501.9554 1505.4725
1508.9234 1509.6328 1510.2386
1513.7499 1514.4341 1516.9845
1517.5671 1523.5123 1527.1960
1530.5133 1534.1712 1537.8793
1539.5901 1544.6996 1546.5155

1548.2029	1553.4931	1598.0581
1655.2069	1676.3798	1678.0070
1681.1633	1685.9983	1686.3766
1693.6621	1699.0906	1701.2516
1703.7146	1723.7702	1736.2017
1809.2871	1834.3610	3060.8739
3071.9348	3072.8252	3075.3418
3075.8334	3076.5819	3084.0113
3085.1757	3085.6095	3087.6756
3090.3629	3091.1558	3094.1560
3100.3936	3114.4677	3127.8553
3129.7053	3138.5487	3141.1751
3142.8314	3147.6392	3147.8624
3155.3509	3157.2092	3157.3218
3158.9963	3160.2717	3163.1731
3166.4911	3167.8695	3169.1276
3171.8386	3171.9162	3173.7878
3175.8828	3176.7944	3179.0910
3181.5309	3184.8974	3187.5844
3197.2570	3197.5586	3198.0291
3200.9478	3203.9652	3206.2549
3206.8406	3207.9578	3212.4502
3217.3341	3218.4089	3223.3217
3226.4316	3227.4462	3232.9805
3233.4660	3237.8947	3242.7579

M6c

Zero-point correction= 1.019804
Thermal correction to Energy= 1.076455
Thermal correction to Enthalpy= 1.077399
Thermal correction to Gibbs Free Energy= 0.926424
Sum of electronic and zero-point Energies= -2568.070086
Sum of electronic and thermal Energies= -2568.013435
Sum of electronic and thermal Enthalpies= -2568.012491
Sum of electronic and thermal Free Energies= -2568.163466
Cartesian coordinates

C	5.688254	-1.729502	0.900121
C	4.683825	-0.767817	0.826137
C	4.981732	0.591635	0.771365
C	6.319610	0.975718	0.789538
C	7.332429	0.015748	0.865593
C	7.025095	-1.340937	0.923968
C	5.117603	-3.121549	0.961398
H	4.194327	1.338685	0.723005

H	6.577361	2.028526	0.746252
H	8.370164	0.332578	0.877033
H	7.814078	-2.084476	0.981218
H	5.248364	-3.552908	1.958624
C	2.724575	-1.423562	-1.597071
C	3.570566	-2.645363	-1.737331
C	3.614874	-2.959478	0.643419
C	3.318714	-1.423127	0.802684
C	1.671874	0.099270	-0.462910
H	3.295292	-3.183030	-2.644224
H	2.742612	-1.229266	1.707408
N	2.051317	-0.745191	-2.485511
N	1.406154	0.200417	-1.762519
N	2.535087	-0.924556	-0.342550
C	0.582064	1.195100	-2.394718
C	-0.613113	0.774979	-2.986533
C	1.009494	2.525944	-2.351000
C	-1.448025	1.775380	-3.481765
C	0.137116	3.481167	-2.869952
C	-1.099088	3.127486	-3.415649
H	-2.392193	1.488094	-3.937882
H	0.434788	4.526329	-2.846020
O	3.272708	-3.474716	-0.632917
H	4.634927	-2.377484	-1.777135
H	2.985111	-3.528017	1.328698
H	5.577240	-3.812130	0.248029
C	-0.954764	-0.685184	-3.111403
H	-0.813379	-1.226085	-2.168469
H	-0.301581	-1.161620	-3.848685
H	-1.986817	-0.800603	-3.444682
C	-2.040679	4.188951	-3.919229
H	-2.675291	4.551744	-3.104042
H	-2.695486	3.799481	-4.701075
H	-1.491936	5.045331	-4.316812
C	2.335608	2.922472	-1.755379
H	3.118924	2.197758	-1.996521
H	2.277964	3.020821	-0.663403
H	2.638680	3.898193	-2.138032
C	1.169427	0.913119	0.708041
O	1.902790	0.930555	1.671399
C	-0.198374	1.579222	0.698740
C	-0.213921	2.659880	1.796837
H	-0.339285	2.085218	-0.260865
H	-1.236514	3.029544	1.897264

H	0.081450	2.227309	2.756694
C	0.694259	3.804238	1.404866
C	1.974454	3.953548	1.944330
C	0.266554	4.708868	0.426744
C	2.812548	4.979021	1.507406
H	2.317146	3.254847	2.701891
C	1.100417	5.733500	-0.010754
H	-0.729895	4.603444	0.001053
C	2.380001	5.867918	0.526509
H	3.804244	5.082882	1.936293
H	0.750564	6.429085	-0.767524
H	3.033083	6.664978	0.186426
N	-0.357159	-1.648537	0.369622
N	0.226051	-2.826472	0.716194
C	0.509413	-3.698203	-0.324525
O	0.471925	-3.414120	-1.498799
O	0.855402	-4.881168	0.188627
C	1.236829	-5.865973	-0.779326
H	2.130499	-5.531374	-1.306955
H	1.440448	-6.770619	-0.210621
H	0.423730	-6.032875	-1.487140
C	-0.786681	-0.849914	1.282076
C	-1.334990	0.461388	0.761740
C	-0.736561	-1.026799	2.732895
C	-2.502802	0.945590	1.586162
H	-1.658766	0.287040	-0.269410
C	-1.547868	-0.285647	3.512295
H	-0.054874	-1.747154	3.173946
C	-3.486518	1.756788	1.033659
C	-2.531831	0.648117	2.959308
H	-1.523698	-0.409244	4.591812
C	-4.484658	2.301363	1.841539
H	-3.459433	1.973139	-0.031902
C	-3.521672	1.215694	3.767290
C	-4.491419	2.044922	3.212230
H	-5.250063	2.932763	1.401961
H	-3.536217	0.989350	4.829669
H	-5.258715	2.479290	3.844041
N	-4.608476	-1.224195	-0.117163
C	-4.285628	-1.997712	1.081056
C	-4.282464	-3.526067	0.911027
C	-5.144046	-1.592699	2.275476
H	-3.251007	-1.718676	1.339847
H	-3.546266	-3.840608	0.165318

H	-4.016981	-4.005100	1.859489
H	-5.263197	-3.901240	0.603065
H	-5.158570	-0.506473	2.392312
H	-6.173892	-1.952495	2.180265
H	-4.722219	-2.029363	3.185497
C	-5.986547	-0.811921	-0.366532
C	-6.988515	-1.939591	-0.671673
C	-6.043688	0.261265	-1.454877
H	-6.331204	-0.323538	0.553454
H	-7.032493	-2.662589	0.146992
H	-7.992741	-1.521548	-0.799611
H	-6.727640	-2.478524	-1.586376
H	-5.349777	1.075835	-1.228401
H	-5.797086	-0.139219	-2.443401
H	-7.054568	0.673712	-1.510036
C	-3.727139	-1.449470	-1.247020
C	-4.130099	-2.503289	-2.291312
H	-2.750982	-1.730859	-0.829421
H	-3.563857	-0.493835	-1.768832
H	-3.288191	-2.710210	-2.960356
H	-4.424260	-3.443609	-1.818976
H	-4.966750	-2.163642	-2.908002
H	0.073939	-3.239159	1.631300

Vibrational frequencies

8.6705	12.1899	16.8268
24.6650	26.8189	28.9389
37.9938	39.1840	44.0894
49.0071	50.6485	55.3648
59.3672	61.9894	73.6025
76.2193	79.7585	84.3481
91.6024	93.7081	96.6907
103.4078	105.2017	107.9183
115.2428	121.4291	125.8745
126.9998	138.9022	148.8572
152.7783	164.4446	172.7792
177.0642	184.0056	193.4779
198.5199	202.5328	209.3075
215.4356	227.3632	229.5388
231.1642	231.8472	238.2106
239.5679	242.8971	250.0127
251.6989	260.3319	275.6254
283.0878	285.1555	289.9670
292.2654	304.3841	324.0132
325.6582	332.4045	336.3465

341.7752	349.1491	352.4882
358.3663	363.3151	382.9200
386.1042	390.4778	390.9089
394.8934	407.7452	412.5726
416.9040	424.6925	435.2788
441.7013	448.9675	490.3344
499.1906	501.1818	504.5390
510.9736	516.6497	520.6646
525.1751	526.0144	530.7272
535.2379	542.7877	547.1199
557.3861	566.1800	571.6188
584.5818	588.5993	596.1804
600.7463	609.4706	625.0738
632.7175	641.4887	652.0754
668.8507	687.5347	704.8289
715.3029	717.8929	721.6184
726.3544	730.0348	747.2837
752.9441	765.5357	771.8774
776.5310	780.3647	783.8332
787.4630	802.1104	808.6687
809.3835	818.8359	834.6710
838.7801	857.8655	861.4385
864.8988	873.4588	881.3675
883.3826	886.7582	889.2051
889.6366	905.5782	909.3305
914.9025	916.1315	920.8497
922.5389	942.2954	949.0209
956.4362	958.7300	960.9660
964.2178	966.8297	976.7306
983.1003	984.6473	985.5312
1010.7118	1017.0643	1018.3965
1018.5574	1026.6470	1027.6859
1028.2627	1029.3519	1030.7707
1033.1561	1039.9267	1041.8113
1053.9371	1056.9138	1058.4707
1061.6632	1063.2319	1066.2950
1071.9106	1072.8604	1077.3480
1078.8183	1080.0939	1102.7133
1114.3324	1119.8554	1124.6938
1127.6896	1136.6035	1138.0744
1152.1759	1156.4740	1157.0385
1163.2022	1170.4542	1177.3745
1180.3264	1183.3095	1184.5596
1193.3799	1194.4664	1198.7849

1199.2623	1205.9177	1207.6411
1213.8661	1224.6947	1225.6858
1232.7766	1240.4284	1246.4500
1250.5229	1251.5135	1261.0795
1268.0783	1270.2488	1280.1158
1284.4082	1287.9968	1293.4747
1298.2622	1306.5708	1315.8955
1319.0340	1331.6875	1335.4997
1339.6941	1342.6395	1348.1603
1352.2137	1353.0494	1353.4317
1356.6458	1363.6319	1367.8428
1372.5845	1373.6106	1374.4048
1382.8186	1383.8943	1390.0260
1394.1508	1399.8994	1401.4121
1408.0678	1412.8405	1418.2007
1421.0036	1422.1014	1426.2695
1429.7998	1430.0083	1441.1246
1445.7725	1461.9325	1466.7698
1474.2852	1476.6533	1480.7786
1484.8021	1487.9800	1489.1658
1489.7220	1490.9545	1491.2872
1491.5890	1494.0290	1494.8267
1494.9826	1496.9575	1498.6692
1505.2052	1506.9047	1508.1859
1509.2751	1509.3401	1512.9860
1515.7928	1519.7845	1522.3473
1525.1478	1528.8987	1535.2656
1537.1040	1542.3500	1544.9105
1549.9133	1557.7127	1597.7339
1652.6393	1675.3783	1676.3279
1681.2016	1684.8946	1689.8108
1691.2885	1697.9936	1701.3271
1705.7214	1744.4184	1837.1197
1861.8447	3022.7789	3036.6445
3055.9490	3060.5940	3063.8644
3065.7269	3065.7828	3066.6238
3069.4416	3071.2483	3077.0531
3081.2568	3089.5181	3096.6626
3101.0278	3103.4716	3113.2702
3131.1377	3131.1750	3131.9365
3138.1726	3139.3671	3139.9711
3141.1822	3141.5768	3141.9381
3145.2501	3150.9008	3152.3695
3161.5103	3161.5211	3165.7962

