Supporting Information

Theoretical Model for N-Heterocyclic Carbene Catalyzed Decarboxylation Reactions

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Part 1: Computational methods

All theoretical calculations were performed with Gaussian 09[1]. All structures were completely optimized by using the B3LYP-D3 method and the 6-31G(d, p) basis set in solvent of THF, which employs the integral equation formalism polarizable continuum model (SMD). Frequency calculations were carried out at the same level to confirm all the optimized structures as minima (no imaginary frequency) or transition states (only one imaginary frequency), and provided the thermal relative Gibbs free energy correction.

All the energies discussed in the main text are the relative Gibbs free energies (GFE), which are obtained by the addition of the thermal Gibbs free energy corrections (GFEC) at the B3LYP-D3[2]/6-31G(d, p)/SMD[3]$_{THF}$ level. To check whether the selected method is reliable, the additional calculations by employing different DFT methods and levels (including M06-2X[4]/6-31G(d, p)/SMD$_{THF}$ and ωB97X-D[5]/6-31G(d, p)/SMD$_{THF}$) have been performed for the key transition states involved in the stereoselectivity-determining step, and the computed and tested results can be found in the **Table S1**. As summarized in **Table S1**, there are small differences between the energies calculated by different methods. Thus, the selected DFT method is appropriate for the system studied in this work.

Table S1. The relative Gibbs free energies (kcal/mol) of transition states **TS5R/S** calculated by the three DFT methods.

Method	B3LYP-D3	M06-2X	ωB97XD
TS5R	0.0	0.0	0.0
TS5S	4.0	4.2	3.7

We further computed the single-point energies for the key transition states **TS5R/S** optimized at the B3LYP-D3/6-31G(d, p)/SMD$_{THF}$ level by using the higher basis set 6-311++G(2df, 2pd). As summarized in **Table S2**, the energies of transition states **TS5R/S** calculated by 6-311++G(2df, 2pd) basis set are close to those calculated by the

selected basis set 6-31G(d, p). Thus, the calculated results should be reliable, and the selected basis set is suitable for the systems studied in this work.

Table S2. The relative Gibbs free energies (kcal/mol) of transition states **TS5R/S** calculated by B3LYP-D3 method with two different basis sets including 6-31G(d, p) and 6-311++G(2df, 2pd).

Basis Set	**6-31G(d, p)**	**6-311++G(2df, 2pd)**
TS5R	0.0	0.0
TS5S	4.0	5.9

Noncovalent interaction (NCI) and atom-in-molecule (AIM)[6] analyses were plotted using NCIplot (version 1.0)[7] and Multiwfn (version 3.3.8)[8]. The three-dimensional structures were illustrated by using CYLview[9].

Part 2: Additionally computational results

2.1 Structural transformation between **NHC•H**$^+$ and **NHC**

Figure S1 depicts the energy profile of the deprotonation process of **NHC•H**$^+$ for the formation of **NHC**. As shown in **Figure S1**, the energy barrier for DBU-assisted deprotonation process of **NHC•H**$^+$ via transition state **TS** is 8.4 kcal/mol, indicating that this process can occur smoothly. Therefore, we think that the free carbene can be easily generated, and the chemical equillium between **NHC** and **NHC•H**$^+$ exists in this reaction system.

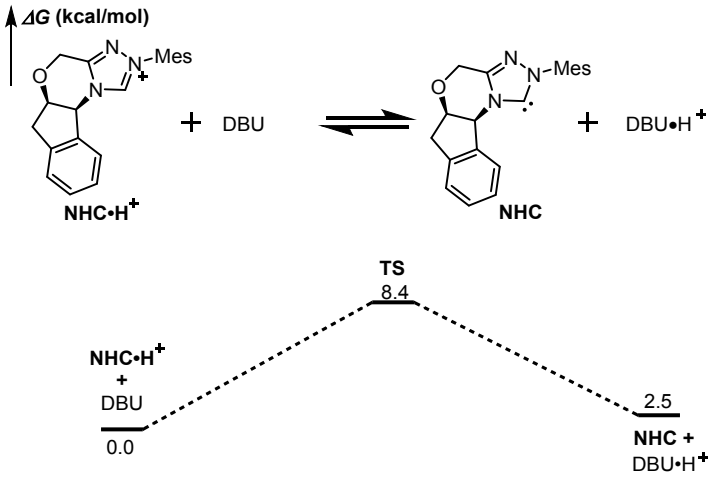


Figure S1. The Gibbs free energy profile for the structural transformation between **NHC•H**$^+$ and **NHC**.

2.2 Different deprotonation pathways of reactant ***pre*-R2**

As shown in **Figure S2**, the α-C(sp^3)-H bond of the other reactant ***pre*-R2** can be deprotonated by DBU to form the real substrate **R2**, which happens through transition state **TS0**. The energy barrier of the deprotonation pathway associated with DBU via **TS0** ($\Delta G^{\neq}$=15.4 kcal/mol) is 10.3 kcal/mol.

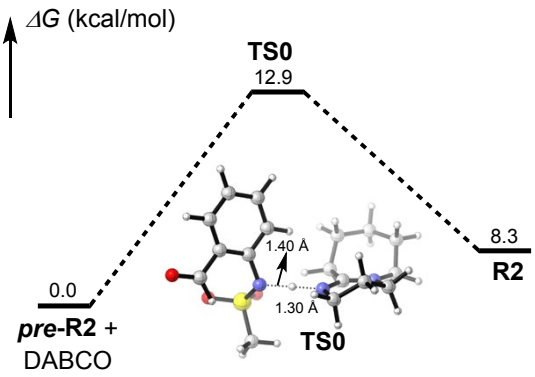


Figure S2. Relative Gibbs free energy profiles of the deprotonation pathway of ***pre*-R2** (distance in angstrom).

2.3 Possible pathways for the former two steps

As shown in **Figures S3** and **S4**, the nucleophilic attack on the carbonyl carbon of **R1** by **NHC** catalyst occurs through either transition state ***Re*-TS1** or ***Si*-TS1** ($\Delta G^{\neq}$=10.9 or 7.9 kcal/mol), which provides the zwitterionic intermediate ***Re*-M1** or ***Si*-M1**, respectively. It should be mentioned that the "***Re*-/*Si*-" represents the attack mode from the *Re* or *Si* face of conjugated dienal **R1**, respectively.

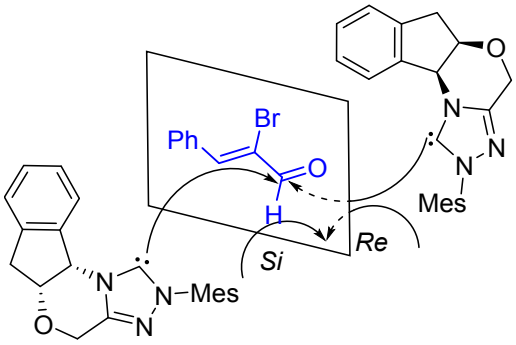


Figure S3. The nucleophilic attack modes of **NHC** to the reactant **R1**.

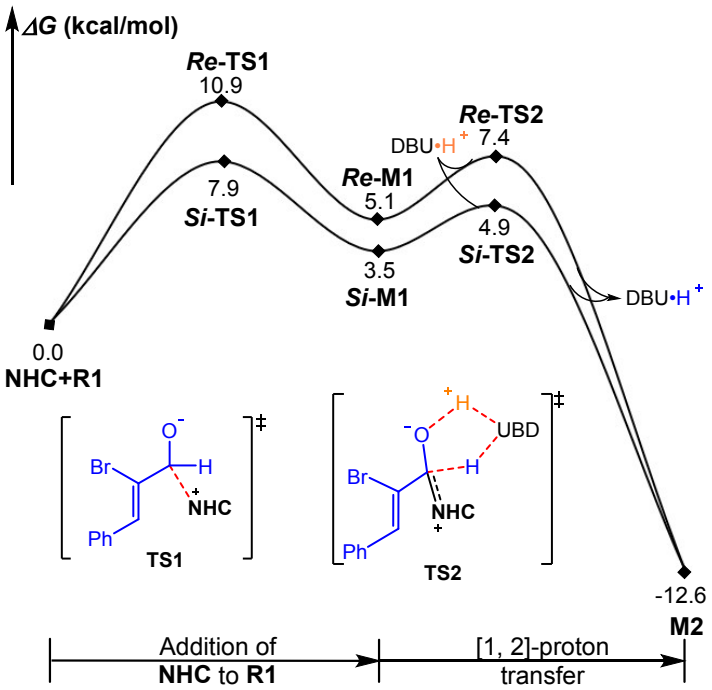


Figure S4. Relative Gibbs free energy profiles for the former two steps of main catalytic cycle and the corresponding 2D-structures of transition states.

The next step is the formation of the Breslow intermediate **M2** through the DBU•H^+-assisted [1, 2]-proton transfer process, and the energy barriers required for this transformation were 2.3 kcal/mol and 1.4 kcal/mol associated with transition states ***Re*-TS2** and ***Si*-TS2** (**Figure S4**), respectively. Obviously, the pathway associated with the *Si*-face attack is more energetically favorable. Thus, the *Re*-face pathway can be excluded in the following discussion.

2.4 Tests of the influence of explicit solvent in proton transfer process

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[10], 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 B3LYP-D3 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[11], 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 S5**, in which 100 THF solvents in a sphere shape were added by using the Packmol software, and both the B3LYP-D3 and M06-2X methods were tested in this part.

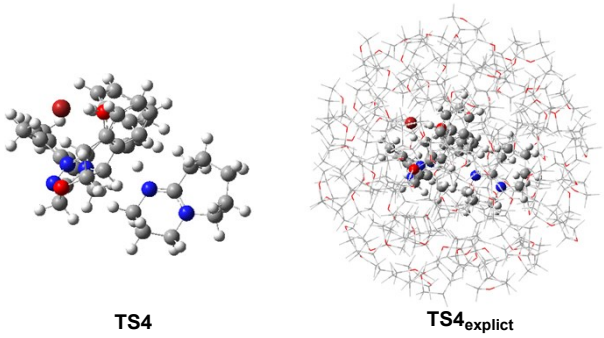


Figure S5. Optimized geometries of transition states with or without explicit solvents involved in proton transfer process.

Table S3. Test the influence of explicit solvent in proton transfer process

Method	**kcal/mol**
B3LYP-D3($\Delta\Delta G_{tot}^{\ddagger}$[TS4-M3]^{a})	19.0
B3LYP-D3($\Delta\Delta G^{\ddagger}$[TS4$_{explicit}$-M3$_{explicit}$]^{b})	18.5
M06-2X($\Delta\Delta G_{tot}^{\ddagger}$[TS4$_{M06\text{-}2X}$ -M3$_{M06\text{-}2X}$]^{a})	21.4
M06-2X($\Delta\Delta G^{\ddagger}$[TS4$_{explicit}$-M3$_{explicit}$]^{b})	20.5

[a]The transition state **TS4** and intermediate **M3** obtained from the IRC calculations were calculated at the level of B3LYP-D3/6-31G(d, p)/ SMD_{THF}.

[b]The transition state **TS4explicit** was first located in the sphere with a radius of 15Å of the explicit solvents at the ONIOM(B3LYP-D3/6-31G(d, p):UFF) level. Then IRC calculation was performed to locate the corresponding intermediate **M3**$_{explicit}$.

As summarized in **Table S3**, the calculated results indicate that the free energy barriers $\Delta\Delta G_{tot}^{\ddagger}$ (with the normal 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[10]. As mentioned above, we believe that the computational errors in this system are not very significant and the calculated results using B3LYP-D3 method are consistent with the experiment.

2.5 Different conformers and configurations of **TS5**s

To ensure the selected and discussed configuration of the enantiochemical transition state **TS5**s with the lowest energy in the main text, we have searched multiple possible conformations for the fifth step. By rotating the dihedral angle Φ(C3−N−Cβ−Cα) with 60° per time in enantio-controlling transition states **TS5R** and **TS5S**, we have totally constructed 2*6=12 conformations as the initial structures, which have been subsequently optimized the structures at the B3LYP-D3/6-31G(d, p)/SMD_{THF} levels, respectively. After the optimization, the corresponding dihedral angles Φ(C3−N−Cβ−Cα) change to 50°/90°/177°/-54°/-128°/-175° and 168°/-61°/-100°/--160°/11°/137° in the **TS5R**s and **TS5S**s, respectively. As revealed by **Figure S6**, the most stable conformations with the lowest energies of the four enantioselective transition states (denoted as **TS5R** and **TS5S**) are associated with the dihedral angles Φ(C3−N−Cβ−Cα) of 50°/168°, separately.

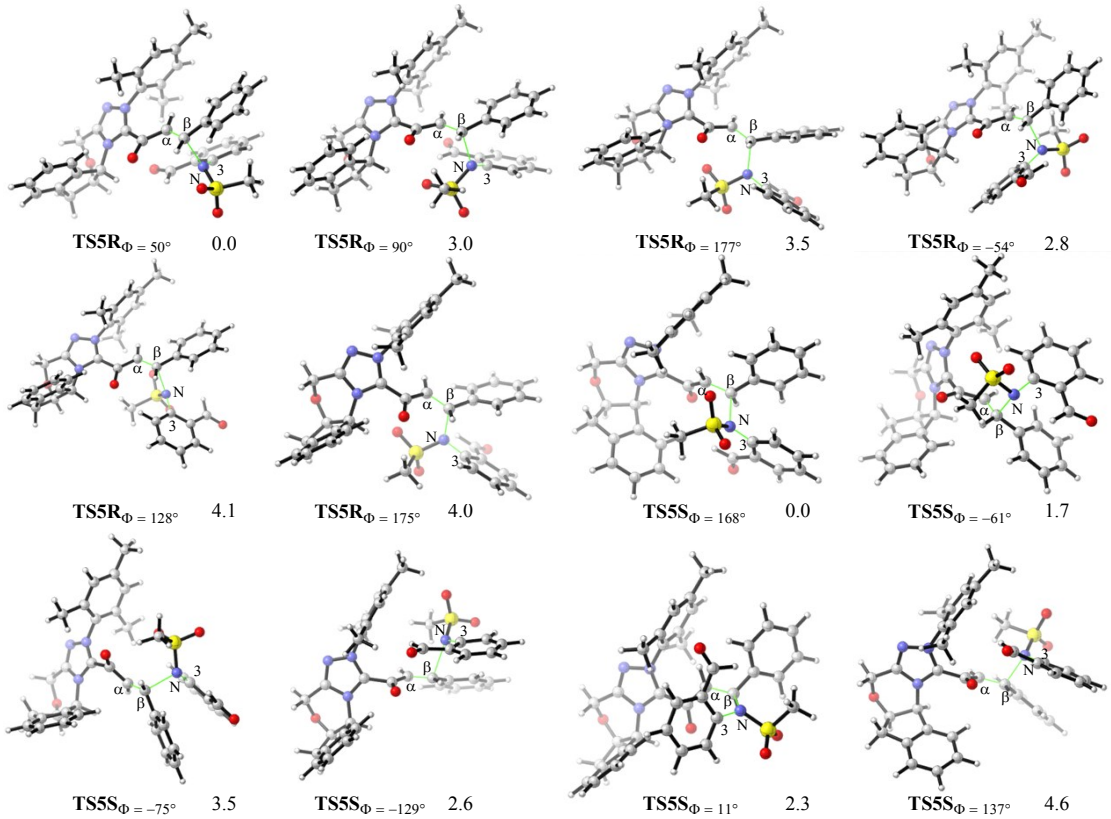
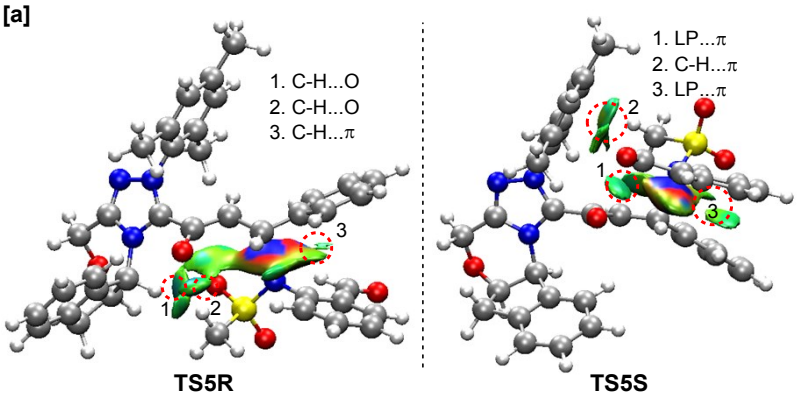


Figure S6. Different configurations and relative energies of the transition states **TS5R**s and **TS5S**s with different dihedral angles Φ(C3−N−Cβ−Cα) (energy in kcal/mol).

Attracted by the puzzle of stereoselectivity, the topology analysis on the key transition states **TS5R/S** was performed to characterize the enantioselectivity-determining factors and electron density distribution by using noncovalent interaction (NCI) method and Bader's atoms-in-molecules (AIM) method. As shown in **Table S4**, the NCI analyses of the transition states **TS5R/S** indicate that the hydrogen bond C-H…O interactions would be significant for determining the enantioselectivity. Correspondingly, the values of Laplacian electron density at the bond critical points (BCPs) along the bond paths were summarized in **Table S4**. The quantitatively calculated results indicate that there are more and stronger hydrogen bond C-H…O interactions in **TS5R** compared with those in the other three transition states. Hence, the C-H…O hydrogen bond interactions would lead to the energetical favorability of *R* configurational transition state **TS5R**, and thus control the enantioselectivity. For the reader's convenience, we have only discussed *R* configurational pathway in the main text.