3169.2329	3169.4650	3170.7443
3171.0706	3174.8331	3175.3089
3188.7243	3191.5443	3194.0956
3194.2780	3197.0979	3202.4630
3206.9613	3207.6078	3209.3930
3213.5344	3213.6931	3215.0238
3216.8828	3217.2785	3221.7550
3227.0101	3228.9366	3230.2158
3234.4907	3239.8049	3597.0726

TS7c

Zero-point correction= 1.018367
Thermal correction to Energy= 1.074144
Thermal correction to Enthalpy= 1.075088
Thermal correction to Gibbs Free Energy= 0.928533
Sum of electronic and zero-point Energies= -2568.055934
Sum of electronic and thermal Energies= -2568.000156
Sum of electronic and thermal Enthalpies= -2567.999212
Sum of electronic and thermal Free Energies= -2568.145768
Cartesian coordinates

C	-6.438556	-0.784336	-0.134950
C	-5.182841	-0.216144	-0.329136
C	-5.000698	1.163639	-0.354327
C	-6.114714	1.978340	-0.174047
C	-7.380470	1.416595	0.019346
C	-7.552063	0.034636	0.037512
C	-6.370655	-2.289604	-0.154136
H	-4.014789	1.590504	-0.520105
H	-5.997831	3.057231	-0.181510
H	-8.238626	2.065830	0.160366
H	-8.535993	-0.397583	0.191579
H	-6.840612	-2.691318	-1.056952
C	-3.180591	-1.410242	1.806327
C	-4.318750	-2.312409	2.153109
C	-4.862038	-2.631389	-0.142278
C	-4.121140	-1.283728	-0.470478
C	-1.905180	-0.306783	0.423779
H	-4.088364	-2.877118	3.055805
H	-3.674396	-1.295802	-1.462120
N	-2.217346	-0.945515	2.545822
N	-1.437965	-0.249931	1.670722
N	-3.035456	-1.033862	0.500564
C	-0.325810	0.514335	2.169468
C	0.854427	-0.161903	2.476093

C	-0.498511	1.894011	2.326943
C	1.936256	0.615510	2.892357
C	0.616581	2.624243	2.732449
C	1.842076	2.004430	3.003196
H	2.872199	0.118980	3.135010
H	0.525144	3.701718	2.845381
O	-4.446952	-3.223043	1.079237
H	-5.238833	-1.733964	2.313528
H	-4.611585	-3.375052	-0.899681
H	-6.867304	-2.757845	0.701540
C	0.945092	-1.658144	2.348140
H	0.582208	-2.010352	1.375762
H	0.323376	-2.144222	3.106522
H	1.975661	-1.986382	2.486217
C	3.040313	2.828145	3.393768
H	3.514061	3.256014	2.502908
H	3.788778	2.220844	3.906966
H	2.753239	3.656957	4.044879
C	-1.817960	2.555346	2.023134
H	-2.645434	2.022171	2.500785
H	-2.018150	2.586532	0.943160
H	-1.816579	3.586441	2.378170
C	-1.359781	0.223460	-0.913930
O	-2.250983	0.360231	-1.771573
C	-0.111388	1.171120	-0.906406
C	-0.243591	2.162819	-2.079172
H	-0.113685	1.759740	0.010217
H	0.746364	2.556473	-2.322629
H	-0.632822	1.647323	-2.959939
C	-1.144672	3.310232	-1.676432
C	-2.499550	3.345860	-2.014132
C	-0.626350	4.333921	-0.875202
C	-3.318415	4.375606	-1.550705
H	-2.912559	2.548091	-2.623268
C	-1.441266	5.361313	-0.408853
H	0.429987	4.321148	-0.611796
C	-2.794665	5.381747	-0.742323
H	-4.368617	4.390822	-1.827264
H	-1.020700	6.145554	0.212916
H	-3.434278	6.180225	-0.380535
N	-0.384215	-1.282090	-1.365693
N	-0.978901	-2.409082	-1.888140
C	-1.431997	-3.328867	-0.958682
O	-1.092742	-3.342443	0.204369

O	-2.251925	-4.199928	-1.545607
C	-2.645965	-5.309094	-0.716968
H	-3.134085	-4.942592	0.187038
H	-3.332743	-5.892498	-1.326077
H	-1.769021	-5.902762	-0.454811
C	0.838244	-0.962897	-1.628233
C	1.182666	0.306846	-0.908804
C	1.770200	-1.636628	-2.484892
C	2.465183	0.961068	-1.338092
H	1.356472	-0.014108	0.130272
C	2.918531	-0.989941	-2.798145
H	1.505831	-2.596763	-2.910599
C	2.874812	2.164391	-0.769337
C	3.297186	0.312415	-2.266467
H	3.611509	-1.456346	-3.494936
C	4.079535	2.748344	-1.154494
H	2.248292	2.643484	-0.018527
C	4.504856	0.910128	-2.649473
C	4.891782	2.125795	-2.103225
H	4.386892	3.689778	-0.710488
H	5.140946	0.404935	-3.371715
H	5.827315	2.584780	-2.404973
N	5.618316	-0.890915	0.058972
C	6.282671	-1.586726	-1.043833
C	6.765327	-3.018214	-0.751156
C	7.420125	-0.764548	-1.647990
H	5.514640	-1.683508	-1.829727
H	5.932473	-3.671643	-0.478672
H	7.234621	-3.439917	-1.645971
H	7.499337	-3.041253	0.059745
H	7.100106	0.258095	-1.862796
H	8.291336	-0.721716	-0.986836
H	7.740537	-1.229655	-2.584130
C	6.407156	-0.044614	0.950690
C	7.457096	-0.759540	1.818714
C	5.496488	0.811617	1.831401
H	6.950605	0.656571	0.305563
H	8.174607	-1.311871	1.207034
H	8.018075	-0.024341	2.405624
H	6.991106	-1.462255	2.514624
H	4.701481	1.273366	1.236879
H	5.038798	0.218633	2.630553
H	6.081295	1.602494	2.309542
C	4.444615	-1.563084	0.586645

C	4.630053	-2.546457	1.756683
H	3.988576	-2.096829	-0.257690
H	3.703545	-0.806199	0.891323
H	3.743923	-3.180587	1.862397
H	5.491003	-3.200465	1.604198
H	4.776431	-2.020886	2.705819
H	-1.505908	-2.281407	-2.746443

Vibrational frequencies

-119.9674	16.4326	19.6981
24.5093	31.9566	35.9046
38.6430	40.0808	47.3544
50.4302	54.2604	55.4737
58.3750	66.7367	70.4120
75.4145	81.0240	82.3977
85.5465	89.9538	94.2435
103.4037	107.9980	108.4786
110.1398	117.5775	122.8748
126.7189	138.4991	139.5124
141.3513	153.2182	160.2019
172.1601	180.6087	181.6748
192.1960	202.1419	207.7087
216.9909	223.0158	225.7403
229.1916	234.9946	237.5234
243.6603	244.9112	251.3231
253.9087	260.2837	272.2682
282.0621	284.4874	291.4032
311.0110	311.4330	322.8375
328.7642	333.3529	341.3331
347.1871	349.3871	359.2977
366.2711	371.2866	382.2270
384.3560	397.5869	404.2408
412.5527	413.5830	416.7612
422.6623	429.9135	435.3686
440.2112	453.5549	461.2037
486.6435	493.0264	495.1755
500.6362	509.6924	515.0984
519.0965	524.6662	528.3621
535.3335	539.7415	550.4579
560.2056	564.8377	569.3357
587.0925	588.3967	595.6316
603.6024	611.8225	624.4198
628.8461	632.5296	650.8231
670.4330	698.0519	703.4227
711.1226	718.8821	722.9835

731.9166	740.4534	751.3289
753.4501	761.5700	773.4708
774.0141	779.6465	785.8605
786.2390	790.7155	804.8138
813.1801	822.4620	835.7170
847.0084	859.6340	860.7750
863.2793	874.6424	876.5986
878.5240	882.1446	885.3787
886.2476	909.7545	915.2937
921.4492	922.6194	923.4221
928.6470	940.0144	949.4048
954.2988	956.2016	958.8690
960.7819	965.0929	980.0413
986.3000	988.0627	996.7915
1002.7245	1012.2975	1013.6786
1019.1524	1022.0529	1023.7903
1026.5131	1029.6313	1031.4117
1037.8937	1039.6966	1046.7386
1055.9057	1057.8088	1060.3343
1062.1248	1064.7946	1069.2093
1070.4438	1070.7046	1071.3179
1078.8952	1086.7452	1095.5852
1109.6708	1119.8302	1122.1498
1122.8540	1131.7995	1143.3378
1146.7320	1149.1156	1153.3970
1155.8626	1161.2163	1176.8268
1178.0854	1178.8501	1191.9160
1192.6077	1197.1520	1198.4947
1199.2005	1203.8476	1204.7285
1206.0428	1222.3010	1224.7821
1230.1925	1235.5129	1236.9891
1242.2841	1246.7897	1250.1079
1259.7906	1263.4467	1281.5215
1283.0137	1289.3732	1290.2262
1294.6813	1302.2845	1306.2614
1310.1967	1323.0511	1327.3032
1337.5941	1339.3235	1342.8270
1348.2113	1350.9534	1356.6399
1358.9070	1359.8325	1364.3613
1368.7088	1372.8165	1373.8368
1384.7538	1384.9333	1385.2945
1395.2611	1399.4236	1401.7228
1405.3726	1407.2293	1418.6639
1420.4129	1423.9154	1428.5978

1429.2201	1433.0956	1435.9739
1449.9486	1456.4594	1460.7163
1472.0975	1472.6032	1477.2544
1481.3335	1486.0185	1486.5462
1489.8837	1491.5958	1492.6843
1493.3028	1495.7052	1495.8576
1496.7685	1497.0697	1500.4542
1504.0575	1505.8623	1506.4301
1508.0606	1512.9680	1515.9355
1516.8157	1517.8453	1519.1615
1520.8645	1523.2819	1528.0792
1531.7941	1537.8899	1540.6745
1542.0890	1551.7672	1587.7648
1622.1498	1633.8058	1675.5174
1680.5071	1681.2798	1683.3133
1688.3321	1692.4642	1694.7168
1698.4304	1701.6627	1727.4233
1846.0675	3004.3378	3026.9977
3050.2305	3055.1389	3059.7291
3060.9722	3061.9359	3062.8878
3067.1655	3070.1119	3071.0347
3074.4059	3080.2038	3080.5401
3087.9493	3104.7210	3106.9286
3128.5290	3132.9300	3133.1908
3136.8778	3137.0068	3138.4534
3140.4591	3144.0366	3148.2036
3150.5997	3152.2414	3159.1667
3161.2738	3161.9158	3166.8615
3167.3319	3170.5650	3177.2680
3177.9963	3178.8388	3183.7706
3190.0329	3191.5594	3192.4746
3200.6393	3202.0411	3203.7880
3204.9916	3205.4734	3206.0781
3213.4609	3216.6589	3217.5285
3219.5519	3219.8828	3224.6455
3228.6110	3229.4484	3230.3312
3232.5930	3243.7328	3580.4876

TS7c1

Zero-point correction= 1.017818

Thermal correction to Energy= 1.073108

Thermal correction to Enthalpy= 1.074053

Thermal correction to Gibbs Free Energy= 0.930616

Sum of electronic and zero-point Energies= -2568.039598

Sum of electronic and thermal Energies= -2567.984307
Sum of electronic and thermal Enthalpies= -2567.983363
Sum of electronic and thermal Free Energies= -2568.126800
Cartesian coordinates

C	4.886379	-2.577872	1.239693
C	3.897422	-1.609453	1.397497
C	4.019374	-0.600405	2.349210
C	5.156156	-0.581940	3.153684
C	6.146813	-1.556335	3.005861
C	6.018982	-2.559864	2.049147
C	4.537666	-3.550794	0.145086
H	3.243168	0.149187	2.464107
H	5.273362	0.195126	3.901497
H	7.027231	-1.527008	3.639514
H	6.793300	-3.311183	1.928678
H	4.262060	-4.525150	0.561208
C	3.264811	-0.172990	-1.351645
C	4.299033	-1.128829	-1.847730
C	3.331057	-2.923054	-0.583207
C	2.772463	-1.829146	0.405026
C	1.509913	0.335649	-0.170528
H	4.572617	-0.879388	-2.872588
H	1.846110	-2.169369	0.875474
N	2.867991	0.974174	-1.817957
N	1.767900	1.276456	-1.077294
N	2.469992	-0.591969	-0.326462
C	1.171145	2.578018	-1.260339
C	0.057103	2.715878	-2.090808
C	1.860107	3.660324	-0.702958
C	-0.424176	4.010532	-2.284410
C	1.359192	4.931637	-0.965904
C	0.210254	5.123367	-1.733480
H	-1.303043	4.150992	-2.909826
H	1.867321	5.792119	-0.539121
O	3.680452	-2.402805	-1.857957
H	5.195441	-1.111330	-1.214719
H	2.552094	-3.653586	-0.799780
H	5.354682	-3.719301	-0.562726
C	-0.548739	1.555017	-2.831829
H	-0.446110	0.602940	-2.304794
H	-0.037745	1.425653	-3.791720
H	-1.603567	1.755750	-3.040003
C	-0.352860	6.502801	-1.950142
H	-1.304710	6.613196	-1.419893

H	-0.547792	6.687612	-3.009835
H	0.329183	7.272479	-1.583773
C	3.127027	3.463810	0.085905
H	3.958668	3.213469	-0.580357
H	3.028017	2.655584	0.817437
H	3.377208	4.375657	0.630259
C	0.475254	0.234901	0.935326
O	0.890133	-0.207225	1.983630
C	-1.000055	0.580875	0.739184
C	-1.352479	1.647276	1.800525
H	-1.122653	1.007249	-0.262215
H	-2.391173	1.944049	1.652861
H	-1.287181	1.171623	2.782664
C	-0.535978	2.923230	1.839212
C	0.668378	2.990962	2.549355
C	-1.071521	4.105843	1.319303
C	1.314144	4.210534	2.740745
H	1.078741	2.090605	2.998952
C	-0.438584	5.327492	1.527507
H	-2.012402	4.069674	0.774206
C	0.757065	5.383911	2.239741
H	2.241700	4.244308	3.304155
H	-0.878399	6.238392	1.131883
H	1.248573	6.337334	2.406316
N	-0.398367	-1.495288	-0.934289
N	0.280418	-2.496847	-1.610238
C	0.951514	-2.153383	-2.754481
O	1.241031	-1.025975	-3.097322
O	1.282451	-3.270959	-3.421682
C	2.113974	-3.060629	-4.564400
H	3.076595	-2.654640	-4.249530
H	2.244251	-4.041378	-5.017353
H	1.634169	-2.376571	-5.265904
C	-1.024508	-1.846102	0.158918
C	-1.783957	-0.780110	0.857611
C	-0.959915	-3.185071	0.732716
C	-2.428331	-1.163312	2.138322
H	-2.983520	-0.769931	0.020497
C	-1.529065	-3.454388	1.924667
H	-0.356376	-3.949793	0.257228
C	-3.330955	-0.317916	2.821522
C	-2.320545	-2.485119	2.641292
H	-1.411884	-4.440908	2.366584
C	-4.008236	-0.722960	3.960703

H	-3.549957	0.666702	2.431722
C	-3.016499	-2.888317	3.794337
C	-3.847956	-2.016127	4.469204
H	-4.689262	-0.029427	4.444049
H	-2.898223	-3.912486	4.138187
H	-4.385140	-2.333173	5.356109
N	-3.999163	-0.918756	-0.799082
C	-4.428347	-2.335737	-0.527225
C	-5.115554	-3.041488	-1.697880
C	-5.266253	-2.482203	0.742453
H	-3.473961	-2.853299	-0.349357
H	-4.479226	-3.098610	-2.582762
H	-5.341902	-4.065936	-1.391041
H	-6.057387	-2.559968	-1.972297
H	-4.834488	-1.964551	1.599622
H	-6.293106	-2.135565	0.600075
H	-5.311050	-3.546091	0.988741
C	-4.958418	0.169258	-0.432554
C	-6.326388	0.131250	-1.117595
C	-4.296028	1.534366	-0.618993
H	-5.122406	0.027806	0.640377
H	-6.852176	-0.809185	-0.949815
H	-6.939195	0.929467	-0.688984
H	-6.261140	0.304747	-2.192031
H	-3.279540	1.547672	-0.218018
H	-4.249082	1.829005	-1.670801
H	-4.880279	2.290191	-0.088620
C	-3.292195	-0.769967	-2.105016
C	-4.097316	-0.465138	-3.366044
H	-2.724250	-1.694681	-2.237981
H	-2.542650	0.011173	-1.960985
H	-3.420939	-0.563556	-4.219868
H	-4.933124	-1.148322	-3.519197
H	-4.482382	0.555977	-3.375791
H	-0.093229	-3.439729	-1.606303

Vibrational frequencies

-1289.2770	10.7597	22.2184
28.1424	30.2346	31.3211
41.8811	49.7573	54.3878
60.7298	62.8726	74.3759
76.0258	78.9599	82.7009
85.4031	88.0283	93.1491
102.9692	104.6609	110.8173
113.6221	117.8189	124.1253

131.0637	137.5021	139.5264
150.6632	154.0218	158.4111
171.5378	179.5623	181.1753
184.7138	186.7804	194.4380
198.7655	208.0956	210.4163
215.0039	217.2520	222.9911
229.4118	233.2686	235.7015
238.3634	247.2201	249.2116
255.2675	258.3928	259.0075
269.4561	273.2305	278.6430
288.0139	299.6993	304.7048
316.9720	325.9914	337.6261
341.0525	345.8732	347.8055
354.5677	358.1452	364.3654
379.7752	386.7668	395.9029
404.4758	412.3675	415.4702
419.2172	423.0956	431.6156
449.7267	453.0767	454.5430
481.3727	490.8494	498.6479
502.0809	504.0744	512.1752
526.4977	528.2011	533.9629
538.3375	543.3904	552.0413
560.0899	561.3073	580.1371
587.4881	591.6434	598.5128
606.1894	616.7098	622.7204
629.7587	634.2842	637.3725
678.1204	687.7159	691.8481
705.6323	719.1769	723.1743
727.7276	732.3730	742.5480
744.5771	752.0586	763.2966
769.4884	772.9318	780.9298
783.7709	792.0652	796.6501
807.3642	809.4950	830.3511
836.7278	842.8025	855.7767
857.8574	864.6274	876.2185
878.7941	880.3449	884.3070
893.2681	897.5626	902.5788
923.8668	926.6283	932.6794
940.1470	946.1997	955.5451
957.4294	958.2292	960.9505
963.6696	969.6339	971.3941
981.5413	986.7645	997.4971
998.5212	1001.0195	1004.9145
1015.3001	1016.9093	1024.2286

1025.0795	1028.9280	1033.6605
1035.7961	1037.5962	1038.8888
1048.6723	1053.7816	1057.3136
1057.4835	1059.4676	1061.3772
1070.5779	1073.2271	1075.3289
1077.5731	1088.2071	1089.7596
1105.7764	1109.0591	1110.4555
1120.4213	1123.4180	1129.5058
1146.7981	1151.7206	1155.2728
1157.6466	1177.5318	1178.0624
1180.7747	1182.9223	1184.2628
1186.9277	1188.4777	1198.6614
1199.4545	1202.4819	1207.3666
1213.3524	1222.7333	1224.6035
1230.7621	1232.3818	1237.3879
1240.0599	1246.0746	1249.3221
1256.3413	1263.5813	1264.2786
1280.5795	1283.1595	1286.4957
1298.1696	1305.9172	1318.2498
1328.1648	1337.1971	1345.4741
1347.1526	1352.3645	1352.8778
1356.4967	1358.6359	1360.7454
1366.3928	1368.6174	1371.8441
1374.0521	1376.1289	1377.7086
1386.1938	1387.4509	1402.0290
1412.3312	1413.8058	1414.7748
1419.9004	1420.7608	1423.4050
1423.7144	1430.1645	1433.0733
1441.3986	1449.9921	1460.1307
1466.1388	1467.8380	1473.1395
1475.3920	1478.1859	1483.0566
1487.2144	1489.0358	1489.7430
1491.5396	1491.9821	1495.1149
1497.3010	1498.4479	1500.9623
1501.8789	1504.0220	1506.3847
1508.8184	1510.8781	1511.5969
1515.3123	1515.5378	1520.1001
1522.4329	1524.9399	1525.2841
1530.4479	1532.5999	1534.3991
1537.6710	1543.1361	1545.2757
1551.0880	1575.1129	1588.6713
1594.9269	1628.5128	1647.0678
1675.0842	1681.7274	1686.2429
1689.5308	1693.2721	1696.2618

1696.8398	1698.8244	1715.2387
1838.9019	1848.2065	3056.3966
3067.3123	3067.8115	3071.0175
3081.7358	3082.0352	3083.4220
3084.7808	3085.4499	3086.5355
3090.5392	3102.7727	3102.8165
3116.2267	3117.8361	3119.8733
3134.7026	3137.9228	3138.5568
3141.1623	3144.4278	3156.7243
3157.8156	3158.8772	3163.5669
3164.4478	3167.0169	3167.3377
3168.2099	3168.6629	3170.1272
3172.7441	3175.5996	3179.7832
3183.1433	3183.7077	3187.3585
3192.1490	3194.3567	3195.6262
3196.7963	3198.8757	3199.3532
3200.3182	3209.8949	3210.1828
3211.7903	3216.4337	3218.6990
3223.0872	3227.6948	3229.1521
3232.4210	3234.2878	3241.4591
3250.9925	3255.0961	3577.8827

M7c1

Zero-point correction= 1.024571

Thermal correction to Energy= 1.079280

Thermal correction to Enthalpy= 1.080224

Thermal correction to Gibbs Free Energy= 0.938094

Sum of electronic and zero-point Energies= -2568.089033

Sum of electronic and thermal Energies= -2568.034324

Sum of electronic and thermal Enthalpies= -2568.033380

Sum of electronic and thermal Free Energies= -2568.175510

Cartesian coordinates

C	6.381299	-0.214610	0.665159
C	5.021834	0.018815	0.841100
C	4.534103	1.257416	1.242026
C	5.446311	2.284745	1.461987
C	6.816482	2.062104	1.289078
C	7.293600	0.813787	0.894900
C	6.640477	-1.635957	0.235823
H	3.465486	1.390241	1.389768
H	5.092195	3.264007	1.769105
H	7.517585	2.872306	1.462409
H	8.358409	0.648602	0.760623
H	7.137153	-2.201823	1.029786