Table S4. NCI Analyses of the Transition States **TS5R** and **TS5S** and Summary of the Values of Laplacian Electron Density ($\nabla^2\rho$, eÅ^{-3}) at the Bond Critical Points (BCPs) in **TS5R/S**



	TS5R		TS5S	
Interactions	Type	$\nabla^2\rho$	Type	$\nabla^2\rho$
1	C-H…O	0.474	LP…π	0.274
2	C-H…O	0.454	C-H…π	0.269
3	C-H…π	0.156	C-H…π	0.245

2.6 Possible [2+2] cycloaddition pathways

To figure out the role of the **NHC** catalyst, we also considered and compared with the [2+2] cycloaddition pathway without the presence of **NHC** for formation of β-lactone ring. As shown in **Figure S7**, intermediate **M5R** releases the catalyst **NHC** via transition state **TS6′** ($\Delta G^{\neq}$ = 13.6 kcal/mol) for generating ketene **M6′**. Then, the intermediate **M6′** undergoes intramolecular concerted Cα-C1 and C(carbonyl)-O2 bonds formation to obtain β-lactone **M7R** via transition state **TS7′** with an energy barrier of 32.2 kcal/mol, which is much higher than that associated with the **TS6R** ($\Delta G^{\neq}$ = 4.7 kcal/mol) in the [2+2] cycloaddition pathway with the presence of **NHC**.

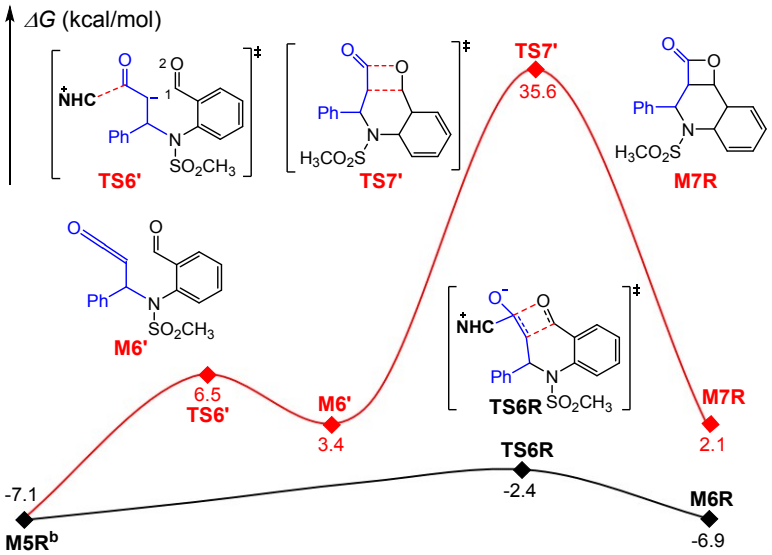


Figure S7. Gibbs free energy profiles for the possible [2+2] cycloaddition pathways.

To discover the role of **NHC** in this process, we tracked and compared the frontier molecular orbital overlap modes along the intrinsic reaction coordinates (IRC) of transition states **TS7′** (**Figure S9** of SI) and **TS6R** (**Figure S10** of SI). As shown in **Figure S8**, the orbital interaction between the center atoms involved in HOMO of **TS7'** along the IRC is gradually changed from a shoulder-to-head overlap mode to a head-to-head overlap mode (**Figure S8a**), which results in the formation of the $\sigma_{C2-C\alpha}$ bond/orbital. We can find that the Cα–C1 σ bond formation involves an unfavorable shoulder-to-head overlap mode[12] between the orbitals in the pathway associated with **TS7′.** In contrast, only the head-to-head overlap mode formation of the $\sigma_{C2-C\alpha}$ bond/orbital can be observed in the HOMO of **TS6R** along the IRC. Therefore, the intramolecular [2+2] cycloaddition reaction with the presence of **NHC** can avoid the unfavorable shoulder-to-head overlap mode, thus the reaction energy barrier is reduced. This opens a new door to explore the new role of catalyst by the so-called frontier molecular orbital overlap mode (FOM) analysis.

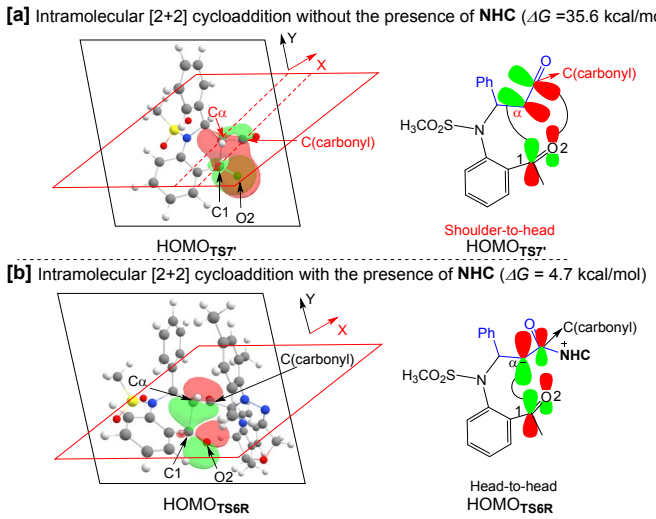


Figure S8 FMO overlap modes involved in the HOMOs of (a) **TS7′** and (b) **TS6R** (only the orbitals of the key C(carbonyl), C1, O2, and Cα atoms of **TS7′** and **TS6R** are shown for clarity).

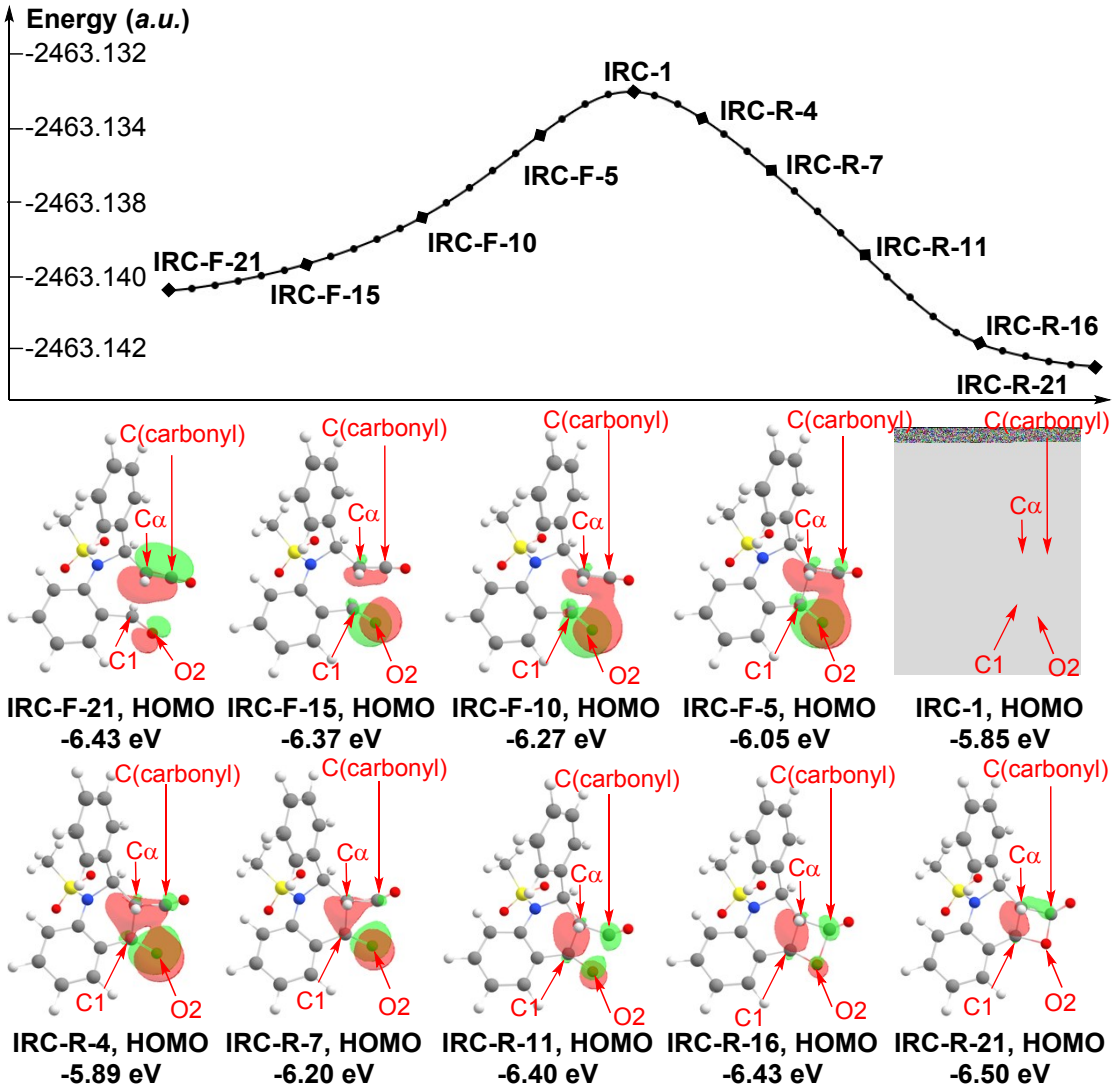


Figure S9. The HOMO changes along the several representative IRC points of **TS7′**. ("F" and "R" represent forward and reverse directions, respectively; IRC-1 is the structure of **TS7′,** only the orbitals of the key C(carbonyl), C1, O2, and Cα atoms of **TS7′** are shown for clarity).

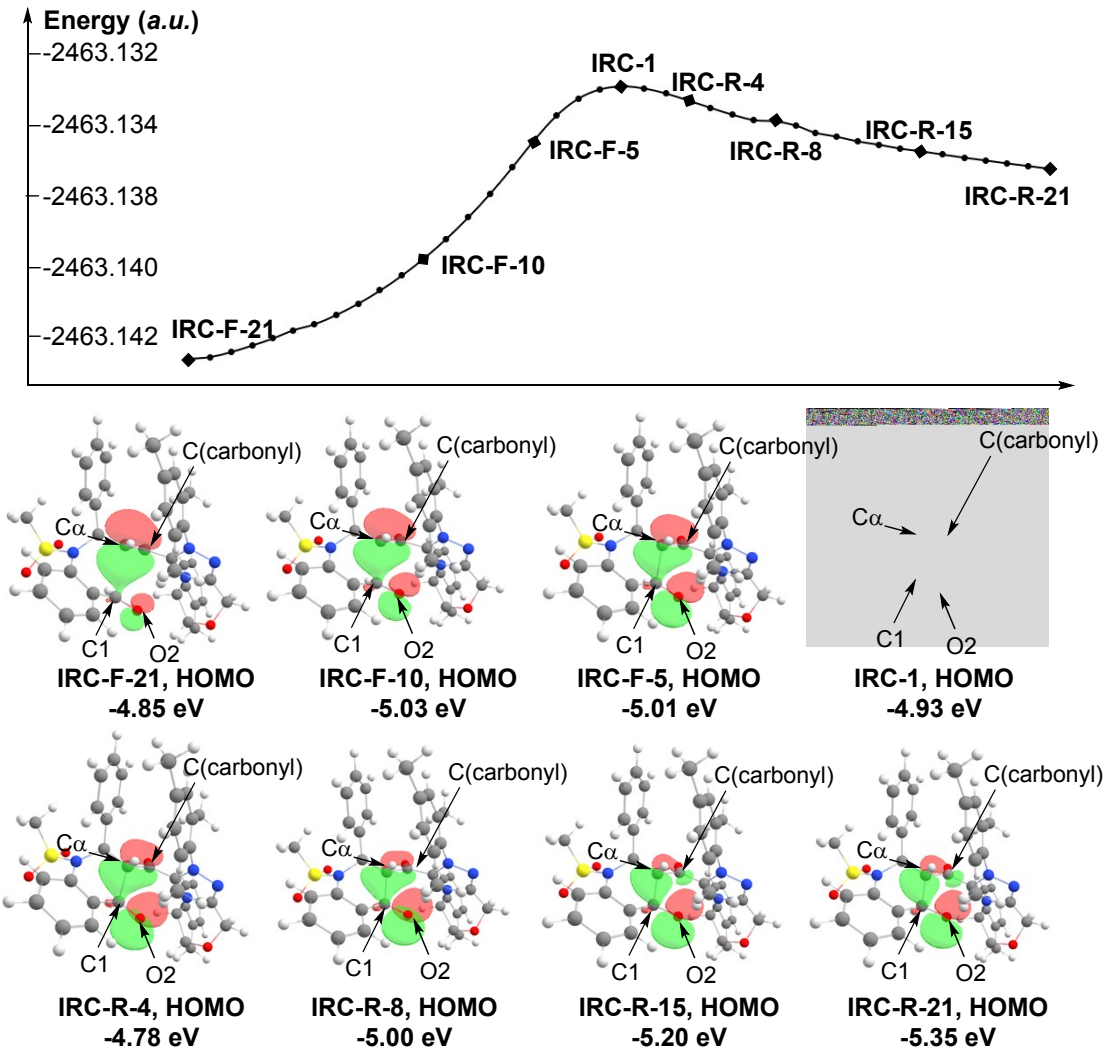


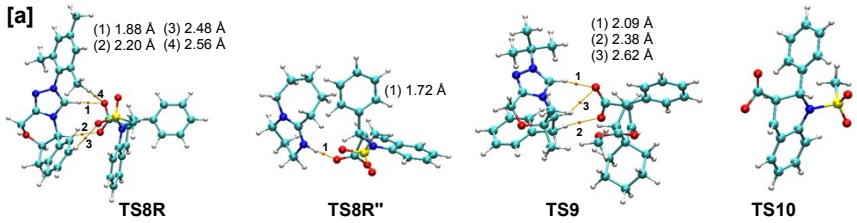
Figure S10. The HOMO changes along several representative IRC points of **TS6R**. ("F" and "R" represent forward and reverse directions, respectively; IRC-1 is the structure of **TS6R**, only the orbitals of the key C(carbonyl), C1, O2, and Cα atoms of **TS6R** are shown for clarity)

2.7 AIM analyses of the transition states **TS8R**, **TS8R''**, **TS9**, and **TS10**

As shown in **Figure S11**, the further intermolecular AIM analyses of the transition states **TS8R/TS8R′′** were performed and compared to explore why the **NHC•H**$^+$ works as NCO would lower the energy barrier of CO_2 releasing. Correspondingly, the values of Laplacian electron density at the bond critical points (BCPs) along the bond paths were summarized in **Figure S11b**. The quantitatively analysis results indicate that there are more and stronger hydrogen bond C-H…O interactions in **TS8R** compared with the

hydrogen bond N-H…O interaction in **TS8R″**. It should be noted that the values of Laplacian electron density of hydrogen bonding C-H…O interaction (1.150, 0.340, 0.276, 0.220) in **TS8R** is more than that of the N-H…O interaction (1.132) in **TS8R″**. Therefore, **NHC•H**$^+$ rather than DABCO•H$^+$ is the better NCO to promote the removal of CO_2. Moreover, we have additionally performed AIM analyses of transition states **TS9** and **TS10** depicted in **Figure 5** to explain why the energy barrier for releasing of CO_2 can also be significantly lowered by the NCO **NHC•H**$^+$.

[a]



[b]

	TS8R		TS8R"		TS9		TS10	
	Type	$\nabla^2\rho$	Type	$\nabla^2\rho$	Type	$\nabla^2\rho$	Type	$\nabla^2\rho$
(1)	C-H...O	1.150	N-H...O	1.169	C-H...O	1.132	——	——
(2)	C-H...O	0.340	——	——	C-H...O	0.291	——	——
(3)	C-H...O	0.276	——	——	C-H...O	0.204	——	——
(4)	C-H...O	0.220	——	——	——	——	——	——

Figure S11. AIM analyses of transition states **TS8R**, **TS8R''**, **TS9**, and **TS10** (distance in Å), summary of the values of Laplacian electron density ($\nabla^2\rho$, eA^{-3}) and electron densities (ρ_{bcp}) at the bond critical points (BCPs) in **TS8R**, **TS8R''**, **TS9**, and **TS10**.

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Part 3: Energies, Cartesian coordinates, and frequencies of all the optimized structures

3.1 Absolute SPE and GFE of the structures optimized by different DFT methods

Table S5. Absolute SPE and GFE of the optimized structures obtained at the /B3LYP-D3/6-31G(d, p)/SMD_{thf} level.