C	3.538361	-0.812826	-1.833295
C	4.852150	-1.391642	-2.239513
C	5.242744	-2.237780	-0.057727
C	4.202692	-1.204108	0.509460
C	1.951988	-0.326395	-0.403606
H	4.818588	-1.706849	-3.281985
H	3.660143	-1.581757	1.372644
N	2.592209	-0.299684	-2.558553
N	1.615245	0.003539	-1.652761
N	3.193302	-0.848817	-0.511060
C	0.478508	0.750667	-2.118727
C	-0.696761	0.089144	-2.465285
C	0.656168	2.135678	-2.245244
C	-1.749005	0.883416	-2.932708
C	-0.426266	2.876380	-2.706671
C	-1.638289	2.267705	-3.049896
H	-2.665317	0.392083	-3.252079
H	-0.318876	3.953117	-2.813583
O	5.059939	-2.534041	-1.434697
H	5.655719	-0.652590	-2.114038
H	5.103425	-3.196281	0.442832
H	7.275017	-1.709648	-0.653442
C	-0.844818	-1.404853	-2.357468
H	-1.462158	-1.666832	-1.489659
H	0.109702	-1.913014	-2.217022
H	-1.332030	-1.794698	-3.255379
C	-2.790212	3.103863	-3.543516
H	-3.278084	3.621074	-2.710368
H	-3.541797	2.490790	-4.046604
H	-2.445619	3.868336	-4.244085
C	1.969438	2.781243	-1.891892
H	2.786786	2.346319	-2.474605
H	2.203092	2.644796	-0.828426
H	1.930752	3.853633	-2.084859
C	1.133354	-0.400419	0.926257
O	1.927983	-0.472043	1.944367
C	-0.092104	0.622534	1.060970
C	0.234891	1.689549	2.124405
H	-0.313001	1.101734	0.101261
H	-0.653115	1.885505	2.732402
H	0.983298	1.248624	2.787941
C	0.740158	3.002650	1.574137
C	1.951066	3.543980	2.016320
C	-0.011556	3.736985	0.648973

C	2.406976	4.772852	1.539436
H	2.536162	2.998846	2.753355
C	0.433611	4.968256	0.176473
H	-0.954997	3.337428	0.281624
C	1.649878	5.488413	0.616145
H	3.348244	5.177036	1.899898
H	-0.168064	5.521822	-0.538517
H	2.001010	6.446096	0.245828
N	0.365837	-1.735565	0.663128
N	1.118006	-2.842914	1.013215
C	1.779463	-3.498803	-0.000654
O	1.537430	-3.416021	-1.185836
O	2.730717	-4.287497	0.526074
C	3.384279	-5.147359	-0.417423
H	3.854495	-4.553154	-1.202248
H	4.131154	-5.693533	0.156140
H	2.663169	-5.839745	-0.855439
C	-0.874199	-1.617513	1.290292
C	-1.231202	-0.296023	1.455121
C	-1.693469	-2.689228	1.714989
C	-2.503503	0.020860	1.993942
H	-5.029997	-0.172017	0.764365
C	-2.879786	-2.394732	2.337211
H	-1.353319	-3.710504	1.584215
C	-3.026134	1.345743	2.057428
C	-3.314527	-1.048404	2.495485
H	-3.508181	-3.193617	2.721944
C	-4.236538	1.605983	2.654372
H	-2.459011	2.159572	1.616548
C	-4.539297	-0.739165	3.147987
C	-4.989229	0.557262	3.239440
H	-4.614256	2.622662	2.689325
H	-5.119019	-1.553045	3.578068
H	-5.919048	0.780472	3.752253
N	-5.468714	-0.564057	-0.082039
C	-6.389223	-1.644249	0.505235
C	-6.852585	-2.702102	-0.487833
C	-7.544264	-1.015750	1.272760
H	-5.726867	-2.136591	1.224663
H	-6.026310	-3.310265	-0.857697
H	-7.526343	-3.369906	0.053846
H	-7.405492	-2.289250	-1.332257
H	-7.203942	-0.240532	1.962182
H	-8.307667	-0.599013	0.612411

H	-8.013861	-1.802734	1.866533
C	-6.142147	0.662485	-0.698784
C	-7.130202	0.363472	-1.818883
C	-5.074364	1.670804	-1.106273
H	-6.699625	1.087181	0.140689
H	-7.979198	-0.229899	-1.480160
H	-7.523578	1.324169	-2.159743
H	-6.673501	-0.129121	-2.676239
H	-4.368238	1.865250	-0.293109
H	-4.514840	1.350178	-1.988098
H	-5.571427	2.611740	-1.351128
C	-4.292311	-1.144668	-0.843701
C	-4.517038	-1.480467	-2.310371
H	-3.996562	-2.030678	-0.274103
H	-3.479477	-0.417227	-0.745850
H	-3.629976	-2.016724	-2.655137
H	-5.378143	-2.123291	-2.483830
H	-4.623879	-0.588903	-2.929479
H	1.628650	-2.729496	1.889087

Vibrational frequencies

17.3120	23.0444	32.2385
34.1094	37.2298	41.4157
44.1260	49.9025	52.6951
55.6004	64.3848	64.9886
69.2705	76.1793	81.5465
85.6571	94.2899	97.5960
103.7139	106.6489	115.1791
123.9612	133.8039	135.1656
139.6042	144.0776	148.9460
151.8378	170.8887	176.6929
177.8022	183.4378	190.4725
199.5648	205.7756	211.4302
213.2981	220.9958	222.3698
228.0786	230.8207	233.9552
238.1237	239.5320	246.7796
253.6074	260.9869	262.3530
269.2300	278.3139	281.6947
286.7688	288.5962	292.5752
304.3301	314.0569	328.4499
334.7790	336.4635	343.2437
345.6412	351.3222	366.7256
375.1998	383.1472	386.5104
398.1388	408.0051	414.4245
416.3443	426.0392	428.4509

439.7723 441.8157 450.4922
457.6905 473.5282 488.8395
495.2799 497.2760 502.4381
516.0349 519.2556 528.2842
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556.6533 563.6747 576.6664
582.0721 588.5820 592.6187
599.6749 604.6907 618.0182
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637.5189 654.7588 682.4987
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718.4986 720.1583 725.2919
739.4312 751.3293 756.2255
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779.1561 784.9619 787.7631
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1124.8875 1127.4474 1132.8111
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1212.1453 1216.6365 1222.8805
1224.5538 1229.0498 1232.9351
1240.2669 1246.5361 1249.8019

1257.0743	1258.6694	1277.8954
1282.5500	1285.2487	1289.7129
1294.8091	1299.6802	1312.8547
1325.6505	1331.2142	1337.6441
1338.4842	1342.8188	1351.8269
1352.2996	1357.8900	1363.2486
1369.2753	1373.3945	1375.3921
1377.4851	1385.5603	1387.2518
1395.8887	1403.1968	1412.0770
1414.9279	1418.2360	1418.8666
1421.2820	1424.0158	1425.5007
1427.2177	1430.5077	1433.7322
1435.4023	1438.3935	1450.8588
1452.0227	1458.6592	1465.2644
1469.7347	1475.1715	1477.2152
1482.7332	1483.1639	1486.2495
1488.1133	1490.7224	1491.4875
1492.4048	1493.9638	1496.2373
1496.8116	1498.3138	1499.6867
1500.3230	1504.6533	1506.9836
1510.6845	1511.7424	1512.9931
1514.7877	1516.7278	1517.8146
1520.3404	1521.8159	1526.5172
1527.9441	1534.7816	1537.5696
1537.9435	1542.1409	1554.5529
1576.7962	1578.7215	1659.7025
1673.9246	1679.4984	1683.3471
1685.1981	1694.7555	1696.9537
1701.1267	1702.0168	1705.2797
1847.6988	3062.7307	3065.1007
3066.2216	3068.3956	3080.9279
3091.0492	3093.0842	3095.3757
3096.4001	3097.5342	3101.3505
3107.2400	3107.9173	3110.1289
3118.0301	3126.5248	3132.3287
3133.4629	3134.0012	3141.4770
3143.6368	3152.1363	3160.1007
3162.8386	3163.8643	3171.4905
3174.8089	3175.7506	3175.7698
3180.1644	3183.1820	3183.3122
3185.3467	3188.6225	3189.9257
3191.3119	3191.7362	3192.6045
3193.9392	3194.1896	3194.9498
3201.5754	3203.4283	3204.5169

3206.4455	3206.4993	3208.6906
3210.8493	3212.0938	3213.5303
3217.7239	3219.9655	3220.6285
3226.3602	3228.0844	3231.5321
3237.2152	3383.4446	3497.6563

TS6d

Zero-point correction= 1.018916
Thermal correction to Energy= 1.074168
Thermal correction to Enthalpy= 1.075113
Thermal correction to Gibbs Free Energy= 0.929994
Sum of electronic and zero-point Energies= -2568.071138
Sum of electronic and thermal Energies= -2568.015886
Sum of electronic and thermal Enthalpies= -2568.014941
Sum of electronic and thermal Free Energies= -2568.160060
Cartesian coordinates

C	-3.997077	-3.636152	0.465913
C	-2.808253	-2.948938	0.691523
C	-1.881543	-3.385352	1.634732
C	-2.165326	-4.542903	2.353956
C	-3.355170	-5.241526	2.130121
C	-4.278898	-4.792804	1.189467
C	-4.840542	-2.958857	-0.582013
H	-0.961629	-2.836210	1.820793
H	-1.454989	-4.899189	3.093409
H	-3.561940	-6.143962	2.696209
H	-5.202322	-5.337798	1.019084
H	-5.748665	-2.536149	-0.142011
C	-1.364624	-2.434545	-2.142509
C	-2.609854	-3.023427	-2.712546
C	-3.953746	-1.832265	-1.165733
C	-2.708155	-1.733118	-0.201215
C	-0.226385	-1.244919	-0.717714
H	-2.488151	-3.194344	-3.781924
H	-2.727570	-0.803950	0.361469
N	-0.164093	-2.380390	-2.638642
N	0.541048	-1.645945	-1.736351
N	-1.445785	-1.757822	-0.963202
C	1.964503	-1.552267	-1.969989
C	2.443854	-0.640828	-2.912835
C	2.766017	-2.532303	-1.365756
C	3.812421	-0.689980	-3.196341
C	4.120105	-2.534070	-1.684478
C	4.659552	-1.620512	-2.598568

H	4.216996	0.014050	-3.918882
H	4.767240	-3.276774	-1.225487
O	-3.620641	-2.055478	-2.524843
H	-2.851854	-3.975080	-2.219574
H	-4.474225	-0.874636	-1.174808
H	-5.158919	-3.635232	-1.381962
C	1.553656	0.341880	-3.627045
H	1.644901	1.342221	-3.191059
H	0.503457	0.053225	-3.572713
H	1.850486	0.409363	-4.675796
C	6.124128	-1.665830	-2.944962
H	6.471490	-0.700573	-3.317978
H	6.308440	-2.412674	-3.723673
H	6.724906	-1.941738	-2.075257
C	2.168660	-3.559208	-0.439978
H	1.385406	-4.130274	-0.949423
H	1.718682	-3.102436	0.449065
H	2.934790	-4.255701	-0.096840
C	0.094586	-0.421378	0.516489
O	-0.806680	-0.266535	1.314835
C	1.521175	-0.000864	0.839322
C	1.657763	0.114300	2.369436
H	2.191065	-0.794237	0.488376
H	2.653963	0.511662	2.585821
H	0.922888	0.830215	2.748107
C	1.495110	-1.224183	3.052433
C	0.382630	-1.512152	3.845602
C	2.469848	-2.212911	2.876762
C	0.242407	-2.763095	4.444927
H	-0.383243	-0.753926	3.980455
C	2.329202	-3.466577	3.465836
H	3.349575	-1.994017	2.272358
C	1.211518	-3.745348	4.251074
H	-0.629795	-2.973104	5.056576
H	3.093425	-4.222803	3.316697
H	1.099872	-4.720492	4.714541
N	-0.085794	2.483449	-0.269432
N	-0.358519	1.414515	-1.066883
C	-1.231340	1.687528	-2.061141
O	-1.620908	2.776726	-2.467739
O	-1.637807	0.518901	-2.635475
C	-2.449924	0.675983	-3.797863
H	-1.907233	1.218169	-4.575700
H	-2.692643	-0.333002	-4.125576

H	-3.365024	1.220856	-3.556126
C	1.061761	2.453825	0.351360
C	1.996835	1.300898	0.092347
C	1.459626	3.512221	1.254613
C	3.435678	1.579746	0.467926
H	1.937871	1.075655	-0.977232
C	2.733719	3.614956	1.678271
H	0.735666	4.263111	1.532914
C	4.433060	0.695118	0.067784
C	3.775967	2.686822	1.261365
H	3.019809	4.439332	2.325158
C	5.759608	0.905438	0.434701
H	4.169377	-0.166439	-0.538226
C	5.111603	2.891291	1.629684
C	6.100752	2.007748	1.218683
H	6.525091	0.209392	0.106462
H	5.364900	3.752720	2.240909
H	7.132986	2.175279	1.506875
H	-1.010082	3.264455	0.028959
N	-2.142380	3.926215	0.607385
C	-2.145601	5.393269	0.285233
C	-2.261408	5.613820	-1.223595
C	-0.895753	6.116474	0.781269
H	-3.011180	5.845951	0.784230
H	-3.220037	5.293255	-1.634449
H	-2.152782	6.680688	-1.432127
H	-1.474992	5.064076	-1.746550
H	-0.748181	6.051798	1.861559
H	-0.001224	5.752801	0.266248
H	-1.000066	7.176556	0.538993
C	-3.361737	3.245375	0.034432
C	-4.707306	3.930348	0.299343
C	-3.417718	1.779335	0.454506
H	-3.191324	3.259698	-1.042263
H	-4.741831	4.955752	-0.073073
H	-5.474408	3.367246	-0.239971
H	-4.986276	3.937325	1.353496
H	-2.446610	1.291402	0.331652
H	-3.742552	1.652184	1.492202
H	-4.144519	1.269611	-0.184640
C	-1.930117	3.638332	2.052963
C	-2.992714	4.105566	3.044436
H	-0.982767	4.095170	2.332240
H	-1.773790	2.558889	2.144038

H	-2.573927	4.047522	4.052167
H	-3.291280	5.142890	2.869002
H	-3.885633	3.479384	3.025520

Vibrational frequencies

-997.3044	17.9366	23.0840
26.2722	26.5414	32.6664
37.1679	41.4466	45.5086
51.5249	55.9240	57.7855
65.6616	68.2993	73.4243
76.0181	77.0304	82.9949
90.9022	94.5696	95.1614
99.4778	102.4916	105.7494
111.3417	117.9162	125.6883
135.0199	143.0367	147.1073
159.6872	169.7321	173.1044
176.0208	185.8479	186.9775
191.7212	200.4804	213.0756
216.1779	219.5548	223.9080
232.6033	235.7982	239.7159
241.8817	253.2345	263.3303
270.5202	279.4298	284.2754
285.8678	289.3935	295.8331
309.5668	315.1182	320.9650
322.4263	330.1544	333.0207
351.2370	358.6062	361.4647
365.1983	383.4039	389.2820
393.5101	408.1435	415.0387
418.3749	419.6810	425.0063
439.6146	445.8229	447.4112
453.2358	455.4833	471.3862
472.5771	485.2754	496.3552
497.4156	503.1649	511.7551
516.3702	521.9725	529.1896
532.8234	537.9953	551.6142
558.6314	565.8402	588.9318
596.1113	600.2584	610.6773
619.6184	623.0063	630.8644
635.8705	649.1573	657.0096
676.0918	701.1105	713.9898
719.0261	721.8484	723.9997
734.6920	749.2835	754.4796
758.2127	765.2090	772.9779
775.5153	778.5868	785.5747
791.9935	796.3649	809.7317

813.2418	821.7906	835.6259
839.0825	863.5466	866.0567
870.1466	873.9091	878.4456
886.9458	888.9479	896.1479
906.7181	915.4416	915.7029
933.0324	935.5038	944.3488
945.6466	959.4460	960.8195
963.3990	965.9293	969.3878
970.2631	981.5223	982.6090
986.7546	991.6208	995.7203
996.2147	1005.6420	1015.5273
1017.6868	1025.4144	1027.2374
1029.3391	1030.4758	1037.3345
1040.7553	1042.5841	1050.2643
1053.6910	1058.5405	1063.4482
1065.9524	1067.3122	1068.7825
1069.6143	1073.6833	1082.1877
1086.5148	1088.7732	1109.7107
1114.0362	1117.9070	1123.9784
1126.6315	1139.9372	1146.6715
1150.6790	1154.2202	1161.5740
1168.5874	1180.8675	1182.0030
1183.9751	1185.8663	1186.3552
1199.6000	1200.6984	1202.8837
1206.9710	1209.6408	1211.2852
1215.3331	1218.8980	1221.4537
1229.2305	1232.8035	1240.5515
1242.0759	1246.8529	1249.2282
1255.5458	1257.4509	1265.3867
1278.8805	1283.5368	1286.5744
1311.6173	1314.6844	1316.3408
1326.4535	1333.3870	1334.7102
1345.4122	1346.9858	1349.9362
1352.6843	1356.7289	1361.2469
1363.6823	1364.2860	1372.3799
1374.8592	1376.4521	1379.2011
1384.2961	1389.7964	1396.8657
1399.5899	1400.0730	1416.7894
1421.4751	1422.8161	1423.3049
1427.6064	1431.7995	1434.2547
1435.6871	1439.6052	1446.5835
1461.7394	1464.9239	1466.0651
1476.0637	1477.8015	1481.7982
1485.5688	1485.7395	1488.8309

1493.8831	1496.1457	1496.7887
1496.8828	1498.4541	1499.9972
1500.9220	1503.8286	1504.2953
1506.3995	1509.4093	1512.9857
1515.0820	1515.3870	1518.8628
1520.1665	1521.0804	1523.3521
1528.7416	1529.8004	1535.6669
1537.7119	1546.8143	1549.1849
1552.6163	1555.4822	1579.8947
1632.2367	1654.5844	1676.6011
1680.3016	1686.1407	1689.5160
1695.3585	1697.9465	1698.9639
1699.5098	1714.0258	1738.2714
1775.0487	1808.9195	3063.8875
3065.9570	3069.9851	3070.6088
3074.9849	3080.7935	3083.3222
3084.2111	3085.5026	3086.5373
3086.7933	3091.7566	3098.3827
3111.2127	3115.9436	3120.7235
3129.1259	3130.8005	3137.2050
3153.2966	3153.4832	3153.7610
3154.8877	3155.2431	3156.4871
3157.9630	3161.6787	3163.9251
3165.6067	3168.1471	3170.5538
3171.7876	3174.6220	3176.6145
3181.3665	3181.9164	3189.9641
3192.7119	3195.6594	3201.0702
3202.8538	3203.5358	3206.3184
3210.0382	3210.2788	3210.8335
3210.8685	3218.4536	3220.4683
3220.4796	3220.6887	3225.9555
3231.1699	3232.3239	3232.9336
3240.8440	3249.5516	3286.2173

M6d

Zero-point correction= 1.021814
Thermal correction to Energy= 1.077934
Thermal correction to Enthalpy= 1.078878
Thermal correction to Gibbs Free Energy= 0.929960
Sum of electronic and zero-point Energies= -2568.073757
Sum of electronic and thermal Energies= -2568.017637
Sum of electronic and thermal Enthalpies= -2568.016693
Sum of electronic and thermal Free Energies= -2568.165610
Cartesian coordinates

C	2.776790	4.510293	0.755606
C	1.745406	3.587214	0.901108
C	0.762322	3.737030	1.874106
C	0.830817	4.843388	2.716690
C	1.866629	5.771624	2.582393
C	2.845509	5.612509	1.603625
C	3.705434	4.119080	-0.365650
H	-0.042834	3.013734	1.975913
H	0.073275	4.987427	3.479819
H	1.904521	6.630682	3.244173
H	3.642671	6.341694	1.497690
H	4.657878	3.751223	0.029763
C	0.232246	3.033469	-1.856380
C	1.208438	4.051653	-2.343422
C	2.973931	2.987155	-1.123920
C	1.875423	2.479838	-0.120097
C	-0.398449	1.373431	-0.596727
H	0.954466	4.359266	-3.357444
H	2.178198	1.537143	0.330166
N	-0.937483	2.691548	-2.315341
N	-1.323356	1.663402	-1.513953
N	0.596756	2.251661	-0.803245
C	-2.640938	1.117332	-1.722731
C	-2.830336	0.268715	-2.814160
C	-3.672043	1.567827	-0.890483
C	-4.133264	-0.178810	-3.040673
C	-4.947420	1.072119	-1.149066
C	-5.195555	0.206352	-2.220368
H	-4.318381	-0.848403	-3.876296
H	-5.771047	1.384327	-0.512174
O	2.469369	3.416882	-2.378351
H	1.204812	4.932090	-1.686969
H	3.643211	2.162515	-1.374801
H	3.931735	4.940679	-1.051184
C	-1.688485	-0.106514	-3.721321
H	-1.956913	-0.969607	-4.331880
H	-0.779210	-0.338460	-3.157459
H	-1.450370	0.726630	-4.390110
C	-6.592896	-0.285968	-2.489058
H	-6.582222	-1.208400	-3.072735
H	-7.158551	0.461962	-3.053681
H	-7.129985	-0.468829	-1.555387
C	-3.401695	2.548738	0.220503
H	-2.855454	3.419568	-0.156092

H	-2.810112	2.103087	1.030716
H	-4.338284	2.891811	0.661248
C	-0.390521	0.360099	0.529829
O	0.484740	0.494588	1.357327
C	-1.489228	-0.682704	0.687465
C	-1.637959	-1.008678	2.187881
H	-2.428876	-0.241268	0.343111
H	-2.234462	-1.918703	2.286472
H	-0.655345	-1.197001	2.626814
C	-2.346341	0.127832	2.887131
C	-1.644379	1.148090	3.534154
C	-3.741444	0.207831	2.813502
C	-2.324170	2.236476	4.081222
H	-0.561709	1.088298	3.605567
C	-4.421975	1.288367	3.366024
H	-4.291462	-0.584822	2.308907
C	-3.712368	2.310754	3.995239
H	-1.767272	3.021955	4.583055
H	-5.504612	1.335839	3.302951
H	-4.239842	3.156856	4.423475
N	1.075646	-2.042254	-0.575598
N	0.917987	-0.901019	-1.286932
C	1.948454	-0.687518	-2.144518
O	2.898912	-1.422260	-2.381433
O	1.765465	0.503087	-2.766812
C	2.672764	0.761254	-3.840180
H	2.626193	-0.043160	-4.576850
H	2.354917	1.706756	-4.272943
H	3.696866	0.845068	-3.468730
C	0.040197	-2.599065	-0.012451
C	-1.301314	-1.957288	-0.220034
C	0.176789	-3.815640	0.747541
C	-2.459166	-2.897418	0.037374
H	-1.334213	-1.606971	-1.259518
C	-0.918597	-4.525115	1.083362
H	1.172167	-4.176203	0.969653
C	-3.746801	-2.512550	-0.325109
C	-2.265101	-4.117420	0.704379
H	-0.806903	-5.461196	1.623011
C	-4.837327	-3.331145	-0.042412
H	-3.899210	-1.565383	-0.835055
C	-3.367429	-4.934069	0.988609
C	-4.647800	-4.544949	0.618287
H	-5.833665	-3.020324	-0.340339