	SPE (a.u.)	GFEC (a.u.)	GFE (a.u.)
NHC+R1+R2	-5035.404344	0.553684	-5034.850660
R1	-2994.118251	0.096197	-2994.022054
R2	-988.069181	0.115291	-987.953890
pre-R2	-988.865242	0.126423	-988.738819
NHC	-1052.420851	0.331064	-1052.089787
CO_2	-188.582334	-0.009290	-188.591624
DBU	-462.156275	0.211535	-461.944740
DBU-H^+	-462.645280	0.227056	-462.418224
NHC-H^+	-1052.911592	0.344734	-1052.566858
Br^-	-2571.839774	-0.016176	-2571.855950
HBr	-2572.310297	-0.013128	-2572.323425
Re-TS1	-4046.546976	0.452533	-4046.094443
Si-TS1	-4046.553275	0.454030	-4046.099245
Re-M1	-4046.555814	0.452023	-4046.103791
Si-M1	-4046.561235	0.455041	-4046.106194
Re-TS2	-4509.22108	0.702844	-4508.518236
Si-TS2	-4429.349662	0.615142	-4428.734520
M2	-4046.565638	0.450057	-4046.115581
TS3	-4046.564868	0.451830	-4046.113038
M3	-4046.580277	0.451770	-4046.128507
TS4	-4429.336759	0.612799	-4428.723960

M4	-1474.734638	0.456073	-1474.278565
M05R	-2463.153695	0.595908	-2462.557787
M05S	-2463.133600	0.593957	-2462.539643
TS5R	-2463.128047	0.593620	-2462.534427
TS5S	-2463.121784	0.595946	-2462.525838
M5R	-2463.135620	0.601113	-2462.534507
M5S	-2463.138348	0.597451	-2462.540897
TS6R	-2463.132086	0.600962	-2462.531124
TS6R	-2463.124295	0.601012	-2462.523283
M6R	-2463.135178	0.603366	-2462.531812
M6S	-2463.129805	0.602456	-2462.527349
TS7R	-2463.100370	0.602337	-2462.498033
TS7S	-2463.098536	0.600368	-2462.498168
M7R	-1410.666807	0.244466	-1410.422341
M07R	-2463.644808	0.616840	-2463.027968
M07R'	-1873.364383	0.495263	-1872.869120
M07R'	-2925.833064	0.855576	-2924.977488
TS8	-2463.615987	0.610754	-2463.005233
TS8'	-2925.775332	0.849213	-2924.926119
TS8''	-1873.337524	0.491390	-1872.846134
TS8'''	-1410.628185	0.243156	-1410.385029
TS8''''	-2463.110990	0.603210	-2462.507780
P	-1222.133294	0.233346	-1221.899948

Table S6. Absolute SPE and GFE of the optimized structures obtained at the M06-2X/6-31G(d, p)/SMD_{thf} level.

	SPE(a.u.)	**GFEC(a.u.)**	**CFE(a.u.)**	***ΔΔG≠***
TS5R	-2462.139173	0.603706	-2461.535467	**0.0**
TS5S	-2462.133825	0.605032	-2461.528793	**4.2**

Table S7. Absolute SPE and GFE of the optimized structures obtained at the ωB97X /6-31G(d, p)/SMD_{thf} level.

	SPE (a.u.)	GFEC (a.u.)	CFE (a.u.)	$\Delta\Delta G^{\neq}$
TS5R	-2462.36915	0.602925	-2461.766225	**0.0**
TS5S	-2462.362003	0.601595	-2461.760408	**3.7**

Table S8. Absolute SPE and GFE of the different conformers of **TS5R/S**.

	SPE(a.u.)	GFEC(a.u.)	GFE(a.u.)
TS5R(Φ=90°)	-2463.129401	0.594206	-2462.535195
TS5R(Φ=177°)	-2463.128047	0.59362	-2462.534427
TS5R(Φ=-54°)	-2463.127018	0.591547	-2462.535471
TS5R(Φ=-128°)	-2463.127501	0.594113	-2462.533388
TS5R(Φ=-175°)	-2463.12812	0.594528	-2462.533592
TS5S(Φ=-61°)	-2463.123551	0.593195	-2462.530356
TS5S(Φ=-100°)	-2463.123462	0.595935	-2462.527527
TS5S(Φ=-160°)	-2463.12455	0.595622	-2462.528928
TS5S(Φ=16°)	-2463.125154	0.595766	-2462.529388
TS5S(Φ=137°)	-2463.121784	0.595946	-2462.525838

3.2 Cartesian coordinates and frequencies of all the stationary points

NHC

Zero-point correction= 0.380193

Thermal correction to Energy= 0.400329

Thermal correction to Enthalpy= 0.401273

Thermal correction to Gibbs Free Energy= 0.331064

Sum of electronic and zero-point Energies= -1052.040657

Sum of electronic and thermal Energies= -1052.020521

Sum of electronic and thermal Enthalpies= -1052.019577

Sum of electronic and thermal Free Energies= -1052.089787

Cartesian coordinates

C	0.129090	0.007291	0.819820
C	-0.529640	-1.677454	-0.542713
C	-2.295127	-0.715115	0.965031
H	-2.226480	-0.976660	2.023372
N	0.735814	-1.531627	-0.817012
N	1.107490	-0.486143	0.032400
N	-0.928074	-0.773299	0.414075
C	-1.487290	-2.660835	-1.139498
H	-0.993971	-3.624732	-1.284783
H	-1.825509	-2.309919	-2.124804
C	-3.228731	-1.697188	0.188042
O	-2.582767	-2.884054	-0.256588
C	-3.891073	0.542015	-0.313260
C	-2.964629	0.621039	0.734649
C	-2.754786	1.815353	1.422008
C	-3.488408	2.944028	1.046817
C	-4.417838	2.869055	0.002076
C	-4.627216	1.667939	-0.682142
C	-3.929002	-0.845295	-0.903232
H	-2.030048	1.865625	2.228240
H	-4.985918	3.752423	-0.276191
H	-5.353694	1.613293	-1.488434
H	-3.379317	-0.873436	-1.851530
H	-4.940852	-1.205930	-1.108682
C	2.469983	-0.039362	-0.005507
C	2.788476	1.094995	-0.763033
C	3.441230	-0.768679	0.699196
C	4.126757	1.505774	-0.792626
C	4.763492	-0.323027	0.637708

C	5.124510	0.812180	-0.100758
H	4.392860	2.384971	-1.373992
H	5.530072	-0.873051	1.178728
C	3.055591	-1.985531	1.500979
H	2.581144	-2.743027	0.868073
H	2.331981	-1.727083	2.282267
H	3.929640	-2.434260	1.979727
C	6.563114	1.266948	-0.139706
H	7.218638	0.474976	-0.520106
H	6.922326	1.524711	0.863549
H	6.690744	2.145888	-0.777774
C	1.719992	1.844207	-1.517683
H	0.975143	2.264048	-0.833303
H	1.181470	1.179211	-2.202238
H	2.151806	2.661537	-2.100614
H	-3.985418	-2.042345	0.896917
H	-3.340053	3.883636	1.571041

Vibrational frequencies

-53.4894	29.5785	36.7652
51.1016	56.4802	72.1424
121.8609	135.5949	138.9375
166.0153	171.8857	197.0721
208.9887	236.1233	241.6190
263.6612	284.8158	298.3112
320.2532	332.2008	350.8423
387.4406	412.7105	454.2852
469.9195	497.5081	513.5028
520.4031	526.7938	530.0568
563.8743	581.1743	599.5598
604.5850	617.2101	628.3103

647.2845	677.3956	694.5868
728.5276	758.8036	767.8657
785.6076	818.9337	841.7270
876.2648	879.7150	885.9478
901.5992	902.3154	954.9231
958.2697	958.9600	973.5115
979.4856	1001.3134	1011.4805
1035.4191	1036.6371	1044.8912
1050.2427	1052.1559	1064.4767
1066.0489	1067.6651	1069.7846
1072.1071	1124.4343	1133.0428
1159.7023	1183.5969	1187.4304
1193.2274	1216.6889	1233.7539
1247.3793	1253.1404	1269.4957
1286.4437	1290.1125	1300.9680
1322.4167	1328.2050	1338.4258
1344.6961	1354.4925	1367.9162
1379.6859	1411.6639	1415.6266
1418.6685	1422.5477	1425.8442
1440.4742	1447.9425	1479.2914
1479.8901	1480.9482	1482.5724
1486.8158	1491.3894	1500.6758
1502.4689	1507.1053	1521.2490
1535.6126	1627.5518	1638.8366
1639.5488	1657.7807	1663.0831
3026.5892	3039.4177	3045.4605
3046.2726	3056.9680	3096.6384
3097.2588	3103.9434	3105.3258
3105.4987	3115.3078	3125.6116
3126.3542	3134.0385	3135.0176

3173.8050	3179.8248	3181.5926
3192.8825	3203.0011	3216.3615

NHC·H$^+$

Zero-point correction= 0.393737

Thermal correction to Energy= 0.413922

Thermal correction to Enthalpy= 0.414866

Thermal correction to Gibbs Free Energy= 0.344734

Sum of electronic and zero-point Energies= -1052.517855

Sum of electronic and thermal Energies= -1052.497671

Sum of electronic and thermal Enthalpies= -1052.496726

Sum of electronic and thermal Free Energies= -1052.566858

Cartesian coordinates

C	0.119125	-0.088215	0.746614
C	-0.553848	-1.721984	-0.525273
C	-2.338823	-0.717930	0.983716
H	-2.257452	-0.993002	2.036607
N	0.717702	-1.572616	-0.802774
N	1.122228	-0.537815	0.004274
N	-0.959579	-0.814460	0.422727
C	-1.525721	-2.695302	-1.115723
H	-1.043203	-3.666948	-1.240763
H	-1.836023	-2.343700	-2.108908
C	-3.269731	-1.680688	0.183477
O	-2.627699	-2.878508	-0.237724
C	-3.861046	0.576911	-0.329086
C	-2.958129	0.634650	0.740990
C	-2.729592	1.820098	1.437943
C	-3.419956	2.968959	1.044454
C	-4.325894	2.917489	-0.021997

C	-4.556553	1.723158	-0.711245
C	-3.929331	-0.810509	-0.917484
H	-2.039439	1.849734	2.276566
H	-4.863269	3.815787	-0.311706
H	-5.268248	1.689648	-1.531031
H	-3.372103	-0.856040	-1.860335
H	-4.948372	-1.142634	-1.131127
C	2.482667	-0.061784	-0.025891
C	2.764117	1.095224	-0.762407
C	3.456310	-0.801285	0.663131
C	4.094389	1.527888	-0.779036
C	4.766416	-0.324245	0.611711
C	5.102943	0.836078	-0.100174
H	4.345458	2.421545	-1.343403
H	5.544468	-0.872811	1.136129
C	3.099160	-2.059028	1.412405
H	2.724903	-2.830255	0.730404
H	2.312686	-1.876368	2.153370
H	3.970840	-2.459332	1.934293
C	6.531495	1.317212	-0.128166
H	7.200516	0.537380	-0.508800
H	6.877361	1.571992	0.880258
H	6.646741	2.202442	-0.758919
C	1.685333	1.835753	-1.510887
H	0.968479	2.304502	-0.826909
H	1.118845	1.160591	-2.161574
H	2.118433	2.623351	-2.130836
H	-4.041974	-2.010876	0.881290
H	-3.261714	3.903149	1.574522
H	0.162211	0.719446	1.460643

Vibrational frequencies

-54.6958	31.1020	37.1524
49.7373	61.0386	70.2219
124.7157	142.6444	144.7866
169.5255	173.8496	199.1729
210.8628	235.0694	241.5529
263.4421	286.3736	295.9185
319.1765	329.2969	342.8344
384.2023	411.7496	450.2562
469.8110	492.4314	513.1471
517.6573	527.4099	528.6083
559.4478	581.2865	594.1567
602.0204	612.1389	626.7170
645.1611	677.9952	701.2827
725.2868	746.2520	769.6501
785.0295	817.8354	837.3277
862.8469	878.7950	880.6678
884.0870	905.1008	911.6746
959.1709	963.9900	969.9857
974.9510	997.9024	1010.7032
1011.5594	1037.8687	1042.9746
1046.5625	1053.7741	1058.7623
1065.2123	1067.9962	1068.4835
1071.8935	1074.2744	1129.1021
1133.8581	1168.0915	1176.4454
1190.9147	1194.4928	1212.5231
1228.1795	1234.2682	1253.9783
1267.7449	1274.3187	1290.7653
1295.0979	1324.2082	1332.3172
1343.2876	1349.6182	1352.2482

1368.6494	1376.3441	1411.4942
1418.1317	1421.6016	1423.0973
1426.5772	1447.3921	1455.6797
1476.7454	1477.1039	1482.3633
1484.6188	1485.4468	1490.4386
1493.1004	1503.3456	1506.7705
1522.4414	1524.4612	1568.2711
1622.3050	1639.3590	1642.7142
1653.3975	1663.9068	3044.4522
3045.0674	3048.2810	3048.8698
3061.3544	3102.8031	3104.1301
3106.5898	3114.5152	3124.6046
3132.3218	3134.3623	3139.9606
3143.9913	3145.8911	3185.4593
3190.0393	3191.1979	3198.1167
3205.4036	3215.9695	3305.6027

DBU

Zero-point correction= 0.246467

Thermal correction to Energy= 0.256135

Thermal correction to Enthalpy= 0.257079

Thermal correction to Gibbs Free Energy= 0.211535

Sum of electronic and zero-point Energies= -461.909808

Sum of electronic and thermal Energies= -461.900140

Sum of electronic and thermal Enthalpies= -461.899196

Sum of electronic and thermal Free Energies= -461.944740

Cartesian coordinates

C	-1.953710	-1.267641	0.573448
C	-2.791087	0.001903	0.368371
C	-1.993239	1.310728	0.327441

C	-0.900813	-1.533381	-0.525067
C	-0.903589	1.332729	-0.755309
C	0.395285	-0.762803	-0.353538
H	-1.454117	-1.236715	1.550516
H	-3.344419	-0.096503	-0.576755
H	-1.520488	1.502878	1.299616
H	-1.306005	0.945269	-1.699562
H	-1.342446	-1.329107	-1.509692
H	-2.635274	-2.126145	0.603748
H	-3.546022	0.065447	1.162053
H	-2.685867	2.141155	0.140601
H	-0.614992	-2.587170	-0.516970
H	-0.604324	2.365236	-0.954383
C	1.485892	1.431728	-0.054246
H	1.144675	2.298096	0.524022
H	1.948204	1.817849	-0.974752
C	2.497561	0.622677	0.749088
H	3.432419	1.184790	0.844620
H	2.107290	0.449395	1.759267
C	2.716192	-0.725243	0.058655
H	3.395805	-1.351630	0.649374
H	3.213386	-0.562324	-0.911325
N	1.467708	-1.459464	-0.141127
N	0.317609	0.610223	-0.390792

Vibrational frequencies

65.9646	79.6461	161.9266
238.1719	249.5353	313.1440
352.2702	367.7084	397.5303
430.3198	486.1334	513.6320
519.8321	646.4028	693.1913

697.8761	803.6114	847.8307
861.3841	872.7441	900.5101
903.4752	932.0409	969.6440
996.3212	1009.3560	1019.0809
1076.2454	1105.1384	1108.6374
1122.5126	1135.4995	1177.7156
1209.0328	1226.9673	1234.4139
1257.3539	1263.4821	1290.5990
1309.4440	1318.8170	1347.1903
1358.7536	1374.1162	1377.1555
1390.3869	1399.2661	1404.0719
1404.6346	1463.2666	1479.4699
1483.0671	1489.3983	1491.6753
1497.8254	1503.3493	1512.6327
1530.1852	1672.4266	2985.0562
3002.2618	3016.7142	3028.7051
3032.0000	3034.7416	3041.0979
3042.4883	3053.2456	3064.9935
3065.7838	3072.8141	3077.8062
3099.6327	3103.0403	3122.2546

DBUH+

Zero-point correction= 0.261597

Thermal correction to Energy= 0.271293

Thermal correction to Enthalpy= 0.272238

Thermal correction to Gibbs Free Energy= 0.227056

Sum of electronic and zero-point Energies= -462.383683

Sum of electronic and thermal Energies= -462.373987

Sum of electronic and thermal Enthalpies= -462.373043

Sum of electronic and thermal Free Energies= -462.418225

Cartesian coordinates

C	1.975113	1.282225	0.557298
C	2.817072	0.014249	0.370910
C	2.024161	-1.297977	0.364057
C	0.917905	1.513018	-0.546519
C	0.951787	-1.369858	-0.728396
C	-0.330535	0.692218	-0.361207
H	1.480616	1.273167	1.536197
H	3.366417	0.096083	-0.576812
H	1.546160	-1.468081	1.336963
H	1.337470	-0.997875	-1.683070
H	1.346332	1.287873	-1.529952
H	2.641716	2.150667	0.552345
H	3.571100	-0.028086	1.164966
H	2.718386	-2.130057	0.201880
H	0.623981	2.565192	-0.568441
H	0.645802	-2.403840	-0.891995
C	-1.485456	-1.451435	-0.098477
H	-1.149712	-2.339958	0.440800
H	-1.917911	-1.775927	-1.051670
C	-2.498332	-0.675850	0.734927
H	-3.427795	-1.246165	0.798354
H	-2.113343	-0.539245	1.750657
C	-2.758432	0.685207	0.100876
H	-3.346831	1.330159	0.756114
H	-3.292535	0.582230	-0.850354
N	-1.468707	1.339826	-0.135529
N	-0.286278	-0.633535	-0.386849
H	-1.424661	2.349042	-0.090149

Vibrational frequencies

83.2170	106.6467	180.8697
217.9903	275.6556	314.0440
344.4487	373.4182	411.9274
437.9428	480.7772	517.5424
532.6530	538.1032	646.5901
701.4706	710.4854	805.2040
843.0100	865.9826	876.2857
906.3438	912.8577	929.2961
982.2451	1002.4330	1012.4742
1024.0933	1090.7034	1102.7261
1115.8412	1125.3279	1135.5424
1180.9592	1214.2669	1233.8804
1248.5990	1251.9688	1271.2015
1297.6397	1310.3466	1321.5799
1352.5917	1357.2421	1372.8390
1388.0624	1393.4657	1402.1560
1404.3138	1419.0784	1428.0890
1478.8468	1481.3682	1491.5519
1494.7427	1500.8578	1502.7886
1510.5933	1536.7246	1620.9778
1684.8759	3033.7695	3045.1298
3050.2680	3061.7025	3065.0671
3069.3672	3077.1228	3078.3937
3086.5146	3094.9295	3100.4616
3124.6533	3128.2492	3135.5843
3141.4921	3145.3489	3633.9744

R1

Zero-point correction= 0.134121

Thermal correction to Energy= 0.143886

Thermal correction to Enthalpy= 0.144831

Thermal correction to Gibbs Free Energy= 0.096197

Sum of electronic and zero-point Energies= -2993.984130

Sum of electronic and thermal Energies= -2993.974365

Sum of electronic and thermal Enthalpies= -2993.973421

Sum of electronic and thermal Free Energies= -2994.022054

Cartesian coordinates

C	-0.059273	1.165341	0.000027
C	1.218933	0.717010	0.000027
H	-0.109253	2.254872	0.000050
C	2.322941	1.695210	0.000023
O	3.510818	1.432074	0.000034
C	-1.375220	0.539952	0.000012
C	-2.484493	1.416173	0.000011
C	-1.627345	-0.848914	0.000003
C	-3.787679	0.930874	0.000000
H	-2.312205	2.489094	0.000020
C	-2.933586	-1.329668	-0.000007
H	-0.804870	-1.550963	0.000007
C	-4.017411	-0.447345	-0.000010
H	-4.622345	1.625446	0.000000
H	-3.106375	-2.401822	-0.000013
H	-5.033204	-0.831638	-0.000018
H	1.963723	2.745382	-0.000587
Br	1.782765	-1.109107	-0.000007

Vibrational frequencies

19.0451	63.9836	119.8025
173.2176	190.9065	240.6045
326.2772	339.8547	411.4528
450.2425	533.7661	542.4675

622.0178	630.7401	701.6842
703.1108	780.8852	856.6102
862.9029	922.1130	959.5715
992.4922	1012.9188	1018.9596
1021.1633	1058.5355	1108.4574
1133.2817	1193.6099	1223.9991
1246.2268	1326.1583	1373.4323
1389.3072	1453.3103	1489.7106
1538.2080	1621.9672	1647.1920
1660.4811	1779.0827	2938.6905
3148.5914	3186.6694	3192.9476
3202.6617	3213.0955	3249.7332

R2

Zero-point correction= 0.153857

Thermal correction to Energy= 0.165529

Thermal correction to Enthalpy= 0.166473

Thermal correction to Gibbs Free Energy= 0.115291

Sum of electronic and zero-point Energies= -987.915323

Sum of electronic and thermal Energies= -987.903652

Sum of electronic and thermal Enthalpies= -987.902708

Sum of electronic and thermal Free Energies= -987.953890

Cartesian coordinates

C	-0.578060	-0.575977	-0.478748
C	-1.303506	0.599398	-0.167282
C	-2.642491	0.529004	0.236065
C	-3.300188	-0.688179	0.316404
C	-2.604918	-1.855730	-0.019473
C	-1.274052	-1.799698	-0.406686
H	-3.152903	1.460892	0.464648

H	-4.339841	-0.736002	0.624693
H	-3.107758	-2.817987	0.031449
H	-0.727560	-2.705177	-0.652889
C	-0.695644	1.933443	-0.362253
H	0.230668	1.941867	-0.958958
O	-1.196530	2.969038	0.036180
N	0.751908	-0.557983	-0.902192
S	1.838453	-0.230725	0.207453
O	1.585535	1.025237	0.957293
O	2.170083	-1.376216	1.085814
C	3.275837	0.053895	-0.808894
H	3.097140	0.919228	-1.448003
H	4.116955	0.245428	-0.140138
H	3.470116	-0.832164	-1.413788

Vibrational frequencies

38.6470	68.6151	90.9165
124.8040	193.1735	239.9769
247.7084	266.4765	284.7884
318.2656	343.6358	450.8388
454.8404	491.1383	505.3738
541.3278	564.3364	614.7321
642.7619	744.5023	769.1788
803.9328	813.7195	848.0463
904.3097	981.1039	985.7132
989.7717	1006.0518	1013.5470
1029.0178	1068.7116	1118.9923
1139.4333	1165.3391	1212.6344
1239.9242	1281.5524	1304.1289
1350.9608	1369.4254	1420.4372
1461.2731	1463.3570	1502.3742

1516.6786	1642.9561	1685.1628
1822.9736	3058.6777	3091.9110
3195.2413	3198.4701	3203.6603
3205.5952	3218.6788	3225.7717

HBr

Zero-point correction= 0.006086

Thermal correction to Energy= 0.008446

Thermal correction to Enthalpy= 0.009390

Thermal correction to Gibbs Free Energy= -0.013128

Sum of electronic and zero-point Energies= -2572.304212

Sum of electronic and thermal Energies= -2572.301851

Sum of electronic and thermal Enthalpies= -2572.300907

Sum of electronic and thermal Free Energies= -2572.323426

Cartesian coordinates

Br	0.000000	0.000000	0.039324
H	0.000000	0.000000	-1.376324

Vibrational frequencies

2671.3493

Br-

Zero-point correction= 0.000000

Thermal correction to Energy= 0.001416

Thermal correction to Enthalpy= 0.002360

Thermal correction to Gibbs Free Energy= -0.016176

Sum of electronic and zero-point Energies= -2571.839774

Sum of electronic and thermal Energies= -2571.838357

Sum of electronic and thermal Enthalpies= -2571.837413

Sum of electronic and thermal Free Energies= -2571.855949

Cartesian coordinates

Br 0.000000 0.000000 0.000000

Vibrational frequencies

co2

Zero-point correction= 0.011439

Thermal correction to Energy= 0.014107

Thermal correction to Enthalpy= 0.015051

Thermal correction to Gibbs Free Energy= -0.009290

Sum of electronic and zero-point Energies= -188.570894

Sum of electronic and thermal Energies= -188.568227

Sum of electronic and thermal Enthalpies= -188.567282

Sum of electronic and thermal Free Energies= -188.591624

Cartesian coordinates

C 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.170172

O 0.000000 0.000000 -1.170172

Vibrational frequencies

619.9790 619.9790 1367.2044

2414.1819

pre-R2

Zero-point correction= 0.165257

Thermal correction to Energy= 0.177312

Thermal correction to Enthalpy= 0.178256

Thermal correction to Gibbs Free Energy= 0.126423

Sum of electronic and zero-point Energies= -988.699986

Sum of electronic and thermal Energies= -988.687930

Sum of electronic and thermal Enthalpies= -988.686986

Sum of electronic and thermal Free Energies= -988.738820

Cartesian coordinates

C	0.648439	-0.562482	0.498332
C	1.339478	0.625585	0.184919
C	2.671501	0.546869	-0.248325
C	3.322183	-0.678060	-0.338661
C	2.636432	-1.850109	-0.001200
C	1.303407	-1.795089	0.401892
H	3.182217	1.472860	-0.492720
H	4.356024	-0.724996	-0.666073
H	3.135422	-2.812233	-0.067381
H	0.760863	-2.706462	0.636282
C	0.714406	1.958416	0.347126
H	-0.241548	1.972140	0.901109
O	1.217293	2.996341	-0.052213
N	-0.713057	-0.510356	0.933024
S	-1.927844	-0.264648	-0.264514
O	-1.362651	0.643696	-1.269252
O	-2.479893	-1.563403	-0.679399
C	-3.163632	0.597301	0.703947
H	-2.740414	1.540758	1.050310
H	-4.019492	0.772293	0.048218
H	-3.454777	-0.033120	1.546394
H	-0.972679	-1.342030	1.463650

Vibrational frequencies

38.3400	64.8546	94.9883
126.6387	202.5581	230.7055
240.8279	256.4502	280.9674
305.4657	340.5777	379.7875
451.8856	467.4593	476.2868
509.3039	527.3578	588.6387
639.4246	645.2274	731.3703

758.5740	784.9177	828.3171
867.0975	881.2688	896.3471
977.1757	990.6047	995.9448
1008.3532	1043.7524	1070.3296
1115.3316	1127.3055	1190.9935
1222.0100	1241.1688	1279.1319
1309.5631	1351.1802	1365.3117
1417.2345	1445.0897	1451.8147
1452.0926	1494.9037	1529.5669
1634.1294	1651.1716	1777.0253
2989.5768	3077.3920	3180.8744
3191.9019	3197.0277	3201.0138
3210.6294	3219.3246	3514.7072

TS0

Zero-point correction= 0.412925

Thermal correction to Energy= 0.435721

Thermal correction to Enthalpy= 0.436665

Thermal correction to Gibbs Free Energy= 0.359730

Sum of electronic and zero-point Energies= -1450.080540

Sum of electronic and thermal Energies= -1450.057745

Sum of electronic and thermal Enthalpies= -1450.056800

Sum of electronic and thermal Free Energies= -1450.133735

Cartesian coordinates

C	-1.929996	-0.677988	-0.029121
C	-3.267672	-0.976260	-0.353484
C	-3.773301	-2.260766	-0.130323
C	-2.963691	-3.263885	0.382968
C	-1.628866	-2.979002	0.680068
C	-1.121268	-1.700114	0.485061
H	-4.811156	-2.452418	-0.387000

H	-3.361227	-4.260396	0.545560
H	-0.982785	-3.756026	1.078151
H	-0.089742	-1.469026	0.734907
C	-4.139182	0.028030	-1.010657
H	-3.624900	0.923629	-1.396569
O	-5.331620	-0.131962	-1.175506
N	-1.381701	0.606297	-0.256023
S	-1.793974	1.766750	0.806518
O	-3.251947	1.826572	0.986365
O	-1.000679	1.704786	2.047378
C	-1.259615	3.208571	-0.084533
H	-1.836060	3.289933	-1.006155
H	-1.434555	4.073333	0.557725
H	-0.193955	3.110453	-0.302960
C	2.511483	-0.797923	1.925372
C	4.013129	-0.920921	2.183542
C	4.874411	-0.948973	0.922153
C	2.090220	0.500441	1.211874
C	4.696593	0.290796	0.045324
C	2.260998	0.434995	-0.283119
H	2.163268	-1.662266	1.345107
H	4.330860	-0.073311	2.805552
H	4.649349	-1.839547	0.321503
H	4.686387	1.195142	0.663056
H	2.668544	1.345230	1.606398
H	1.984908	-0.833244	2.884157
H	4.202112	-1.827674	2.768033
H	5.928735	-1.014140	1.211584
H	1.038121	0.717904	1.412752
H	5.535821	0.390693	-0.646198

C	3.695544	-0.009839	-2.219743
H	4.486681	-0.760364	-2.307187
H	4.046885	0.908100	-2.706672
C	2.414761	-0.511177	-2.865664
H	2.540097	-0.543100	-3.950045
H	2.196412	-1.525699	-2.516183
C	1.269650	0.411378	-2.476344
H	0.308958	0.034348	-2.836969
H	1.418888	1.407715	-2.911380
N	1.188115	0.513975	-1.025212
N	3.490581	0.252267	-0.789867
H	-0.012262	0.585609	-0.539873

Vibrational frequencies

-1320.3209	27.4568	34.9060
37.4894	58.9058	65.8095
79.5717	86.3811	91.2071
98.1221	102.5604	126.7801
141.2979	184.7365	227.0667
246.5274	251.9502	261.9593
269.2198	278.7458	287.6692
316.2925	317.9463	354.9196
358.4492	379.1760	414.9473
436.6324	452.2986	456.5099
490.6923	499.4890	501.4372
521.3038	525.4010	545.2535
577.2270	639.1655	646.9785
655.0123	714.9266	731.8883
742.6884	781.3008	812.4296
821.1091	832.3999	848.6458
856.8327	868.2237	888.4456

900.6078	907.5360	923.1493
940.6034	959.2457	989.4763
993.5596	997.6598	1004.6980
1007.9316	1021.7304	1024.7058
1039.2646	1039.3029	1080.1218
1108.2310	1119.6648	1122.3976
1127.9034	1137.5334	1147.2974
1149.5603	1169.3910	1190.4101
1221.5384	1227.5217	1244.9200
1251.8283	1264.3774	1274.2078
1276.8113	1290.3284	1297.0279
1300.5553	1319.3481	1328.0325
1347.0171	1355.6774	1369.7280
1374.7296	1382.0053	1386.6366
1395.4727	1407.6451	1413.5217
1420.6176	1424.6733	1449.0214
1461.5063	1466.6235	1475.6466
1480.8127	1482.3720	1487.8153
1492.6488	1498.0085	1504.5109
1511.5070	1521.1263	1535.0646
1553.7556	1634.8967	1656.7966
1691.6220	1725.5281	1836.2259
3058.7929	3064.9580	3067.1658
3070.5151	3073.6558	3078.9661
3088.2298	3090.1437	3091.2491
3092.8494	3111.2510	3119.0287
3122.3271	3128.3681	3141.6163
3148.4485	3150.1068	3156.3029
3198.0524	3205.1280	3211.7907
3221.2777	3233.0551	3241.8788

Re-TS1

Zero-point correction= 0.516268

Thermal correction to Energy= 0.547282

Thermal correction to Enthalpy= 0.548226

Thermal correction to Gibbs Free Energy= 0.452533

Sum of electronic and zero-point Energies= -4046.030708

Sum of electronic and thermal Energies= -4045.999694

Sum of electronic and thermal Enthalpies= -4045.998750

Sum of electronic and thermal Free Energies= -4046.094443

Cartesian coordinates

C	5.453047	0.782764	-0.267545
C	4.146050	0.497024	-0.668713
C	3.878652	-0.388346	-1.713788
C	4.960608	-0.997785	-2.354658
C	6.275122	-0.720657	-1.956640
C	6.530093	0.173293	-0.913384
C	5.477510	1.777682	0.864464
C	4.000106	1.930793	1.313451
C	3.138366	1.260423	0.167489
H	2.853161	-0.592187	-2.019995
H	4.780259	-1.692827	-3.169873
H	7.104659	-1.205491	-2.463904
H	7.550441	0.386294	-0.606230
H	6.095733	1.457264	1.709435
H	3.720233	2.979936	1.416707
H	5.871929	2.744249	0.529833
H	2.625357	2.026651	-0.417017
N	2.105835	0.389154	0.735950
O	3.762730	1.382228	2.613979

C	0.866351	0.097808	0.260528
C	2.328727	-0.320851	1.892751
N	0.407022	-0.789405	1.154545
N	1.298798	-1.059637	2.192270
C	3.585709	-0.036118	2.644824
H	4.440856	-0.565956	2.203382
H	3.489637	-0.337228	3.689133
C	-0.872366	-1.442901	1.162674
C	-0.996962	-2.678749	0.518677
C	-1.940069	-0.813785	1.817464
C	-2.249618	-3.299062	0.550785
C	-3.175670	-1.464695	1.807662
C	-3.348340	-2.703723	1.177304
H	-2.373405	-4.255551	0.049378
H	-4.022249	-0.992830	2.299955
C	-1.703376	1.808322	-0.950728
C	-1.229846	0.641049	-1.416647
H	-0.917978	2.548885	-0.784711
C	-3.045502	2.281542	-0.594055
C	-3.252284	3.674425	-0.524500
C	-4.118408	1.435759	-0.247697
C	-4.486457	4.204248	-0.155385
H	-2.431062	4.343478	-0.768611
C	-5.348448	1.969070	0.132979
H	-3.980886	0.363386	-0.259510
C	-5.543306	3.352056	0.174974
H	-4.621680	5.281499	-0.119014
H	-6.158369	1.297526	0.404390
H	-6.505338	3.761141	0.469903
Br	-2.321126	-0.832889	-1.947150

C	0.263362	0.404880	-1.635492
H	0.774861	1.388032	-1.682628
O	0.679116	-0.557081	-2.321837
C	0.153957	-3.258903	-0.258283
H	0.351893	-2.625833	-1.132542
H	1.070801	-3.297738	0.339768
H	-0.075629	-4.270695	-0.602211
C	-1.755633	0.520226	2.491439
H	-0.960616	0.478211	3.244351
H	-1.472563	1.288855	1.764966
H	-2.677532	0.843500	2.980279
C	-4.708153	-3.356121	1.142753
H	-4.637215	-4.428381	0.938272
H	-5.242191	-3.221680	2.089136
H	-5.329382	-2.911384	0.354913

Vibrational frequencies

-212.5375	17.8273	24.9505
27.8069	37.2764	47.6823
56.5251	60.3382	69.0769
80.2724	82.9186	101.6326
107.4164	118.7651	124.7613
127.8618	140.5563	164.8790
180.7781	195.4547	202.1046
210.3376	216.1866	220.1536
232.6220	249.7182	264.5861
282.9685	290.6364	301.2342
324.8598	334.7843	356.3494
381.3658	399.3493	417.6377
427.4465	447.9566	452.4329
483.1992	487.2175	499.1749

507.5979	515.8714	526.8265
532.4981	535.4091	573.6619
581.9670	589.7443	598.4134
606.6112	614.9566	615.4757
624.7559	634.5333	696.3954
704.4871	708.4193	716.9854
722.7551	741.5544	752.8399
768.4748	774.0741	794.8940
821.6241	842.7614	844.3851
862.1332	869.9508	873.1553
879.0682	898.2659	899.9910
910.7339	942.8697	950.7129
963.2361	966.5956	978.1146
984.7813	986.2246	991.7847
1005.6283	1013.8838	1026.5910
1032.7492	1035.7637	1042.5111
1044.8609	1048.0869	1054.6842
1058.0860	1058.5427	1064.8511
1067.9941	1074.3650	1075.9527
1097.0055	1117.6978	1119.3817
1133.4572	1182.8983	1188.2711
1188.6831	1198.1843	1200.8370
1219.7606	1225.4402	1231.1229
1237.7823	1249.9269	1267.5425
1272.9252	1291.8348	1296.5524
1308.8036	1309.7673	1322.2869
1333.3684	1343.1018	1347.9947
1358.4418	1369.3062	1370.6838
1376.6805	1383.6703	1400.2254
1408.8880	1421.4888	1423.3078