H	-3.207200	-5.877119	1.502952
H	-5.495639	-5.182818	0.842992
H	2.037903	-2.443270	-0.429724
N	3.774013	-2.902883	0.597031
C	4.414444	-4.146343	0.099458
C	4.763553	-4.016145	-1.385314
C	3.509230	-5.367193	0.266724
H	5.342891	-4.345622	0.659405
H	5.571387	-3.306711	-1.574492
H	5.083003	-4.988346	-1.768385
H	3.884372	-3.682987	-1.945777
H	3.264094	-5.592555	1.306846
H	2.580964	-5.235434	-0.300240
H	4.020103	-6.244661	-0.137260
C	4.566705	-1.688068	0.257620
C	6.052686	-1.697103	0.649991
C	3.889851	-0.427946	0.789324
H	4.517913	-1.619318	-0.830094
H	6.568350	-2.597847	0.308300
H	6.541497	-0.842173	0.172535
H	6.206527	-1.605744	1.726411
H	2.819235	-0.430549	0.558148
H	4.004289	-0.312695	1.872144
H	4.347326	0.446718	0.315507
C	3.356168	-2.974499	2.008905
C	4.440389	-3.051434	3.088699
H	2.718062	-3.851511	2.119564
H	2.702432	-2.117406	2.206612
H	3.984948	-3.357693	4.034486
H	5.211988	-3.785159	2.836922
H	4.925711	-2.087868	3.254650

Vibrational frequencies

11.4698	21.5324	24.3344
29.5940	31.9743	34.4921
37.1044	41.1598	45.1086
48.5796	54.5966	55.0285
56.6581	65.1887	67.8384
71.1456	74.1235	78.9115
83.4183	89.6362	92.0823
97.5135	98.2650	107.5979
111.1659	119.3630	123.0790
133.2818	140.3586	149.3091
151.2408	162.5857	166.3019
174.4829	176.9667	185.8180

189.5149 204.4237 210.2305
212.2404 215.0169 217.8780
232.2824 241.2790 242.5850
251.8791 253.1438 259.1812
267.3812 277.5800 285.8017
288.3713 294.2324 298.3401
305.2334 310.1744 314.4792
316.6316 328.8835 342.5107
348.7405 359.5360 368.3991
372.8764 390.5770 396.9383
408.8566 412.0062 419.9646
421.5621 427.6796 431.1954
442.9242 445.4839 447.0994
449.5354 460.7937 474.4396
489.4642 496.1493 496.8471
501.9930 507.6905 514.1822
522.2542 525.5448 531.1543
536.5867 548.8444 556.7079
568.6342 588.0494 591.9617
598.8468 605.6469 612.1517
621.0039 629.4487 635.6625
636.3722 640.7756 662.4504
697.8485 717.2306 718.7143
720.0501 724.5075 728.4831
738.5969 747.8964 754.4044
764.5195 774.0454 774.6398
776.5867 779.6105 789.0746
794.3301 796.5226 807.2826
815.9302 828.1384 837.2753
857.1918 860.7208 866.8757
874.5945 878.0997 889.5179
891.0167 894.2741 903.6802
909.6987 920.0261 927.0848
932.1703 935.5536 944.5652
948.3223 956.3651 959.1262
966.9956 968.1214 969.7622
978.4788 983.2125 985.8117
992.3396 993.3263 1000.7262
1011.1807 1013.8786 1017.5551
1024.5519 1025.5858 1027.5759
1028.1165 1031.0431 1034.7678
1036.2877 1041.5274 1044.2308
1051.2016 1060.2404 1063.6885
1067.3965 1068.5257 1069.7565

1073.8582	1074.8459	1081.3508
1083.2638	1085.1017	1109.8424
1114.2527	1115.7262	1122.7756
1124.6446	1136.3241	1143.1168
1146.7976	1156.8106	1163.0873
1167.1177	1174.0422	1177.3879
1184.1892	1185.4036	1187.9331
1190.7915	1197.2818	1203.0429
1206.3938	1208.3114	1209.2450
1209.4276	1215.8288	1222.2961
1233.2032	1239.8296	1241.7285
1246.2944	1252.3301	1253.4800
1257.5445	1262.1294	1265.7218
1280.9760	1282.7207	1284.1052
1298.8461	1307.4343	1311.9680
1324.3764	1325.3061	1340.1537
1342.1499	1346.2825	1351.2826
1352.8224	1355.2713	1359.4500
1361.0281	1363.5747	1372.4976
1375.4622	1375.8474	1378.1808
1381.9619	1385.6223	1388.8765
1392.8094	1398.0074	1413.1453
1417.9075	1421.0750	1421.9202
1426.3808	1427.6628	1429.1842
1433.9934	1434.0828	1443.6474
1459.7842	1463.7205	1467.3105
1476.2640	1479.4068	1481.8848
1485.6582	1489.7053	1491.8493
1494.0053	1494.3321	1496.2570
1496.5484	1497.5585	1498.9517
1499.0949	1500.7744	1502.0157
1506.6802	1508.7777	1508.8993
1511.4532	1511.7767	1521.5874
1522.6925	1522.9176	1524.0781
1528.6444	1538.9820	1540.0565
1542.2719	1542.7537	1548.5108
1550.6167	1551.6010	1588.3637
1651.9897	1674.2133	1685.7724
1688.1186	1688.9134	1691.4621
1692.6343	1695.7645	1701.0223
1706.0827	1727.3564	1770.4243
1825.9384	2991.3486	3020.7645
3059.8562	3065.0869	3065.4829
3070.2731	3072.7408	3073.1692

3073.4158	3077.9342	3080.7769
3085.8551	3089.0655	3090.3325
3092.9367	3112.1351	3130.8332
3133.7345	3139.0302	3141.4889
3141.7997	3142.3026	3144.1806
3145.6910	3147.1009	3147.3212
3147.7397	3150.0129	3161.1807
3162.0023	3164.6771	3168.7396
3169.3047	3169.5869	3171.5351
3174.1300	3179.4372	3183.7952
3185.6916	3189.8430	3192.0604
3201.5034	3204.2347	3205.3452
3207.2790	3209.1444	3212.6389
3213.5079	3215.5501	3216.2427
3217.1124	3222.3947	3223.5412
3227.2915	3229.1028	3232.4698
3236.7277	3243.6052	3270.1319

TS7d

Zero-point correction= 1.019406
Thermal correction to Energy= 1.073699
Thermal correction to Enthalpy= 1.074643
Thermal correction to Gibbs Free Energy= 0.933505
Sum of electronic and zero-point Energies= -2568.065353
Sum of electronic and thermal Energies= -2568.011060
Sum of electronic and thermal Enthalpies= -2568.010116
Sum of electronic and thermal Free Energies= -2568.151253
Cartesian coordinates

C	-5.184823	-1.578934	0.507002
C	-3.804439	-1.531158	0.684419
C	-3.162579	-2.275873	1.666393
C	-3.942974	-3.091670	2.483668
C	-5.328480	-3.147441	2.314482
C	-5.960823	-2.390730	1.328967
C	-5.614321	-0.672413	-0.620514
H	-2.083548	-2.219076	1.799883
H	-3.466521	-3.684720	3.257247
H	-5.920871	-3.790567	2.957310
H	-7.037688	-2.441555	1.200135
H	-6.086471	0.235299	-0.229833
C	-2.218572	-2.141778	-1.948648
C	-3.616694	-2.342941	-2.430722
C	-4.307072	-0.311838	-1.361708
C	-3.172182	-0.591145	-0.314554

C	-0.687909	-1.080499	-0.810737
H	-3.609432	-2.816888	-3.411755
H	-2.819187	0.326194	0.151707
N	-1.091939	-2.584895	-2.421782
N	-0.144028	-1.923263	-1.697147
N	-2.014434	-1.228148	-0.956669
C	1.224286	-2.336115	-1.902835
C	2.023813	-1.675149	-2.839206
C	1.622199	-3.510705	-1.247195
C	3.309320	-2.181035	-3.037708
C	2.906142	-3.983783	-1.500999
C	3.768862	-3.320344	-2.379444
H	3.960502	-1.680129	-3.751602
H	3.240988	-4.890118	-1.001095
O	-4.162233	-1.042862	-2.573977
H	-4.195459	-2.958272	-1.730547
H	-4.282662	0.733855	-1.673321
H	-6.321649	-1.135752	-1.314047
C	1.537687	-0.499287	-3.645803
H	1.880977	0.447887	-3.217170
H	0.447637	-0.470089	-3.694548
H	1.930524	-0.567612	-4.662769
C	5.178289	-3.805286	-2.591422
H	5.883672	-3.153056	-2.052591
H	5.447755	-3.781545	-3.655606
H	5.306758	-4.830622	-2.217824
C	0.678982	-4.246729	-0.332631
H	-0.128451	-4.710005	-0.908365
H	0.214452	-3.580730	0.404439
H	1.204595	-5.032195	0.212687
C	-0.062100	-0.068179	0.172542
O	-0.880392	0.430199	0.971537
C	1.349457	-0.458824	0.723918
C	1.349013	-0.288391	2.252061
H	1.532646	-1.512156	0.489085
H	2.385573	-0.351801	2.600298
H	0.971647	0.706095	2.503386
C	0.540082	-1.339136	2.974386
C	-0.556416	-0.993231	3.766525
C	0.911594	-2.684990	2.893404
C	-1.257038	-1.966628	4.474710
H	-0.864063	0.047142	3.814962
C	0.200580	-3.665237	3.582052
H	1.779868	-2.966730	2.298582

C	-0.881746	-3.305706	4.382929
H	-2.106127	-1.681331	5.088048
H	0.503008	-4.705315	3.508178
H	-1.426235	-4.065432	4.935265
N	1.115466	2.187532	-0.409829
N	0.421457	1.218538	-1.088972
C	-0.340350	1.756679	-2.098149
O	-0.190593	2.862573	-2.583912
O	-1.262211	0.878344	-2.531778
C	-2.030969	1.314521	-3.661579
H	-1.383034	1.438156	-4.531742
H	-2.765881	0.527839	-3.826818
H	-2.519199	2.264711	-3.437949
C	2.195824	1.792548	0.201119
C	2.528241	0.339481	0.070165
C	2.991641	2.673736	1.015292
C	3.865645	-0.053064	0.642044
H	2.510674	0.099901	-1.001267
C	4.142442	2.222845	1.557563
H	2.680106	3.700086	1.156709
C	4.336654	-1.351600	0.469050
C	4.633119	0.866017	1.375248
H	4.751312	2.900986	2.151380
C	5.556927	-1.738741	1.013927
H	3.743001	-2.062532	-0.095374
C	5.862173	0.470379	1.918245
C	6.323444	-0.826350	1.742186
H	5.910087	-2.755546	0.871302
H	6.448919	1.188808	2.482616
H	7.274079	-1.128588	2.165679
H	0.589140	3.176537	-0.225859
N	-0.227251	4.418680	0.340177
C	0.721415	5.538586	0.074145
C	0.583086	6.786214	0.952715
C	0.764171	5.886093	-1.412800
H	1.709859	5.121788	0.309784
H	0.779457	6.561824	2.003601
H	1.327646	7.520230	0.631263
H	-0.401262	7.251159	0.874646
H	0.841438	4.982182	-2.022649
H	-0.118084	6.447237	-1.732547
H	1.638350	6.514061	-1.601148
C	-1.541733	4.494001	-0.360135
C	-2.387541	5.749485	-0.112460

C	-2.364510	3.233430	-0.085991
H	-1.290656	4.477173	-1.422481
H	-1.909231	6.651177	-0.498929
H	-3.336412	5.634411	-0.645585
H	-2.616552	5.906068	0.942831
H	-1.752160	2.327825	-0.106152
H	-2.857400	3.265212	0.890567
H	-3.146665	3.149396	-0.846848
C	-0.272696	3.990542	1.758845
C	-1.210610	4.697386	2.741702
H	0.752903	4.078383	2.135621
H	-0.510312	2.918112	1.763172
H	-0.981467	4.336827	3.748546
H	-1.094301	5.781799	2.738750
H	-2.259128	4.466786	2.546526

Vibrational frequencies

-136.9577	18.4669	24.5862
27.8660	31.6651	34.9769
38.1990	44.2775	49.5066
52.0761	57.5887	67.0153
74.3406	76.0605	81.2922
86.2878	88.4401	90.8705
97.1974	109.7331	116.7994
118.3470	119.9057	127.2830
133.7033	137.0536	146.6706
158.5858	165.3010	166.6752
179.2110	181.9639	185.8859
190.4890	196.2586	202.8719
216.1583	218.8932	224.3095
228.6758	230.9478	235.3660
239.7071	241.0782	244.4917
246.2796	251.4251	252.5323
263.8723	271.7443	282.5388
291.5601	293.5539	298.5700
304.6992	309.9866	324.1661
329.1109	331.7829	337.6344
348.7738	353.3143	359.6285
365.0930	373.2316	380.5158
388.8812	401.7135	411.4120
416.6330	421.4718	422.0127
428.9112	436.0697	442.8093
453.1216	468.7579	480.5453
487.6147	492.4985	499.0694
507.2708	511.4373	516.6672

525.1407 528.1485 535.1531
545.0219 557.7583 563.8594
569.8831 579.1849 588.8314
594.4229 606.0887 610.2531
615.3789 624.1799 629.5899
631.9625 651.1148 659.7279
682.7023 698.1270 716.5752
720.8177 725.5530 734.9130
744.0637 751.7565 753.6210
762.2155 766.5192 774.3893
776.6757 780.2031 789.1536
793.2690 802.0972 813.9527
815.6413 836.0745 838.3996
853.7290 863.0824 867.0639
876.3688 878.7158 887.5912
888.5302 893.0970 896.3885
907.1629 919.6639 923.2673
927.5256 932.3257 940.9422
942.6826 954.0505 956.5779
962.7814 967.0368 972.4718
975.2051 980.0328 981.8917
986.8028 997.3797 1008.2342
1010.0354 1019.0650 1020.5170
1023.3969 1025.2347 1029.3394
1030.2120 1031.6630 1032.6675
1043.7816 1046.8285 1052.7777
1057.4034 1060.3818 1064.8859
1065.9227 1067.0428 1070.3072
1075.0524 1077.2257 1080.2952
1087.4670 1091.3795 1097.0534
1116.3147 1117.2974 1119.4702
1130.5636 1139.6481 1142.7525
1149.3109 1155.6851 1169.8043
1175.3824 1175.7253 1176.9994
1177.6003 1183.7064 1190.5589
1193.2914 1193.6204 1195.3654
1201.6304 1207.6375 1208.8921
1216.8179 1222.3297 1225.0881
1229.0229 1234.1598 1246.0229
1248.4577 1249.4344 1250.2477
1252.6662 1264.9117 1270.2969
1274.1695 1280.4519 1281.5425
1288.6527 1299.4689 1306.6331
1321.8783 1334.4974 1336.1739

1338.2825	1340.1808	1348.1092
1351.4534	1353.3678	1361.0264
1362.1924	1366.1805	1369.1235
1370.5963	1374.1343	1376.7920
1386.2771	1388.5285	1394.9751
1408.1019	1410.1365	1413.8584
1419.4185	1420.9915	1423.9259
1425.5933	1430.2206	1431.2159
1438.0628	1440.1945	1442.1704
1458.4248	1463.1770	1467.1496
1471.1420	1474.7130	1483.1858
1487.1567	1489.7939	1492.0604
1492.5545	1493.3659	1494.1986
1496.4706	1496.9877	1500.2917
1503.4652	1504.4850	1505.3614
1507.4985	1510.3634	1512.0262
1514.5747	1515.2110	1515.3507
1517.2003	1522.1672	1523.2526
1528.4599	1530.0713	1532.6429
1535.2346	1538.4642	1546.1229
1554.2128	1570.9040	1589.0600
1607.2329	1647.9105	1675.4095
1679.4692	1682.3606	1690.7540
1693.9698	1694.7993	1697.6115
1699.8208	1704.8874	1749.5150
1799.4047	1809.9551	3019.6423
3063.5000	3066.5396	3069.7412
3072.5419	3077.3290	3078.3450
3079.4581	3084.1001	3084.2308
3086.1565	3087.1541	3087.6156
3090.3535	3091.2614	3091.4926
3108.7941	3119.0207	3124.6240
3136.0566	3137.4529	3141.3950
3144.6066	3149.3019	3150.6736
3154.9353	3157.9067	3158.3145
3160.1229	3163.8889	3171.6037
3173.5198	3177.4304	3178.0029
3180.4131	3181.3488	3186.3212
3186.9799	3188.8016	3190.0797
3190.5359	3193.1375	3198.3211
3198.6074	3205.5929	3206.1064
3210.1047	3211.9962	3212.4739
3214.0292	3215.3999	3220.3244
3222.9559	3234.8176	3235.2796

3237.9172 3238.4458 3254.1102

TS7d1

Zero-point correction= 1.019164
Thermal correction to Energy= 1.073743
Thermal correction to Enthalpy= 1.074687
Thermal correction to Gibbs Free Energy= 0.934040
Sum of electronic and zero-point Energies= -2568.021389
Sum of electronic and thermal Energies= -2567.966811
Sum of electronic and thermal Enthalpies= -2567.965866
Sum of electronic and thermal Free Energies= -2568.106513
Cartesian coordinates

C	5.422056	-1.393488	1.315130
C	4.292747	-0.583553	1.220456
C	4.347642	0.775653	1.518635
C	5.564939	1.316484	1.923449
C	6.699726	0.507931	2.028523
C	6.636370	-0.850075	1.726673
C	5.112532	-2.817581	0.931909
H	3.464160	1.403619	1.443304
H	5.631499	2.373541	2.159017
H	7.641704	0.944736	2.344144
H	7.521983	-1.473842	1.799468
H	5.114917	-3.467208	1.812684
C	2.962458	-0.843364	-1.652525
C	4.068544	-1.822959	-1.859571
C	3.701220	-2.775234	0.305963
C	3.101442	-1.389357	0.746587
C	1.433604	0.157486	-0.471543
H	4.121318	-2.111308	-2.909374
H	2.342242	-1.537601	1.514264
N	2.319819	-0.090088	-2.501651
N	1.371323	0.523961	-1.756414
N	2.454868	-0.716507	-0.395404
C	0.571073	1.562734	-2.355105
C	-0.423084	1.210516	-3.271343
C	0.930323	2.884123	-2.070728
C	-1.198166	2.251809	-3.781625
C	0.136751	3.884372	-2.627283
C	-0.951695	3.586160	-3.449936
H	-1.993615	2.012772	-4.482249
H	0.385572	4.922129	-2.420611
O	3.731005	-2.963840	-1.101851
H	5.030306	-1.387451	-1.554718

H	3.053201	-3.575192	0.662859
H	5.826285	-3.237619	0.217102
C	-0.569301	-0.191858	-3.797069
H	-0.335830	-0.965427	-3.059899
H	0.131881	-0.330144	-4.627223
H	-1.577221	-0.347066	-4.188106
C	-1.825763	4.687672	-3.986417
H	-2.574072	4.977464	-3.238540
H	-2.358335	4.369489	-4.886430
H	-1.236523	5.577536	-4.224675
C	2.167967	3.201287	-1.274408
H	3.019495	2.613205	-1.631682
H	2.035975	3.000527	-0.206199
H	2.414970	4.258268	-1.372860
C	0.626464	0.553076	0.757409
O	1.226738	0.465934	1.803248
C	-0.844375	0.983107	0.721100
C	-0.941868	2.211072	1.677839
H	-1.096969	1.288359	-0.302040
H	-1.946198	2.621635	1.596458
H	-0.834087	1.827983	2.695796
C	0.030936	3.350522	1.480360
C	1.206658	3.423236	2.238008
C	-0.279951	4.412872	0.626070
C	2.061657	4.517166	2.127112
H	1.441379	2.620144	2.930454
C	0.569208	5.512377	0.519469
H	-1.201533	4.383740	0.048993
C	1.744388	5.565509	1.265976
H	2.965623	4.555565	2.725364
H	0.307287	6.333654	-0.141943
H	2.403222	6.424045	1.185464
N	-0.341788	-1.951442	0.357396
N	0.409431	-3.102955	0.355410
C	0.747489	-3.364211	-0.916911
O	0.524254	-2.645499	-1.912279
O	1.381891	-4.550362	-1.021069
C	1.757114	-4.918951	-2.343182
H	2.432584	-4.178064	-2.772412
H	2.262876	-5.879151	-2.249816
H	0.875329	-5.018711	-2.980661
C	-1.015621	-1.486566	1.388964
C	-1.753849	-0.222030	1.237740
C	-0.993761	-2.232866	2.620427

C	-2.671538	0.077875	2.375351
H	-2.759000	-0.624775	0.306278
C	-1.774686	-1.839446	3.648958
H	-0.348027	-3.099612	2.675830
C	-3.648742	1.084603	2.276191
C	-2.687450	-0.724191	3.539056
H	-1.761626	-2.397821	4.581054
C	-4.566914	1.314229	3.289640
H	-3.713533	1.679938	1.370305
C	-3.622370	-0.484462	4.561311
C	-4.555234	0.529572	4.447998
H	-5.308819	2.097000	3.170230
H	-3.610417	-1.124470	5.439019
H	-5.278928	0.702935	5.236493
N	-3.690105	-1.203896	-0.492428
C	-4.098152	-2.406749	0.318783
C	-4.548503	-3.627434	-0.487698
C	-5.132140	-2.084255	1.397791
H	-3.168882	-2.694885	0.831654
H	-3.782721	-3.979500	-1.181000
H	-4.743568	-4.438849	0.218103
H	-5.470987	-3.441925	-1.043260
H	-4.873283	-1.206986	1.991413
H	-6.130956	-1.942767	0.977658
H	-5.180059	-2.939564	2.077067
C	-4.737402	-0.163037	-0.738670
C	-5.976674	-0.609087	-1.520865
C	-4.108701	1.072911	-1.379431
H	-5.072728	0.120318	0.262141
H	-6.416794	-1.521779	-1.116797
H	-6.727827	0.181370	-1.436777
H	-5.775092	-0.760764	-2.580125
H	-3.217156	1.407444	-0.837546
H	-3.825062	0.897486	-2.421104
H	-4.835368	1.888731	-1.367002
C	-2.833594	-1.552460	-1.657229
C	-3.489109	-1.897604	-2.993391
H	-2.213261	-2.394672	-1.339306
H	-2.157008	-0.701340	-1.806647
H	-2.728636	-2.357877	-3.629106
H	-4.311883	-2.604901	-2.889534
H	-3.862386	-1.011631	-3.512053
H	-0.439349	-1.515305	-0.563382