1428.0430	1441.9171	1450.4082
1453.5751	1468.8122	1479.6689
1485.5344	1488.8344	1492.1735
1493.5265	1497.4053	1498.0808
1498.7702	1512.0300	1531.2147
1535.7653	1536.4833	1570.3653
1624.6143	1640.7184	1642.8403
1644.5419	1654.7024	1657.6557
1659.4606	1684.1061	2882.3939
3031.1338	3036.8988	3038.8764
3048.1180	3054.4685	3096.3465
3098.1071	3100.0985	3108.5585
3113.7167	3114.3380	3126.3113
3127.5321	3130.4366	3138.3386
3144.9324	3147.0046	3177.7347
3178.2006	3180.3013	3181.6147
3185.2059	3191.3612	3194.6519
3204.3727	3207.0053	3249.6416

Si-TS1

Zero-point correction= 0.516913

Thermal correction to Energy= 0.547778

Thermal correction to Enthalpy= 0.548723

Thermal correction to Gibbs Free Energy= 0.454030

Sum of electronic and zero-point Energies= -4046.036362

Sum of electronic and thermal Energies= -4046.005497

Sum of electronic and thermal Enthalpies= -4046.004553

Sum of electronic and thermal Free Energies= -4046.099245

Cartesian coordinates

C	-5.289624	-0.080577	-0.114001

C	-4.030377	-0.019547	-0.715911
C	-3.828924	0.687053	-1.902361
C	-4.912052	1.359842	-2.471529
C	-6.174738	1.314134	-1.865589
C	-6.372775	0.587254	-0.689364
C	-5.274347	-0.927915	1.130510
C	-3.819317	-1.464335	1.241726
C	-2.997334	-0.800315	0.065467
H	-2.852691	0.667204	-2.376934
H	-4.777939	1.914256	-3.396151
H	-7.009783	1.839880	-2.320513
H	-7.356077	0.541980	-0.228810
H	-5.547100	-0.354566	2.023658
H	-3.801034	-2.544287	1.090571
H	-5.986627	-1.757319	1.068822
H	-2.494958	-1.542240	-0.555428
N	-1.921427	0.059769	0.598673
O	-3.249120	-1.288472	2.539388
C	-0.812980	0.491766	-0.053504
C	-1.880301	0.511457	1.896715
N	-0.161525	1.193242	0.883514
N	-0.805722	1.216941	2.116475
C	-2.937124	0.067958	2.850529
H	-3.819581	0.719871	2.787631
H	-2.561490	0.096916	3.874762
C	1.125318	1.810148	0.737669
C	1.243344	2.960058	-0.055029
C	2.225698	1.208552	1.370195
C	2.523262	3.500856	-0.224135
C	3.479299	1.792260	1.176051

C	3.649293	2.930430	0.378777
H	2.639835	4.388324	-0.841045
H	4.348707	1.330415	1.635884
C	2.233575	-0.663548	-1.401697
C	0.959535	-1.045529	-1.220287
H	2.301417	0.251296	-1.991577
C	3.542648	-1.161088	-0.968395
C	4.660319	-0.361776	-1.291074
C	3.771203	-2.346843	-0.242516
C	5.946721	-0.719830	-0.897552
H	4.507759	0.558182	-1.848418
C	5.060311	-2.703161	0.150394
H	2.942147	-2.990082	0.016203
C	6.153408	-1.894526	-0.170054
H	6.786714	-0.082102	-1.157992
H	5.210032	-3.621963	0.710393
H	7.154744	-2.178321	0.140588
Br	0.377582	-2.574525	-0.213264
C	-0.207251	-0.276377	-1.819016
H	0.163352	0.688254	-2.222022
O	-1.157366	-0.879343	-2.365970
C	2.070592	-0.040569	2.199226
H	3.047034	-0.464135	2.444805
H	1.539553	0.167565	3.134189
H	1.494659	-0.803585	1.668621
C	0.040288	3.590002	-0.711463
H	-0.776858	3.728017	0.004326
H	0.296027	4.566159	-1.130725
H	-0.347575	2.965778	-1.524044
C	5.020816	3.529251	0.189241

H	5.791422	2.752200	0.165499
H	5.083792	4.105275	-0.738773
H	5.270841	4.207745	1.014593

Vibrational frequencies

-209.7391	23.7710	28.0781
31.7902	38.7615	44.6684
49.0890	60.9233	69.5857
83.3220	89.8804	92.9399
125.3101	128.4309	134.4929
137.2096	164.0801	171.9785
184.9008	190.8317	196.6503
213.6915	220.1734	231.4879
239.1069	246.8409	266.1519
286.8422	290.9780	300.3706
328.2076	333.5831	347.2004
367.8564	396.7209	408.6736
423.3096	441.2328	446.0816
484.8167	499.1316	503.9300
517.3022	524.3172	530.7530
535.3165	539.7041	556.8427
579.3893	580.8362	601.6139
606.1960	612.9198	619.5066
630.9977	633.9677	674.3837
688.7131	705.8438	713.8187
722.6490	734.7797	751.3378
765.5981	780.7846	791.8046
822.7403	842.5186	856.8027
860.7516	870.0438	876.5649
883.3558	902.3276	903.0282
909.4252	954.8052	956.3446

959.8593	969.4630	976.4591
984.5570	994.5585	996.8626
1003.1521	1013.6035	1017.9320
1040.2798	1042.2841	1045.5304
1047.8382	1049.2103	1054.0312
1057.4361	1059.3723	1066.8405
1070.5851	1071.4997	1074.3613
1097.1120	1113.0389	1122.4898
1122.5763	1179.3116	1186.7971
1190.2914	1196.2365	1200.0034
1221.9905	1224.8733	1232.8850
1234.7950	1242.5736	1269.6281
1275.9371	1291.3947	1297.7184
1309.7474	1319.4626	1325.8945
1329.3122	1343.6936	1345.0243
1362.7398	1369.5377	1371.3972
1376.5107	1394.0829	1400.4504
1406.1759	1422.6065	1426.2927
1434.2470	1439.9943	1450.1725
1460.0876	1477.6976	1480.7961
1484.3931	1487.2479	1491.0602
1491.9897	1495.5960	1499.2370
1499.9312	1513.1285	1524.6438
1535.2293	1538.1175	1576.6455
1625.8626	1635.3681	1640.9072
1641.8342	1654.5752	1656.7349
1659.5463	1686.6642	2894.1855
3030.5850	3038.3492	3047.9648
3055.7274	3058.7669	3091.1429
3100.1449	3108.2022	3121.3766

3121.7823	3127.3735	3131.9007
3133.7796	3134.3925	3142.3760
3144.0197	3178.2683	3179.5805
3182.6046	3185.2080	3189.4475
3190.6062	3198.8552	3199.8184
3206.9880	3209.8756	3254.2871

Re-M1

Zero-point correction= 0.517230

Thermal correction to Energy= 0.548587

Thermal correction to Enthalpy= 0.549531

Thermal correction to Gibbs Free Energy= 0.452023

Sum of electronic and zero-point Energies= -4046.038584

Sum of electronic and thermal Energies= -4046.007227

Sum of electronic and thermal Enthalpies= -4046.006283

Sum of electronic and thermal Free Energies= -4046.103791

Cartesian coordinates

C	5.481050	0.742404	-0.273107
C	4.193164	0.390675	-0.683595
C	3.964390	-0.628774	-1.608112
C	5.073620	-1.309189	-2.117512
C	6.370976	-0.967224	-1.712360
C	6.584163	0.062417	-0.791491
C	5.453384	1.887026	0.707556
C	3.961952	2.061663	1.093581
C	3.153361	1.258638	-0.003249
H	2.939746	-0.861708	-1.905712
H	4.929593	-2.110914	-2.836484
H	7.221479	-1.507841	-2.118714
H	7.591626	0.324884	-0.480170

H	6.055028	1.709610	1.604793
H	3.661649	3.110118	1.080305
H	5.831551	2.806645	0.245607
H	2.674994	1.948636	-0.700806
N	2.087753	0.466616	0.626024
O	3.690297	1.642252	2.435446
C	0.860182	0.117817	0.168388
C	2.266145	-0.117567	1.855659
N	0.346401	-0.654199	1.138830
N	1.216938	-0.804055	2.208701
C	3.507209	0.235521	2.605174
H	4.367416	-0.340863	2.239309
H	3.381577	0.040386	3.671095
C	-0.938051	-1.300380	1.204242
C	-1.079669	-2.563867	0.617729
C	-1.976652	-0.645963	1.880952
C	-2.336567	-3.169505	0.704377
C	-3.214148	-1.291385	1.932599
C	-3.411615	-2.549764	1.349274
H	-2.480189	-4.142186	0.241065
H	-4.041794	-0.797532	2.434819
C	-1.711124	1.704355	-0.844017
C	-1.158710	0.566761	-1.293986
H	-0.971526	2.452825	-0.549623
C	-3.101392	2.135224	-0.645916
C	-3.366421	3.518311	-0.598113
C	-4.173002	1.247995	-0.424588
C	-4.654492	3.999367	-0.372795
H	-2.548400	4.219180	-0.745064
C	-5.458710	1.731952	-0.188830

H	-3.991601	0.181949	-0.421873
C	-5.709610	3.106334	-0.168351
H	-4.834049	5.070634	-0.350991
H	-6.268268	1.028692	-0.013312
H	-6.714347	3.477471	0.012579
Br	-2.149363	-0.870619	-2.064664
C	0.384398	0.326911	-1.292070
H	0.790655	1.338990	-1.553949
O	0.856808	-0.688981	-1.998569
C	-1.763534	0.700924	2.518106
H	-2.691191	1.077483	2.954819
H	-1.004880	0.648005	3.307113
H	-1.414765	1.433720	1.783474
C	0.065103	-3.197702	-0.123149
H	-0.214036	-4.184452	-0.501223
H	0.359349	-2.550316	-0.961652
H	0.940825	-3.314039	0.527003
C	-4.756699	-3.227807	1.435837
H	-4.908367	-3.926637	0.607760
H	-4.849260	-3.799409	2.368057
H	-5.571802	-2.497370	1.421738

Vibrational frequencies

11.5579	18.7124	22.3489
38.0761	47.0893	54.0221
56.9507	63.2042	71.8993
80.4195	86.1743	95.8552
112.0898	120.5049	125.7289
146.3302	164.1916	179.6157
180.6816	200.2890	211.5524
215.8085	228.1168	233.2983

252.1979	257.1912	285.2702
292.0358	304.8664	315.5585
325.8689	349.3390	381.9491
401.1953	405.9607	420.1246
436.1475	445.5262	457.2900
488.6409	492.5387	502.0950
514.6748	527.4915	531.6141
534.5128	561.7230	581.2572
585.2612	597.0626	600.0264
606.4543	613.4286	628.4065
637.8367	681.9615	708.3625
710.9073	711.8474	720.7376
733.9377	753.6128	769.6932
772.7503	790.4374	796.0884
825.5036	843.1343	848.0918
864.3506	869.7481	872.2405
877.0101	888.1742	898.1623
912.4651	940.8101	949.5378
964.4752	975.9809	984.0752
987.2960	988.3169	1003.6439
1007.8816	1014.7795	1029.5707
1035.2257	1042.8848	1045.8124
1050.3778	1055.3652	1058.0956
1058.6664	1065.5892	1068.2654
1078.1581	1080.6378	1089.5692
1097.7061	1114.3385	1118.3349
1180.3249	1186.4865	1188.9527
1198.6186	1203.9222	1218.1609
1219.8550	1225.0696	1230.7837
1242.9139	1251.8677	1269.7719

1292.8767	1293.1416	1299.4788
1303.0031	1313.9094	1322.0162
1330.8634	1342.4998	1344.2680
1348.7169	1353.8285	1369.4061
1370.2163	1378.0329	1379.3330
1409.7934	1421.2673	1427.5429
1437.0726	1443.9901	1448.9788
1459.4671	1473.0515	1476.4752
1480.0686	1485.4084	1486.3856
1490.8612	1497.4292	1501.9630
1503.7302	1510.8998	1519.9914
1531.0483	1535.7653	1537.2326
1624.9239	1639.5933	1641.0562
1647.5589	1655.1080	1656.1588
1658.1403	1683.0159	2729.8962
2996.3845	3037.6203	3042.5947
3049.7157	3054.4266	3075.9900
3099.3364	3099.3966	3102.0559
3106.1909	3109.9983	3118.7117
3126.0063	3126.9065	3130.5297
3141.4953	3153.0967	3175.6397
3179.0064	3180.6329	3182.4325
3182.5665	3191.3165	3192.7280
3203.1347	3205.2747	3249.5431

Si-M1

Zero-point correction= 0.518161

Thermal correction to Energy= 0.549172

Thermal correction to Enthalpy= 0.550116

Thermal correction to Gibbs Free Energy= 0.455041

Sum of electronic and zero-point Energies= -4046.043074

Sum of electronic and thermal Energies= -4046.012064

Sum of electronic and thermal Enthalpies= -4046.011120

Sum of electronic and thermal Free Energies= -4046.106194

Cartesian coordinates

C	5.287666	-0.350942	0.130054
C	4.041794	-0.117052	0.714680
C	3.908360	0.663271	1.863261
C	5.055794	1.245470	2.405569
C	6.308508	1.035181	1.812411
C	6.434171	0.228057	0.678820
C	5.178975	-1.281713	-1.049809
C	3.656341	-1.500901	-1.270844
C	2.937068	-0.829734	-0.031505
H	2.925848	0.754419	2.319089
H	4.980142	1.857824	3.299852
H	7.192821	1.494777	2.245462
H	7.409190	0.053790	0.231527
H	5.640029	-0.881432	-1.959442
H	3.404700	-2.561650	-1.294454
H	5.673238	-2.237458	-0.842722
H	2.418702	-1.544381	0.606658
N	1.889764	0.108147	-0.496678
O	3.215562	-1.018196	-2.545315
C	0.732936	0.473892	0.090553
C	1.971763	0.764335	-1.701458
N	0.167811	1.335539	-0.764883
N	0.929794	1.524825	-1.903100
C	3.092733	0.401180	-2.615932
H	4.022614	0.912366	-2.331292

H	2.845383	0.669445	-3.644231
C	-1.130928	1.940780	-0.644495
C	-1.280263	3.063008	0.178073
C	-2.198930	1.346405	-1.337146
C	-2.572634	3.581393	0.326423
C	-3.465393	1.902753	-1.154799
C	-3.672563	3.010766	-0.321589
H	-2.718790	4.448147	0.965333
H	-4.314361	1.450535	-1.660268
C	-2.287561	-0.696442	1.261839
C	-0.998589	-0.983504	1.027164
H	-2.397465	0.248077	1.795517
C	-3.576661	-1.303053	0.909923
C	-4.728781	-0.539532	1.197559
C	-3.757933	-2.551092	0.281318
C	-6.002486	-0.991476	0.863304
H	-4.612539	0.425841	1.682430
C	-5.034786	-3.002780	-0.049205
H	-2.902164	-3.168442	0.047536
C	-6.162427	-2.228773	0.234364
H	-6.869408	-0.378775	1.094214
H	-5.147274	-3.968588	-0.534011
H	-7.153543	-2.586044	-0.029825
Br	-0.367736	-2.547312	0.084632
C	0.187645	-0.071585	1.459388
H	-0.338128	0.819521	1.893834
O	1.124637	-0.633323	2.185884
C	-1.988997	0.147322	-2.224953
H	-2.944760	-0.228162	-2.597252
H	-1.358763	0.399866	-3.084674

H	-1.492299	-0.669147	-1.693040
C	-0.100305	3.679508	0.885328
H	0.736769	3.840479	0.197873
H	-0.371880	4.641597	1.326038
H	0.264118	3.032504	1.691910
C	-5.062107	3.569755	-0.143151
H	-5.424959	4.024767	-1.072528
H	-5.771274	2.778006	0.123046
H	-5.092813	4.333653	0.638501

Vibrational frequencies

23.1526	26.8051	29.8860
40.2484	44.3072	48.9710
53.3608	68.5781	88.5102
92.7910	96.9779	107.9769
126.2568	134.2171	152.4754
157.6008	168.5734	186.8646
192.0863	197.2825	221.1256
230.2188	232.2540	242.4298
244.6548	262.3034	286.0270
289.1235	305.6964	314.5959
333.1421	345.0523	361.2308
388.1645	400.6257	417.7546
439.1052	453.0946	464.4179
493.6690	506.5091	513.2887
518.2813	530.4921	533.3450
539.9781	546.3639	577.6201
582.1243	593.0969	601.4053
609.8190	617.4186	632.1025
634.1412	682.2760	689.3901
707.2901	709.3960	719.1320