Vibrational frequencies

-1403.5432	21.2802	24.0830
28.7873	34.7787	42.4753
49.6040	55.2018	57.1261
57.9399	64.3014	66.9469
73.5562	77.2196	85.5497
93.6151	93.7413	96.0830
104.6270	108.8782	116.1321
117.3135	119.4611	124.0374
128.6809	137.3530	141.9457
143.0603	153.4189	155.2594
166.9964	179.4419	180.4347
189.4196	194.1282	203.3050
206.4660	209.2436	212.2596
219.4534	230.5136	236.9013
241.9439	243.5709	248.1113
252.7702	253.7735	258.5809
266.1719	270.1372	275.2622
283.8500	290.3566	296.4603
303.9166	307.6208	312.0531
327.9133	333.1137	340.9450
345.4374	349.5654	350.9968
355.8468	361.7508	369.5331
384.4452	390.9684	398.1265
402.5592	409.4417	413.3910
429.3610	431.6689	432.3363
444.2684	452.4121	458.4811
480.4614	490.4517	502.1554
506.2453	511.4595	515.0270
524.2355	528.1046	535.9163
542.0712	548.3113	558.3312
566.8599	576.1162	592.3722
593.3768	597.8697	607.9865
615.4304	627.8461	633.2418
644.7902	652.1970	677.2139
686.2427	689.8207	706.8949
719.6381	722.6612	725.1780
729.9409	736.1321	748.4335
752.2305	754.5731	769.2111
773.1509	784.4531	787.6593
792.7405	803.8341	813.2288
819.8110	829.7807	834.6288
848.6785	856.9988	860.4435
871.8650	875.0845	879.9505
883.1497	890.3394	892.3031

898.5051 914.3886 917.4918
919.4575 925.4175 932.4491
937.0272 943.4958 951.5136
959.2514 960.1466 963.5954
967.4517 969.7923 971.2795
984.6724 989.7793 992.9216
999.4953 1003.2791 1012.6733
1017.0040 1018.7329 1023.4307
1027.7642 1028.6816 1031.6728
1035.2806 1037.5757 1040.6870
1045.1224 1047.6839 1054.7917
1056.2567 1061.5083 1062.2438
1065.5104 1066.7367 1072.2471
1077.0904 1088.2438 1096.7698
1106.6594 1112.9326 1116.8749
1119.9138 1121.9091 1134.9988
1150.1282 1157.5356 1158.2996
1161.1487 1177.0053 1177.1050
1180.7139 1181.3723 1183.9587
1191.7517 1193.0764 1194.0352
1202.4608 1207.8609 1208.9008
1210.3457 1214.2820 1227.9453
1232.3199 1237.4950 1238.2733
1241.9474 1248.9707 1251.0175
1259.5966 1263.3448 1274.0830
1280.6609 1284.3345 1289.9153
1302.0946 1311.0392 1312.3193
1330.7550 1342.3257 1344.6452
1345.3608 1346.8548 1350.0641
1353.9992 1363.4643 1366.7060
1368.8320 1372.5177 1373.1786
1375.0267 1376.7353 1379.0264
1384.5485 1389.8771 1394.1730
1407.9001 1410.2139 1418.8703
1419.6897 1420.0518 1420.3288
1425.2139 1426.2378 1434.7535
1437.7169 1443.2068 1446.3945
1464.4902 1465.9228 1473.7854
1476.9725 1482.6821 1484.3759
1489.3656 1491.9587 1493.3209
1493.6035 1493.6939 1495.4259
1497.4191 1498.8194 1499.1434
1499.6182 1501.8216 1503.6064
1506.8056 1508.6926 1514.0037

1514.7846	1515.7360	1516.3383
1519.9788	1522.6454	1524.7235
1530.8771	1531.7778	1532.5740
1536.7061	1539.7467	1552.0695
1553.1477	1567.9691	1571.4527
1593.6470	1633.2764	1672.7320
1674.3163	1679.5641	1680.8630
1684.4980	1689.8422	1691.6163
1697.4747	1697.9278	1700.6570
1711.2884	1839.3689	3056.6380
3058.4326	3069.3746	3071.4673
3074.9706	3076.4039	3076.8788
3083.7962	3086.6142	3089.9336
3090.1064	3092.8645	3098.1609
3098.3248	3117.0094	3129.1632
3131.5282	3140.2225	3142.1252
3143.6872	3145.2698	3152.0561
3159.6721	3160.2672	3160.8741
3162.4821	3166.3476	3172.9586
3174.9902	3175.7052	3177.9081
3178.9566	3182.2961	3183.6940
3187.8593	3188.0430	3191.3509
3191.4054	3199.7019	3201.0103
3203.3948	3204.7641	3206.6043
3206.8110	3207.2961	3209.4898
3211.4008	3212.6563	3214.1587
3218.5958	3218.6708	3220.4337
3230.3369	3231.1675	3236.7143
3243.8929	3266.5070	3452.9711

M7d1

Zero-point correction= 0.741970

Thermal correction to Energy= 0.784060

Thermal correction to Enthalpy= 0.785004

Thermal correction to Gibbs Free Energy= 0.668803

Sum of electronic and zero-point Energies= -2197.006072

Sum of electronic and thermal Energies= -2196.963982

Sum of electronic and thermal Enthalpies= -2196.963038

Sum of electronic and thermal Free Energies= -2197.079240

Cartesian coordinates

C	5.305037	-0.450374	-0.592336
C	3.935054	-0.688189	-0.658407
C	3.423311	-1.961958	-0.880106
C	4.321220	-3.015613	-1.033557

C	5.698518	-2.786612	-0.972777
C	6.200091	-1.504669	-0.754647
C	5.589094	1.010483	-0.348668
H	2.349237	-2.122259	-0.933297
H	3.950433	-4.022097	-1.198855
H	6.386069	-3.617896	-1.092048
H	7.271119	-1.333313	-0.702956
H	5.972095	1.486731	-1.257156
C	2.423259	0.449211	1.900492
C	3.816969	0.837645	2.267042
C	4.227262	1.630868	0.042230
C	3.156647	0.589269	-0.446884
C	0.803682	0.111480	0.478039
H	3.853598	1.176183	3.302291
H	2.654464	0.930257	-1.351964
N	1.377335	0.231036	2.644721
N	0.375876	0.020796	1.741169
N	2.114805	0.388992	0.572108
C	-0.937466	-0.379823	2.166326
C	-1.918772	0.592469	2.365400
C	-1.184476	-1.755478	2.230599
C	-3.219942	0.137795	2.580705
C	-2.499778	-2.155419	2.452332
C	-3.530416	-1.222660	2.605694
H	-4.013833	0.869335	2.712736
H	-2.727465	-3.218150	2.479211
O	4.160194	1.924398	1.433720
H	4.500052	-0.013495	2.139938
H	4.047608	2.589621	-0.447658
H	6.322002	1.185441	0.444513
C	-1.627016	2.070917	2.329274
H	-0.556070	2.286651	2.289028
H	-2.024245	2.549391	3.227851
H	-2.118745	2.539303	1.469111
C	-4.958666	-1.664417	2.783741
H	-5.046697	-2.751866	2.751533
H	-5.584683	-1.242128	1.991217
H	-5.359474	-1.314407	3.739219
C	-0.083239	-2.748647	1.972547
H	0.809912	-2.513646	2.558283
H	0.196979	-2.751426	0.910079
H	-0.413483	-3.757807	2.221701
C	0.069887	0.040318	-0.857188
O	0.811136	-0.197976	-1.820568

C	-1.433053	-0.362793	-0.896133
C	-1.631953	-1.382813	-2.044390
H	-1.709078	-0.866243	0.033178
H	-2.693991	-1.428217	-2.297309
H	-1.092838	-1.022365	-2.922184
C	-1.147816	-2.755906	-1.642775
C	0.113748	-3.222964	-2.020377
C	-1.948671	-3.573611	-0.836718
C	0.566377	-4.472348	-1.596315
H	0.741288	-2.592536	-2.643415
C	-1.500554	-4.821099	-0.411346
H	-2.937450	-3.229854	-0.538884
C	-0.236690	-5.273070	-0.787203
H	1.545639	-4.823218	-1.908418
H	-2.137358	-5.440526	0.213241
H	0.116510	-6.244489	-0.456579
N	-0.251468	2.022798	-0.801403
N	0.641661	2.722272	-1.624537
C	1.564747	3.397924	-0.937754
O	2.449133	4.105716	-1.423570
O	1.503520	3.246569	0.454622
C	2.222313	4.215722	1.206616
H	1.772918	5.205692	1.084452
H	2.155836	3.899165	2.248238
H	3.268173	4.254579	0.902004
C	-1.628517	2.066744	-1.188547
C	-2.287763	0.871485	-1.069643
C	-2.278636	3.270468	-1.544182
C	-3.715176	0.861786	-1.139008
H	-0.179859	2.349420	0.167279
C	-3.636085	3.258338	-1.713365
H	-1.683345	4.168058	-1.673173
C	-4.494325	-0.282975	-0.821930
C	-4.387976	2.070375	-1.481830
H	-4.166703	4.164510	-1.990729
C	-5.866026	-0.241566	-0.883653
H	-3.994996	-1.190892	-0.495972
C	-5.805150	2.074155	-1.558568
C	-6.530249	0.944993	-1.272410
H	-6.444993	-1.124161	-0.630446
H	-6.307216	2.996968	-1.835648
H	-7.613565	0.962132	-1.328368

Vibrational frequencies

18.0916	32.8462	34.2918

42.5512 46.7146 50.8174
56.1638 62.0689 67.9358
71.2834 79.6035 84.9247
94.5480 99.5296 102.2052
103.6175 110.9780 121.6091
133.8134 142.7174 151.6223
164.8235 165.6825 171.2298
178.9264 189.6226 198.9154
207.7172 215.0081 220.0101
233.8452 239.0022 246.1559
247.1373 260.2484 262.0941
272.2046 284.6145 292.2941
308.2846 315.6688 328.1342
336.2536 345.1052 366.2622
384.6740 394.9306 398.0784
407.1210 419.6671 420.7353
427.4507 442.5212 445.7967
451.6595 462.0376 490.2924
492.7604 495.4449 512.3093
518.3259 527.1409 529.6013
533.9935 548.7422 566.0386
567.9163 577.5832 587.5007
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987.7727 989.5604 1000.3174
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1050.9254 1054.6371 1057.1309
1060.3807 1061.6142 1063.0465
1063.6320 1065.2755 1068.0573

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1207.8442	1211.1607	1212.0813
1219.9365	1231.9619	1234.8788
1243.0882	1247.2232	1255.5703
1268.2661	1278.7194	1286.2987
1287.6361	1296.3317	1303.9322
1317.2580	1328.1092	1334.1106
1341.9593	1350.7821	1352.4413
1359.1007	1363.4708	1366.5312
1372.8350	1374.5899	1381.6809
1384.6982	1395.5297	1413.6178
1417.7445	1424.9386	1427.2931
1442.4536	1443.9309	1445.5204
1465.1873	1469.8218	1479.4879
1482.3078	1485.0102	1485.8061
1488.1881	1489.4933	1492.7162
1497.7786	1498.1369	1499.5462
1502.1499	1508.3904	1514.2520
1517.6644	1521.4232	1522.0475
1531.7113	1539.7686	1542.6590
1555.1357	1577.5078	1578.4667
1650.7683	1668.1716	1675.1756
1683.3720	1685.3366	1690.0575
1691.7211	1695.0499	1700.5819
1701.1397	1718.0520	1757.2213
3060.0469	3061.3167	3069.8312
3070.6552	3084.2021	3085.3508
3111.8190	3134.7220	3135.0634
3137.0317	3140.3713	3142.9442
3156.2511	3163.4670	3169.0915
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3177.3213	3180.2140	3183.4066
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3202.5173	3202.6218	3205.1032
3206.5087	3207.7297	3209.3558
3214.1007	3219.7382	3219.8611
3224.1893	3227.2363	3234.3558
3236.0103	3238.6784	3418.5543

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