738.8971 751.0637 771.7457

775.9640 796.5329 801.3564

827.2219 841.5244 855.1182

864.1161 873.7576 877.6226

887.2959 905.2728 907.7524

908.7483 947.2904 952.2839

959.1206 975.3093 980.2532

984.5414 988.0805 989.9779

1010.3340 1012.7728 1018.7054

1031.6359 1036.5268 1038.1382

1046.5152 1053.3074 1058.4495

1059.1561 1064.3763 1066.6220

1070.6962 1074.7304 1083.8537

1101.5755 1117.2424 1120.2673

1181.5610 1184.2198 1189.0743

1194.0699 1196.6752 1214.0330

1219.9585 1220.4147 1231.0160

1243.3237 1257.3471 1275.9604

1285.2039 1286.9749 1291.5676

1305.9990 1312.4689 1321.1343

1329.8323 1335.7639 1348.4612

1354.2878 1367.1380 1370.0926

1371.3578 1383.7648 1388.1803

1409.8081 1418.6153 1426.9238

1433.6437 1439.7946 1449.0323

1466.0592 1475.2420 1478.8588

1481.6975 1486.1310 1487.0388

1491.4277 1493.3343 1498.1405

1499.8708 1506.2985 1517.3066

1522.9367 1532.9352 1537.0029

1625.3114	1637.1849	1640.9400
1642.1534	1654.1189	1654.4502
1657.1961	1685.0353	2738.6228
3039.1957	3040.5495	3044.4251
3055.3090	3055.3819	3091.3916
3098.6972	3104.6267	3121.1688
3129.7494	3131.1355	3132.8895
3136.6836	3145.9453	3147.2579
3150.1268	3175.9010	3180.1196
3181.0276	3183.4000	3186.4425
3187.3867	3189.7319	3196.2352
3201.8696	3207.7412	3254.1067

SiTS2

Zero-point correction= 0.775225

Thermal correction to Energy= 0.815241

Thermal correction to Enthalpy= 0.816186

Thermal correction to Gibbs Free Energy= 0.702844

Sum of electronic and zero-point Energies= -4508.445855

Sum of electronic and thermal Energies= -4508.405838

Sum of electronic and thermal Enthalpies= -4508.404894

Sum of electronic and thermal Free Energies= -4508.518236

Cartesian coordinates

C	-1.322005	-4.031524	1.835386
C	-0.742162	-3.154052	0.915309
C	-0.547685	-3.529855	-0.413033
C	-0.961807	-4.799477	-0.819004
C	-1.558980	-5.676743	0.094289
C	-1.739675	-5.298879	1.426801
C	-1.389220	-3.429376	3.214502

C	-0.637530	-2.078240	3.115322
C	-0.426452	-1.821398	1.565734
H	-0.086717	-2.856766	-1.124105
H	-0.819670	-5.105685	-1.851136
H	-1.877282	-6.661817	-0.234506
H	-2.191092	-5.985229	2.137694
H	-0.912359	-4.060758	3.971738
H	-1.223333	-1.261097	3.539500
H	-2.423863	-3.270479	3.537615
H	-1.111486	-1.044896	1.228296
N	0.939078	-1.341220	1.299323
O	0.578165	-2.070409	3.867585
C	1.418944	-0.384934	0.451150
C	2.000307	-1.809385	2.040330
N	2.747449	-0.357345	0.688495
N	3.114046	-1.227424	1.703563
C	1.681729	-2.691695	3.201906
H	1.445515	-3.713684	2.880531
H	2.523096	-2.726181	3.895002
C	3.793368	0.370707	0.014096
C	4.457873	-0.262430	-1.044251
C	4.132035	1.648801	0.477698
C	5.501854	0.438879	-1.656466
C	5.185175	2.303654	-0.163943
C	5.877727	1.718200	-1.231789
H	6.036713	-0.029455	-2.478587
H	5.468212	3.296177	0.176723
C	-1.702646	-0.008743	-1.060448
C	-0.378015	-0.081718	-1.249494
H	-1.939044	0.620690	-0.203445

C	-2.889949	-0.559590	-1.713123
C	-4.125133	-0.000016	-1.322729
C	-2.906117	-1.618288	-2.642806
C	-5.327310	-0.458819	-1.852866
H	-4.131599	0.806334	-0.594490
C	-4.112562	-2.086901	-3.157733
H	-1.984406	-2.086533	-2.958083
C	-5.325249	-1.507884	-2.774842
H	-6.263496	-0.004332	-1.542826
H	-4.104274	-2.911363	-3.864646
H	-6.260365	-1.876401	-3.185850
Br	0.437347	-0.948145	-2.831211
C	0.639712	0.543874	-0.373873
H	-0.012173	1.369939	0.524069
O	1.451747	1.487897	-1.050347
H	1.840340	1.070309	-1.838318
C	3.354370	2.301051	1.589771
H	2.342216	2.547246	1.246313
H	3.256618	1.639978	2.457525
H	3.837730	3.225425	1.915065
C	4.057169	-1.641519	-1.502811
H	4.087073	-2.361105	-0.677362
H	3.036620	-1.644128	-1.898481
H	4.723998	-1.999872	-2.290611
C	6.975438	2.471768	-1.940880
H	6.553578	3.229708	-2.613403
H	7.622047	2.995869	-1.230410
H	7.595708	1.806189	-2.547370
C	-2.469125	3.469881	-1.394761
C	-3.443795	4.645915	-1.259338

C	-3.972265	4.885389	0.159733
C	-1.172254	3.604963	-0.565975
C	-2.865959	5.145456	1.189300
C	-1.315953	3.233225	0.892044
H	-2.980417	2.535508	-1.135926
H	-2.943366	5.561455	-1.603907
H	-4.577982	4.034210	0.497779
H	-2.124310	5.841268	0.781240
H	-0.806262	4.637582	-0.629584
H	-2.178323	3.371908	-2.446219
H	-4.291738	4.482870	-1.935004
H	-4.634542	5.759195	0.148648
H	-0.386357	2.977144	-0.986526
H	-3.280514	5.620366	2.081126
C	-2.520834	3.484656	3.026060
H	-3.598771	3.612299	3.163070
H	-2.014504	4.143316	3.742527
C	-2.115363	2.033501	3.258011
H	-2.196924	1.794960	4.322128
H	-2.786187	1.362027	2.708374
C	-0.688833	1.846880	2.749416
H	-0.351911	0.813095	2.847511
H	0.005504	2.464917	3.334545
N	-0.606798	2.221130	1.339949
N	-2.185362	3.923853	1.658400

Vibrational frequencies

-1488.8132	-43.3365	-37.2434
-19.7472	21.2680	25.4606
27.6001	32.5576	39.0867
42.8429	50.6713	54.0426

60.5139	78.1264	83.5939
87.4563	92.2017	94.8382
114.7315	121.0106	127.9035
130.8686	138.0501	146.3378
154.9900	170.1275	181.3838
187.5572	197.7363	209.4045
212.5302	228.0139	238.8206
244.9516	248.4609	255.1737
268.8004	270.7874	284.7108
290.0092	308.7749	313.8537
325.9808	332.2276	354.1399
361.0113	377.5428	385.8574
398.1905	412.2175	413.9914
423.7110	429.7307	435.9298
438.9338	457.1484	477.5628
489.8474	496.9080	503.0701
511.4319	517.4770	526.8666
528.4034	529.7549	530.7134
536.0962	556.5714	580.9698
583.3614	599.6807	610.3900
612.4373	618.5638	631.5021
642.6896	644.8415	660.9858
700.1927	701.6320	702.9123
716.4771	724.9265	733.7254
749.2517	760.9166	771.5244
774.4760	790.0698	803.0505
809.3931	830.0619	847.3077
847.7223	852.0351	863.8365
866.9187	875.2002	876.2701
882.1710	887.2375	896.9840

904.3479	904.7629	915.8971
917.1572	930.3668	939.2249
957.9722	960.8540	974.5834
979.1684	984.0305	987.4707
992.5419	998.2461	1000.0289
1009.2310	1013.5343	1015.3843
1026.7978	1037.3251	1041.0962
1044.8456	1053.9274	1057.4764
1060.6496	1062.3716	1065.8470
1072.2788	1073.9887	1078.1647
1089.6681	1090.0259	1099.8650
1104.0371	1112.8312	1117.0419
1118.8612	1123.8947	1125.5418
1132.0994	1140.5593	1178.3997
1181.8296	1189.5717	1191.2136
1198.0327	1206.5022	1219.5117
1220.1643	1221.7546	1229.1116
1233.1604	1245.8618	1248.7361
1250.0146	1261.3161	1270.5372
1270.8215	1294.5889	1295.0440
1296.3836	1299.4143	1301.1315
1315.2538	1316.4087	1322.2511
1326.2005	1331.7077	1343.2292
1344.8673	1352.7327	1356.5141
1368.1503	1370.2250	1371.9090
1372.6210	1383.2362	1385.5100
1386.7181	1393.3796	1402.6777
1407.3506	1409.6009	1415.2676
1416.1167	1419.6190	1430.0467
1438.3369	1439.7746	1448.9519

1460.6784	1472.5894	1473.7072
1476.5204	1478.5216	1482.1670
1485.3884	1485.7652	1488.2433
1490.6476	1493.9814	1495.6801
1496.7627	1499.9126	1501.7215
1504.6808	1508.9076	1512.8641
1522.9355	1526.4645	1530.4147
1533.1042	1538.0069	1539.4399
1621.9110	1627.4991	1641.8616
1642.6876	1650.1922	1655.7714
1655.8986	1662.0142	1671.1530
1714.9893	3027.5817	3032.5806
3034.8312	3038.5225	3039.2740
3042.9110	3047.5396	3053.3826
3054.7740	3054.8138	3057.9804
3060.2622	3062.7762	3077.2889
3083.8502	3093.5154	3098.9339
3100.5904	3100.9195	3101.1822
3117.3644	3118.4918	3120.9846
3122.4578	3127.7352	3131.7647
3133.8589	3141.0388	3141.5376
3148.9649	3150.1086	3160.8514
3181.8270	3183.1218	3183.9761
3187.4992	3192.2037	3197.3675
3201.1309	3209.5496	3213.2766
3240.4373	3254.4321	3695.8386

M2

Zero-point correction= 0.516288

Thermal correction to Energy= 0.548503

Thermal correction to Enthalpy= 0.549447

Thermal correction to Gibbs Free Energy= 0.450057

Sum of electronic and zero-point Energies= -4046.049350

Sum of electronic and thermal Energies= -4046.017135

Sum of electronic and thermal Enthalpies= -4046.016191

Sum of electronic and thermal Free Energies= -4046.115581

Cartesian coordinates

C	-2.532209	3.172067	0.466334
C	-1.814775	1.982149	0.626050
C	-1.612385	1.434581	1.895831
C	-2.119427	2.109749	3.008348
C	-2.824846	3.308974	2.852794
C	-3.041623	3.841723	1.580120
C	-2.673057	3.555998	-0.982437
C	-1.915131	2.459974	-1.779781
C	-1.368137	1.426148	-0.712198
H	-1.101814	0.487718	2.022060
H	-1.971588	1.694041	4.000917
H	-3.215651	3.822593	3.726729
H	-3.600303	4.765749	1.457114
H	-2.253183	4.545407	-1.197095
H	-2.594256	1.929615	-2.448269
H	-3.724261	3.593064	-1.287312
H	-1.809455	0.445742	-0.894844
N	0.087233	1.266258	-0.831774
O	-0.917767	2.990769	-2.652068
C	0.923560	0.284681	-0.307597
C	0.890691	2.268056	-1.325581
N	2.189123	0.780529	-0.544206
N	2.153244	2.017327	-1.186901

C	0.240360	3.450375	-1.962766
H	-0.008954	4.207852	-1.205530
H	0.911720	3.905722	-2.692973
C	3.457654	0.146014	-0.361049
C	4.331884	0.671019	0.601916
C	3.802652	-0.956853	-1.159226
C	5.582649	0.064180	0.752765
C	5.058069	-1.538705	-0.961443
C	5.962801	-1.041165	-0.015824
H	6.269748	0.458529	1.497283
H	5.339728	-2.395794	-1.568932
C	-1.369850	-1.766676	-0.798147
C	-0.601332	-1.582154	0.311909
H	-0.836929	-1.582565	-1.730273
C	-2.768063	-2.156169	-0.971027
C	-3.162978	-2.662533	-2.228815
C	-3.766748	-2.000568	0.014342
C	-4.482371	-3.029035	-2.481392
H	-2.415334	-2.771577	-3.010773
C	-5.085656	-2.368984	-0.241546
H	-3.506615	-1.583827	0.978970
C	-5.453670	-2.888771	-1.486066
H	-4.754319	-3.421565	-3.457480
H	-5.835115	-2.236839	0.534267
H	-6.484203	-3.171716	-1.680244
Br	-1.132253	-2.389579	2.064227
C	0.630685	-0.890865	0.383323
O	1.647266	-1.344957	1.222209
H	1.862632	-2.258543	0.982510
C	2.851026	-1.506025	-2.191414

H	2.005856	-2.024420	-1.722719
H	2.431718	-0.707279	-2.812055
H	3.357717	-2.218177	-2.847413
C	3.916143	1.832221	1.467251
H	3.698252	2.721626	0.867158
H	3.003512	1.591641	2.024350
H	4.699266	2.084468	2.186692
C	7.322614	-1.675089	0.148185
H	7.252184	-2.767778	0.178897
H	7.979514	-1.419976	-0.692720
H	7.814609	-1.339633	1.065613

Vibrational frequencies

16.0810	17.2068	25.3341
31.1302	36.3359	44.6846
48.6370	51.9628	80.6326
86.3957	94.4993	110.1674
115.2675	125.2808	131.0991
142.4216	148.6224	156.4654
166.0266	188.1445	194.1311
205.4417	211.3582	223.1724
235.1378	242.1010	268.5012
286.6586	293.5763	300.7328
331.0351	332.4539	355.7432
365.2600	381.8465	395.3802
420.0335	421.6723	440.9758
447.7599	482.4411	495.3772
504.9089	515.0134	521.6510
528.2163	533.7084	539.1880
573.1136	581.1798	582.2613
599.7532	608.4447	613.8167

614.0013	631.9481	645.5886
652.0397	685.1409	698.1129
710.2115	727.0073	742.1339
763.9904	768.0951	779.1216
799.4684	814.7779	827.6736
851.9726	857.6666	859.2581
873.3262	877.1411	884.6313
902.8499	902.9238	927.0699
953.9165	959.0099	971.9093
977.4707	979.7178	994.1765
998.4626	1000.3747	1007.5360
1010.7584	1037.6832	1043.0842
1045.4612	1054.4053	1056.0063
1059.3359	1060.8050	1063.4222
1067.0326	1067.6582	1081.9874
1112.9970	1115.0802	1125.2646
1156.4626	1169.6450	1187.1207
1188.2535	1196.0582	1204.8824
1210.0880	1212.7990	1215.6899
1236.3401	1249.4313	1274.0629
1276.1197	1281.2824	1288.2631
1299.0622	1310.2640	1320.1226
1329.1982	1334.2028	1340.1719
1345.9982	1354.9760	1366.8104
1368.9433	1381.2626	1388.2379
1408.6569	1412.5823	1420.1427
1421.6786	1426.8751	1449.5306
1468.2051	1475.7958	1477.8171
1481.0454	1483.4587	1486.3517
1486.9292	1492.7013	1496.7684

1497.9048	1507.8549	1525.3303
1528.1593	1534.0484	1576.3060
1618.6959	1635.4429	1638.6637
1640.3850	1654.2295	1657.0719
1657.5002	1677.8759	3021.5383
3037.1890	3038.8877	3046.6072
3057.4109	3091.4631	3096.4468
3099.3688	3107.7868	3108.3856
3125.2742	3126.9775	3132.3024
3134.7438	3140.6582	3143.3744
3170.8236	3173.8790	3178.2947
3181.1770	3182.0540	3191.1620
3191.1989	3204.1700	3204.9851
3232.4543	3240.5124	3753.2661

TS3

Zero-point correction= 0.516218

Thermal correction to Energy= 0.547383

Thermal correction to Enthalpy= 0.548327

Thermal correction to Gibbs Free Energy= 0.451830

Sum of electronic and zero-point Energies= -4046.048649

Sum of electronic and thermal Energies= -4046.017485

Sum of electronic and thermal Enthalpies= -4046.016541

Sum of electronic and thermal Free Energies= -4046.113038

Cartesian coordinates

C	-2.616115	2.947022	0.664506
C	-1.846678	1.780044	0.686199
C	-1.643686	1.075727	1.875924
C	-2.207800	1.571798	3.053363
C	-2.964509	2.749856	3.039077

C	-3.177825	3.439963	1.843678
C	-2.738250	3.514822	-0.724775
C	-1.860889	2.605932	-1.627986
C	-1.337421	1.435273	-0.698882
H	-1.091364	0.143325	1.890545
H	-2.062165	1.033359	3.985356
H	-3.395730	3.125101	3.962881
H	-3.773838	4.348487	1.830726
H	-2.399483	4.554979	-0.786722
H	-2.450959	2.167661	-2.433419
H	-3.777958	3.504186	-1.068948
H	-1.741867	0.486677	-1.047329
N	0.129280	1.327654	-0.764562
O	-0.829914	3.322604	-2.307529
C	0.973163	0.296743	-0.389964
C	0.915740	2.428737	-1.011968
N	2.222485	0.853391	-0.454823
N	2.178872	2.185405	-0.850409
C	0.251366	3.688263	-1.457024
H	-0.088107	4.273039	-0.589676
H	0.947558	4.299741	-2.033741
C	3.509173	0.241413	-0.287249
C	4.197631	0.458217	0.911257
C	4.034345	-0.527433	-1.334904
C	5.467008	-0.115714	1.043035
C	5.297937	-1.091623	-1.151343
C	6.028965	-0.894388	0.027947
H	6.018964	0.039107	1.966864
H	5.723313	-1.697861	-1.948011
C	-1.408926	-1.751514	-1.174682

C	-0.536919	-1.640292	-0.150608
H	-0.956072	-1.662421	-2.162379
C	-2.853570	-1.980232	-1.172186
C	-3.457540	-2.510682	-2.330328
C	-3.685296	-1.639926	-0.085645
C	-4.832580	-2.725335	-2.390396
H	-2.833485	-2.761296	-3.184764
C	-5.059910	-1.857835	-0.148472
H	-3.249645	-1.197509	0.801961
C	-5.641572	-2.403870	-1.296541
H	-5.274074	-3.142314	-3.291403
H	-5.682868	-1.587064	0.699702
H	-6.714331	-2.568272	-1.341871
Br	-1.032495	-2.689532	1.718356
C	0.694636	-1.027307	0.003577
O	1.730109	-1.656768	0.686397
H	1.288996	-2.301901	1.269824
C	3.245812	-0.745843	-2.600149
H	2.351242	-1.353058	-2.407710
H	2.904100	0.204224	-3.025170
H	3.845381	-1.260744	-3.353313
C	3.557263	1.238787	2.028517
H	3.258964	2.240455	1.702038
H	2.649514	0.727701	2.370564
H	4.237600	1.340704	2.879162
C	7.397896	-1.509920	0.184947
H	7.371648	-2.592712	-0.017870
H	8.115762	-1.064951	-0.525886
H	7.791543	-1.360955	1.200103

Vibrational frequencies

-54.7774	16.3105	21.5725
22.7774	32.0697	38.9207
46.5905	50.3692	54.2577
81.9028	89.7377	97.2910
109.5163	122.7253	149.8881
164.6441	174.9563	180.8502
191.2333	201.5621	206.1060
212.3588	229.8660	241.8175
246.7852	268.9258	280.6820
284.1142	290.4053	301.3129
323.0978	329.1690	337.6940
366.6650	379.7335	388.5683
421.3625	423.2396	442.4967
450.8652	470.2568	488.7555
507.1555	510.5374	517.1884
524.5574	526.6117	533.1630
569.4447	579.9748	583.7093
599.2840	609.3669	613.4446
616.0508	632.2614	645.5120
664.6922	693.3968	702.9065
708.8651	727.1061	730.0592
763.4491	771.7747	777.1459
801.8712	809.7798	825.9577
844.3926	855.8099	858.7666
873.3369	875.6356	883.0288
899.1787	907.1605	924.9588
955.9151	961.2940	972.5369
976.9769	980.5682	992.3421
998.7936	1005.8254	1006.8260
1011.5619	1039.6995	1040.4389

1050.0914	1054.5793	1055.3965
1058.4570	1063.2109	1068.2404
1070.1140	1080.8048	1084.3515
1110.3664	1114.5948	1124.9964
1152.0303	1173.8333	1187.9294
1188.8909	1197.6258	1205.0705
1210.2362	1213.7418	1213.9582
1236.2252	1247.3978	1255.7865
1273.3364	1287.4277	1289.1305
1300.8738	1317.2647	1327.7929
1329.8590	1338.6122	1344.5853
1346.3185	1358.1355	1367.0193
1368.4042	1380.2882	1409.4808
1411.0840	1418.0065	1421.9996
1427.1683	1432.5462	1454.0091
1467.1020	1474.8058	1480.4131
1484.2921	1485.9307	1488.3534
1488.9986	1490.8270	1497.9364
1498.2929	1511.4704	1524.4722
1531.2505	1535.8224	1569.6833
1624.0545	1639.4235	1643.8826
1650.8846	1656.6725	1657.4668
1667.7670	1719.4377	2982.1466
3023.2922	3034.4208	3037.0859
3041.4924	3058.1707	3075.4077
3093.5322	3094.0911	3104.9911
3125.4252	3127.7268	3138.9784
3140.3484	3142.0377	3142.6801
3173.3306	3174.5220	3177.6045
3182.4042	3182.6656	3192.1804

3193.2280	3205.1566	3205.8505
3227.4359	3227.9168	3637.2654

M3

Zero-point correction= 0.517176

Thermal correction to Energy= 0.548985

Thermal correction to Enthalpy= 0.549929

Thermal correction to Gibbs Free Energy= 0.451770

Sum of electronic and zero-point Energies= -4046.063100

Sum of electronic and thermal Energies= -4046.031292

Sum of electronic and thermal Enthalpies= -4046.030348

Sum of electronic and thermal Free Energies= -4046.128506

Cartesian coordinates

C	-4.040947	1.204638	-0.124826
C	-2.714198	1.591099	0.103096
C	-2.103449	2.570072	-0.677569
C	-2.824850	3.138828	-1.727766
C	-4.142842	2.737744	-1.975629
C	-4.760816	1.775319	-1.172395
C	-4.492326	0.183479	0.882875
C	-3.470396	0.348069	2.018361
C	-2.169550	0.915957	1.333913
H	-1.080755	2.876411	-0.484481
H	-2.362275	3.897210	-2.352157
H	-4.695872	3.189383	-2.794487
H	-5.789996	1.481226	-1.357493
H	-4.384587	-0.820383	0.457293
H	-3.796547	1.126586	2.722227
H	-5.520527	0.327556	1.225408
H	-1.658399	1.623367	1.992376

N	-1.184150	-0.195170	1.160503
O	-3.318423	-0.886552	2.712692
C	-0.179168	-0.433893	0.285713
C	-1.035505	-1.090436	2.189904
N	0.536508	-1.435466	0.823316
N	0.002442	-1.863048	2.014157
C	-2.037836	-1.070662	3.296858
H	-2.036780	-2.025821	3.824396
H	-1.792448	-0.274327	4.016662
C	1.803673	-1.962292	0.375880
C	1.835843	-2.908420	-0.656158
C	2.957651	-1.477837	1.011297
C	3.094804	-3.361442	-1.063844
C	4.188433	-1.965949	0.565965
C	4.276517	-2.901804	-0.472187
H	3.148990	-4.091449	-1.867376
H	5.097533	-1.599960	1.035863
C	2.582720	1.294612	-0.967130
C	1.359628	0.817312	-1.015271
H	3.391625	0.647935	-1.315050
C	2.999295	2.614086	-0.459790
C	4.351776	2.982842	-0.546928
C	2.091263	3.507322	0.136324
C	4.785029	4.216021	-0.059332
H	5.061929	2.296559	-1.000934
C	2.524563	4.737012	0.622498
H	1.046184	3.224163	0.220813
C	3.873680	5.097317	0.525720
H	5.834083	4.487275	-0.135135
H	1.811818	5.417580	1.079499

H	4.209971	6.057360	0.906209
Br	-2.662002	-1.987435	-1.305635
C	0.166670	0.254859	-0.982057
O	-0.733109	0.288451	-1.983813
H	-1.448410	-0.416941	-1.824021
C	0.576423	-3.392718	-1.317892
H	-0.215922	-3.598455	-0.594544
H	0.158804	-2.637146	-1.990573
H	0.770600	-4.297115	-1.900232
C	2.873174	-0.458293	2.117378
H	2.389592	-0.877622	3.006388
H	3.869353	-0.112133	2.401971
H	2.288356	0.414204	1.807950
C	5.615125	-3.428059	-0.926167
H	5.844278	-4.382958	-0.436813
H	5.627881	-3.607434	-2.005761
H	6.423944	-2.732925	-0.682695

Vibrational frequencies

16.4727	17.8026	32.1797
41.4635	43.3818	48.9131
51.3152	57.9497	62.1799
76.0703	80.0668	83.2031
115.1465	125.8452	140.0048
147.0977	161.9893	173.2239
179.6397	193.6686	202.1920
207.9323	216.6860	235.5153
246.1486	273.7086	276.8125
292.0252	293.2796	306.9879
320.9420	337.7663	352.1063
364.5496	382.2133	414.9986

416.7186	424.9766	456.8627
464.3881	481.7779	503.5117
506.4145	521.1203	521.2908
529.2949	542.1455	573.0791
581.3846	588.7893	600.2596
604.8897	614.9730	622.5390
631.1754	655.0705	662.8034
697.4536	707.5925	713.1436
731.0686	739.9010	756.0210
764.9784	767.4240	789.4934
801.7389	822.4418	834.0513
836.6383	860.7722	872.8797
882.3480	888.1946	894.5005
900.5686	902.0367	942.7837
951.8137	963.7617	974.9110
981.6698	986.3238	996.0666
1007.6728	1012.9674	1014.6601
1020.4962	1042.2749	1042.8626
1047.8271	1053.3336	1055.8349
1056.3947	1065.7274	1067.9324
1073.9175	1086.1959	1094.1730
1110.0539	1119.2239	1132.0694
1151.9027	1179.8052	1186.9216
1187.9657	1189.3893	1201.4624
1206.4610	1214.0623	1236.0046
1237.7111	1258.8653	1264.7331
1284.2209	1288.9815	1296.4385
1306.3899	1328.7560	1333.9583
1341.5219	1344.6099	1357.3879
1363.8543	1365.0585	1373.9796

1386.0227	1403.9518	1408.9045
1413.0921	1413.6715	1420.6132
1424.7643	1446.6287	1466.9535
1474.0858	1481.2302	1485.6666
1487.2363	1488.7197	1494.0222
1496.0785	1498.5406	1502.8766
1505.9605	1519.4728	1522.3621
1524.4539	1532.6811	1540.7640
1633.0833	1633.9097	1640.7413
1642.0653	1653.5322	1653.9738
1664.8032	2039.0987	2848.2911
3011.5626	3027.2041	3039.6550
3049.5081	3056.8741	3060.2290
3094.3011	3101.5516	3110.2400
3118.4415	3120.1370	3123.6045
3128.4424	3141.2073	3146.5605
3148.2796	3182.2891	3183.6752
3183.6944	3185.4579	3186.8181
3194.6524	3196.2899	3201.7101
3205.0995	3211.8186	3216.9607

TS4

Zero-point correction= 0.773214

Thermal correction to Energy= 0.815665

Thermal correction to Enthalpy= 0.816609

Thermal correction to Gibbs Free Energy= 0.695698

Sum of electronic and zero-point Energies= -4508.436384

Sum of electronic and thermal Energies= -4508.393933

Sum of electronic and thermal Enthalpies= -4508.392989

Sum of electronic and thermal Free Energies= -4508.513899

Cartesian coordinates

C	2.421564	3.229732	-1.225895
C	2.141713	1.917859	-0.825281
C	2.245386	0.855492	-1.720644
C	2.585954	1.123877	-3.047669
C	2.844203	2.436820	-3.456600
C	2.773413	3.494772	-2.546584
C	2.274678	4.194757	-0.083894
C	2.299260	3.286197	1.156149
C	1.846585	1.860894	0.650391
H	2.062269	-0.159625	-1.395344
H	2.660812	0.308647	-3.760695
H	3.113372	2.634163	-4.490256
H	2.988244	4.510743	-2.864276
H	1.298321	4.688024	-0.141729
H	3.325482	3.156188	1.524678
H	3.055437	4.959069	-0.050544
H	2.398637	1.064699	1.153180
N	0.424469	1.626968	1.054441
O	1.497386	3.873462	2.177747
C	-0.587324	0.908314	0.531843
C	-0.008911	2.079668	2.278747
N	-1.574480	0.934937	1.437736
N	-1.228426	1.683049	2.532459
C	0.909781	2.945972	3.076149
H	0.345905	3.504700	3.824564
H	1.662744	2.330296	3.591044
C	-2.859718	0.271989	1.373629
C	-3.976119	1.023223	0.968080
C	-2.946138	-1.073360	1.767303

C	-5.194846	0.345852	0.867154
C	-4.191634	-1.694769	1.647810
C	-5.318042	-1.012139	1.180828
H	-6.069366	0.899862	0.537962
H	-4.276270	-2.743843	1.919470
C	-0.841593	-2.434514	-1.022273
C	-0.312123	-1.273771	-0.558432
H	-0.201504	-3.313235	-0.932989
C	-2.189349	-2.727986	-1.493285
C	-2.499623	-4.071061	-1.796013
C	-3.196591	-1.752476	-1.647432
C	-3.767247	-4.426820	-2.247597
H	-1.735151	-4.833445	-1.672210
C	-4.459953	-2.110342	-2.100948
H	-3.001218	-0.717684	-1.400075
C	-4.750712	-3.446484	-2.401811
H	-3.989620	-5.464538	-2.476220
H	-5.225585	-1.348676	-2.208629
H	-5.742124	-3.720616	-2.750149
Br	-1.026980	3.535735	-1.405331
C	-0.648558	0.061295	-0.714246
O	-0.910513	0.626838	-1.842100
H	-0.963067	1.705496	-1.765854
H	0.768650	-1.478466	0.158447
C	-1.788058	-1.844806	2.342560
H	-1.942451	-2.006828	3.415410
H	-1.705224	-2.826676	1.868312
H	-0.835753	-1.337198	2.214212
C	-3.892473	2.504041	0.717049
H	-4.809324	2.864526	0.244168

H	-3.769983	3.039944	1.666287
H	-3.047752	2.784211	0.080795
C	-6.626510	-1.739008	1.006627
H	-6.905857	-2.278398	1.918136
H	-7.439537	-1.054415	0.751072
H	-6.544849	-2.481950	0.204207
C	4.146594	-2.238282	-1.705594
C	5.459720	-3.015294	-1.555144
C	5.980592	-3.132241	-0.118967
C	2.941276	-2.844056	-0.951159
C	4.983166	-3.798278	0.836242
C	2.894455	-2.498490	0.522030
H	4.284350	-1.196952	-1.391965
H	5.315632	-4.027776	-1.957328
H	6.243807	-2.143795	0.279492
H	4.535744	-4.681163	0.367566
H	2.942784	-3.934888	-1.068268
H	3.883892	-2.206099	-2.768599
H	6.225310	-2.539783	-2.179278
H	6.900517	-3.728616	-0.121229
H	2.012421	-2.486394	-1.397701
H	5.497717	-4.150330	1.732479
C	4.035667	-2.448075	2.708476
H	5.088596	-2.217357	2.896412
H	3.753262	-3.274617	3.372189
C	3.166079	-1.225659	2.969177
H	3.108116	-1.036606	4.044691
H	3.612297	-0.343145	2.496416
C	1.779387	-1.474727	2.381599
H	1.136540	-0.596795	2.495664

H	1.288078	-2.299640	2.915410
N	1.876022	-1.793594	0.958946
N	3.916889	-2.897482	1.309025

Vibrational frequencies

-1238.1342	5.8264	17.1873
30.8264	35.5893	38.1053
43.5196	46.2558	49.2858
60.0737	63.5144	71.1000
75.6834	80.7200	88.0892
101.2147	101.5790	105.4057
110.6987	120.8116	121.9048
131.5411	136.2034	145.4586
154.9745	158.5329	167.4614
175.9953	177.5107	189.1310
204.3960	208.1562	218.6698
240.1948	246.8504	248.0734
264.8287	281.3445	285.8603
292.5318	295.0915	320.3013
329.4758	346.1530	357.6852
360.5763	365.9018	372.0855
380.4692	409.4230	416.9470
418.6102	425.0532	435.9958
446.8516	465.1678	481.7228
482.5955	495.7075	503.9072
509.6536	513.9659	525.5984
530.3035	536.5491	544.6813
546.5683	580.6835	581.2727
592.3811	597.7291	607.1513
624.3636	626.8597	637.5199
647.2453	657.5618	689.1257

698.2684	701.0926	715.3139
717.2666	729.4616	750.4685
761.4702	766.9628	773.6192
795.9016	804.0224	811.7453
829.9136	839.8342	851.8908
860.2280	864.6942	868.8078
873.3405	883.7706	889.2838
894.3846	899.9433	902.6024
910.0146	918.1342	940.5066
945.0518	959.5290	968.9086
971.0094	973.4011	974.3728
982.6976	986.4954	991.5281
1000.8060	1001.4610	1011.6557
1012.7982	1015.7726	1019.7482
1025.1128	1032.6828	1041.3870
1044.4532	1053.4689	1056.4844
1058.3857	1065.4866	1068.2305
1073.3447	1075.1035	1084.1568
1090.1080	1094.2372	1108.7610
1114.9673	1118.6131	1123.8768
1127.6726	1130.3509	1133.5329
1152.1944	1179.3403	1185.6375
1187.1280	1189.9562	1193.6638
1200.3629	1203.3102	1212.5045
1222.5423	1223.8957	1232.8901
1237.9019	1241.9090	1251.8353
1257.3014	1263.8637	1270.2969
1272.8581	1290.6133	1295.1456
1300.5564	1301.6344	1314.4074
1324.8711	1331.8139	1336.2440

1338.5252	1346.6322	1348.4346
1358.3720	1366.9209	1369.7678
1373.5425	1374.7381	1379.5953
1380.2421	1390.0345	1392.5330
1397.2756	1400.8934	1401.6519
1404.2822	1408.9311	1409.8103
1420.5848	1421.9464	1425.4437
1441.0762	1451.7040	1466.4139
1469.8766	1473.1367	1478.9578
1479.7248	1483.5772	1483.9126
1487.0531	1487.7587	1489.0366
1490.0889	1494.8249	1497.1710
1499.4527	1502.5981	1503.5269
1505.2232	1511.0869	1517.3178
1521.3847	1524.3872	1528.1401
1530.9414	1540.9215	1546.7802
1557.8045	1625.5277	1629.7655
1638.3293	1642.8570	1645.8325
1652.3698	1655.8925	1665.2964
1708.4804	1925.7989	3020.3034
3024.3021	3028.7940	3037.3558
3038.0144	3038.6929	3042.0375
3044.5765	3047.7188	3055.0587
3057.3669	3058.7844	3066.3277
3067.1993	3077.4441	3086.8783
3093.0815	3098.8004	3101.6566
3102.5893	3104.8425	3117.1372
3117.3381	3124.0094	3126.0771
3127.6553	3132.5078	3136.2808
3136.4925	3142.9560	3149.3314

3181.4368	3187.9266	3188.1844
3190.8180	3196.3350	3199.7252
3208.0325	3209.8528	3216.2444
3230.0881	3251.0443	3258.7520

M4

Zero-point correction= 0.518673

Thermal correction to Energy= 0.548312

Thermal correction to Enthalpy= 0.549256

Thermal correction to Gibbs Free Energy= 0.456073

Sum of electronic and zero-point Energies= -1474.215965

Sum of electronic and thermal Energies= -1474.186326

Sum of electronic and thermal Enthalpies= -1474.185382

Sum of electronic and thermal Free Energies= -1474.278565

Cartesian coordinates

C	1.915573	1.751111	1.072251
C	1.089977	0.836473	0.500150
H	1.645633	2.112064	2.063641
C	-0.076165	0.353059	1.204802
O	-0.483116	0.703683	2.311457
C	3.125133	2.305336	0.495261
C	3.766344	3.366713	1.167702
C	3.689726	1.822877	-0.706943
C	4.922536	3.941947	0.648073
H	3.344335	3.738616	2.097270
C	4.847273	2.395396	-1.217608
H	3.232705	0.988567	-1.229124
C	5.464282	3.458301	-0.545327
H	5.403010	4.762036	1.172398
H	5.276801	2.013871	-2.138843

H	6.368757	3.902254	-0.950395
C	-0.895331	-0.715744	0.515107
C	-2.557906	-2.005985	-0.066818
C	-3.253371	0.221108	0.950095
H	-3.163453	0.261726	2.035083
N	-1.477654	-2.676346	-0.386285
N	-0.446436	-1.851746	-0.022712
N	-2.242178	-0.789042	0.486326
C	-3.978562	-2.438861	-0.255910
H	-4.082066	-3.481297	0.054473
H	-4.242660	-2.379698	-1.320259
C	-4.651879	-0.261754	0.459034
O	-4.843529	-1.665279	0.558979
C	-4.012933	1.632206	-0.824827
C	-3.117670	1.557400	0.253652
C	-2.307298	2.643027	0.590039
C	-2.373035	3.796314	-0.196083
C	-3.244602	3.863249	-1.288599
C	-4.077763	2.785820	-1.603332
C	-4.834917	0.374891	-0.941803
H	-1.650404	2.603666	1.450321
H	-3.287567	4.768651	-1.886914
H	-4.774917	2.851275	-2.433597
H	-4.445289	-0.269711	-1.738276
H	-5.888266	0.562244	-1.164307
C	0.925388	-2.274153	-0.178332
C	1.604044	-2.766608	0.944849
C	1.506846	-2.160248	-1.449718
C	2.943272	-3.124596	0.767017
C	2.847218	-2.532954	-1.568713

C	3.580586	-3.009821	-0.474144
H	3.498975	-3.504256	1.620053
H	3.329302	-2.446902	-2.538520
C	0.723580	-1.635142	-2.624876
H	0.368624	-0.614003	-2.443443
H	-0.158739	-2.252864	-2.821373
H	1.339678	-1.622576	-3.526415
C	5.019712	-3.426879	-0.637993
H	5.507657	-2.874558	-1.446251
H	5.085536	-4.494180	-0.883243
H	5.588295	-3.268501	0.283028
C	0.925930	-2.902643	2.284490
H	-0.040149	-3.409695	2.191686
H	0.740321	-1.925648	2.745977
H	1.548152	-3.479381	2.971820
H	-5.383433	0.173572	1.143289
H	-1.750960	4.650911	0.052038
H	1.271237	0.447471	-0.493909

Vibrational frequencies

11.4238	19.4031	24.8106
31.1682	44.7699	49.4947
59.1703	71.1854	86.6647
91.1387	115.7185	118.6619
137.7277	145.0107	167.4900
176.7615	187.9924	197.2796
203.2393	206.0260	241.7620
242.6096	255.5474	262.6271
269.9223	292.9869	294.4902
308.8341	328.1925	338.4900
360.1171	375.8264	410.4115

415.0912	435.1911	457.2326
466.9037	484.2687	493.8647
510.4928	522.9372	526.9974
529.6410	536.0634	575.8816
579.5032	584.6044	590.7285
604.0899	626.3710	629.8273
632.3088	649.8395	690.3823
697.4763	710.6849	728.8748
744.5119	761.6438	770.5454
778.3109	794.1976	799.7446
839.1271	840.9648	856.5335
875.0979	881.3714	883.5366
892.4988	906.3363	907.9006
911.1931	952.6913	960.7119
965.8580	974.5700	977.8212
988.4265	1007.3871	1009.9068
1012.0275	1016.5979	1031.0104
1032.4257	1042.0980	1044.8804
1046.0633	1057.0693	1058.6526
1061.3074	1063.2084	1069.6639
1071.5174	1073.3215	1102.1948
1125.0584	1125.4763	1131.3315
1148.3165	1176.3116	1187.5145
1191.4392	1195.3751	1201.4001
1213.6176	1224.0770	1229.8636
1258.5071	1259.1224	1273.5862
1289.1546	1292.4023	1299.8075
1316.1891	1334.5165	1338.2471
1341.3815	1345.4945	1347.0789
1359.6781	1370.5136	1377.3346

1384.9579	1391.6419	1414.0052
1416.0715	1419.0907	1423.7356
1429.5564	1445.3894	1464.8026
1477.6792	1484.8278	1485.8696
1487.0796	1488.1017	1491.5427
1494.1064	1496.8289	1502.7927
1506.8258	1517.1226	1518.9294
1541.1955	1542.9013	1605.9024
1619.9195	1629.0818	1637.7462
1639.5632	1651.0573	1658.7801
1660.7194	1728.2012	3043.0098
3044.7329	3048.9994	3053.3132
3061.3049	3107.0081	3109.7212
3112.9347	3115.9455	3127.8266
3134.9960	3135.3312	3144.6738
3144.7759	3152.5702	3170.6592
3189.2430	3189.5294	3190.0239
3191.6452	3195.3221	3200.7141
3204.5522	3210.4529	3213.4541
3219.4427	3233.3567	3247.6868

TS5R

Zero-point correction= 0.671510

Thermal correction to Energy= 0.713904

Thermal correction to Enthalpy= 0.714848

Thermal correction to Gibbs Free Energy= 0.593620

Sum of electronic and zero-point Energies= -2462.456537

Sum of electronic and thermal Energies= -2462.414144

Sum of electronic and thermal Enthalpies= -2462.413200

Sum of electronic and thermal Free Energies= -2462.534427

Cartesian coordinates

C	1.801830	0.210962	0.781788
C	0.612258	0.797360	0.292233
H	1.709044	-0.270247	1.750756
C	-0.625110	0.317026	0.721230
O	-0.877924	-0.541748	1.606685
C	3.106002	0.873929	0.539311
C	4.056896	0.938829	1.566724
C	3.431690	1.402190	-0.721236
C	5.301143	1.533254	1.348353
H	3.821619	0.513645	2.537971
C	4.676412	1.986337	-0.942462
H	2.716775	1.324087	-1.534320
C	5.615032	2.055542	0.093031
H	6.027684	1.575960	2.154690
H	4.921046	2.378837	-1.925291
H	6.587350	2.506618	-0.083053
C	-1.821111	0.833885	-0.032941
C	-3.727805	0.884145	-1.117565
C	-3.005921	-1.396712	-0.440508
H	-2.009791	-1.822514	-0.337809
N	-3.346606	2.132752	-1.065219
N	-2.152481	2.085836	-0.372283
N	-2.827343	0.062323	-0.489017
C	-4.830079	0.221242	-1.875977
H	-5.262597	0.910056	-2.602694
H	-5.623013	-0.128940	-1.202163
C	-3.685553	-1.900828	-1.774594
O	-4.216207	-0.850135	-2.592519
C	-4.949701	-2.665801	0.158012

C	-3.952679	-1.825582	0.659587
C	-3.897221	-1.484949	2.010864
C	-4.878377	-1.994282	2.864506
C	-5.884858	-2.833796	2.369246
C	-5.924307	-3.178690	1.015630
C	-4.777510	-2.903399	-1.320832
H	-3.094890	-0.851240	2.373753
H	-6.641988	-3.221745	3.044932
H	-6.705166	-3.831766	0.635689
H	-5.695596	-2.745790	-1.895955
H	-4.450238	-3.931030	-1.517021
C	-1.431110	3.300119	-0.094169
C	-0.733586	3.906676	-1.149600
C	-1.466139	3.820998	1.205826
C	-0.039784	5.084025	-0.862472
C	-0.753224	5.001032	1.438123
C	-0.035047	5.642122	0.422685
H	0.513586	5.573258	-1.659777
H	-0.762636	5.427975	2.437365
C	-2.222932	3.132376	2.312852
H	-1.701737	2.225783	2.641758
H	-3.225990	2.833102	1.990926
H	-2.324088	3.790714	3.178732
C	0.756075	6.893342	0.711179
H	1.806187	6.647862	0.913376
H	0.367398	7.420275	1.587348
H	0.742370	7.581647	-0.139635
C	-0.724933	3.300040	-2.529246
H	-1.729151	3.291106	-2.965965
H	-0.378522	2.260457	-2.505081

H	-0.066449	3.862030	-3.195171
H	-2.931348	-2.371201	-2.405732
H	-4.859066	-1.740971	3.920553
H	0.653086	1.506118	-0.524152
C	3.348285	-2.089231	0.351785
C	4.525973	-2.157309	-0.429282
C	5.702322	-2.683806	0.124864
C	5.730525	-3.138347	1.438295
C	4.567931	-3.070129	2.215597
C	3.391708	-2.550142	1.678893
H	6.588836	-2.721384	-0.501008
H	6.646462	-3.542158	1.859142
H	4.580409	-3.420501	3.243926
H	2.492875	-2.486867	2.284219
C	4.541328	-1.672665	-1.827243
H	3.589835	-1.250945	-2.189282
O	5.526841	-1.721267	-2.551253
N	2.185476	-1.465508	-0.161085
S	1.051951	-2.427939	-0.837475
O	0.012586	-1.562297	-1.438235
O	1.709469	-3.415995	-1.721147
C	0.253397	-3.378393	0.474743
H	-0.201682	-2.677262	1.175582
H	-0.502631	-4.016377	0.011015
H	1.008435	-3.996108	0.963551

Vibrational frequencies

-294.0774	13.9377	21.8239
22.6988	26.6613	34.0563
38.4393	43.5599	48.3633
51.2431	53.7310	60.8912

64.6546 69.0361 72.3853

82.4810 87.7981 103.5605

108.8689 121.3418 129.9805

134.5483 139.1497 141.5142

160.5891 176.3011 182.1326

194.5953 203.6342 207.6608

215.1578 217.4407 237.2641

241.2898 251.1204 265.3479

270.0035 280.1627 281.0950

287.4518 295.6160 298.5888

314.3423 318.5534 328.7406

354.6430 369.6094 389.0677

394.2728 401.5137 406.4781

417.0446 443.6695 447.0933

465.4775 478.6154 482.4222

487.7523 492.6045 509.3115

513.9425 524.1376 529.6356

530.7132 535.9410 542.0306

560.8164 580.6827 587.4125

597.7749 602.5348 606.4959

618.2039 624.3568 633.6214

637.1583 645.6234 693.5491

700.3710 705.6659 707.3918

718.3250 731.6319 737.9009

750.5686 761.0964 766.4738

768.1791 782.1590 789.0042

793.8009 800.6048 813.3131

829.0346 838.7437 844.7820

857.9335 871.6432 877.6121

886.1105 906.5331 906.8484

907.2710 912.0385 928.4873

933.6943 948.5915 960.5502

976.0710 978.1250 979.5094

981.7672 987.8051 989.0823

1000.7016 1003.9178 1006.9114

1007.4260 1015.0545 1032.4454

1033.6137 1041.7831 1044.2517

1046.0649 1053.1012 1054.6592

1057.3102 1064.5548 1067.5307

1069.3592 1070.9289 1071.2592

1079.2754 1088.7832 1097.5171

1109.3844 1117.1542 1118.7292

1141.1870 1164.2232 1184.4707

1186.8251 1187.0111 1188.0419

1194.0079 1203.0060 1210.1087

1216.8364 1219.7359 1227.1150

1236.0243 1245.3737 1252.7141

1256.7375 1268.9129 1280.0665

1292.7767 1296.1957 1297.6206

1305.0392 1311.1982 1323.9159

1331.9876 1338.6193 1342.9177

1344.0304 1354.3830 1359.4541

1364.1471 1369.7853 1377.4448

1381.8791 1411.0163 1423.1029

1425.6945 1428.5450 1431.4888

1445.1354 1448.7110 1458.4188

1470.9381 1472.6070 1479.1769

1480.9516 1481.9563 1485.2373

1485.6390 1489.0309 1490.4074

1492.1520 1494.9954 1499.1516

1507.5032	1511.3105	1518.1713
1522.5833	1533.4960	1538.3240
1565.9124	1615.9643	1623.2817
1635.4810	1639.1968	1641.1709
1642.6659	1643.9514	1654.2980
1656.8323	1658.6530	1764.0847
3024.7106	3040.0760	3045.7224
3046.5809	3048.3453	3057.4435
3066.8416	3101.1886	3102.5376
3106.9751	3107.0855	3129.5044
3133.1880	3139.8795	3144.0008
3154.4084	3167.5403	3170.1514
3182.0921	3182.7109	3183.5319
3184.7592	3184.9038	3186.3709
3188.0125	3189.5663	3192.7971
3196.8140	3197.0226	3204.3188
3204.4938	3206.3021	3211.1878
3212.8721	3214.3309	3247.2070

TS5S

Zero-point correction= 0.671845

Thermal correction to Energy= 0.713988

Thermal correction to Enthalpy= 0.714932

Thermal correction to Gibbs Free Energy= 0.595946

Sum of electronic and zero-point Energies= -2462.449940

Sum of electronic and thermal Energies= -2462.407797

Sum of electronic and thermal Enthalpies= -2462.406852

Sum of electronic and thermal Free Energies= -2462.525839

Cartesian coordinates

C	1.114490	-1.430821	-0.326626

C	-0.035922	-0.713258	-0.762810
H	1.127317	-1.571706	0.750326
C	-0.804229	-0.042672	0.190168
O	-0.660125	0.017157	1.433846
C	1.645017	-2.594574	-1.071229
C	2.318694	-3.600998	-0.358249
C	1.485133	-2.749189	-2.458433
C	2.829161	-4.721449	-1.012170
H	2.440220	-3.498060	0.715429
C	1.990906	-3.869749	-3.111844
H	0.962406	-1.992213	-3.033856
C	2.668901	-4.858467	-2.392497
H	3.346997	-5.488796	-0.443825
H	1.859368	-3.972386	-4.185295
H	3.064406	-5.731052	-2.904441
C	-2.011584	0.722315	-0.325064
C	-4.005742	1.376988	-0.957252
C	-3.713246	-1.142205	-0.756365
H	-3.132835	-1.590855	-1.563784
N	-3.312587	2.478971	-0.836358
N	-2.069569	2.050134	-0.432245
N	-3.244078	0.272512	-0.641184
C	-5.430051	1.236083	-1.395735
H	-5.634663	1.946735	-2.199388
H	-6.104876	1.469306	-0.561555
C	-5.243890	-1.123058	-1.054932
O	-5.652796	-0.067752	-1.915472
C	-4.910137	-1.942239	1.153768
C	-3.647683	-1.909425	0.543700
C	-2.555993	-2.568963	1.106963

C	-2.736612	-3.245977	2.315035
C	-3.990216	-3.266654	2.937106
C	-5.087207	-2.622679	2.356916
C	-5.935022	-1.205265	0.329080
H	-1.590211	-2.560946	0.614548
H	-4.115163	-3.799516	3.875461
H	-6.063151	-2.658584	2.832452
H	-6.122746	-0.209084	0.745947
H	-6.898417	-1.718069	0.268366
C	-0.963057	2.960599	-0.275537
C	-0.229022	3.292836	-1.425259
C	-0.645118	3.425812	1.004864
C	0.895551	4.099630	-1.251562
C	0.499464	4.223195	1.123470
C	1.287787	4.551312	0.017342
H	1.491812	4.364576	-2.120863
H	0.791953	4.565977	2.110766
C	-1.467844	3.045631	2.205548
H	-1.281191	1.998048	2.457915
H	-2.538832	3.161623	2.005757
H	-1.207068	3.664862	3.066058
C	2.563732	5.337798	0.175448
H	2.637957	5.794230	1.166119
H	2.643197	6.129885	-0.576789
H	3.430890	4.678789	0.044613
C	-0.629283	2.771168	-2.781292
H	-1.648189	3.077153	-3.041644
H	-0.603650	1.675717	-2.802672
H	0.047737	3.139257	-3.555185
H	-5.459579	-2.038343	-1.611027

H	-1.897917	-3.762735	2.771611
H	-0.322047	-0.662015	-1.806519
C	3.316546	-0.465674	1.063086
C	2.883670	0.161082	2.258275
C	3.478707	-0.184211	3.481843
C	4.505293	-1.118969	3.540047
C	4.955145	-1.717205	2.355702
C	4.365670	-1.403318	1.133855
H	3.122755	0.315988	4.377616
H	4.960811	-1.376774	4.491511
H	5.762971	-2.443453	2.387026
H	4.698306	-1.885144	0.221592
C	1.872775	1.244628	2.230681
H	1.503649	1.521677	1.233496
O	1.497264	1.839125	3.232951
N	2.619673	-0.180288	-0.135086
S	3.579897	0.172814	-1.445228
O	4.528318	1.245122	-1.063919
O	4.162999	-1.010799	-2.120204
C	2.371019	0.891174	-2.556399
H	1.932267	1.759319	-2.068984
H	2.913090	1.186663	-3.457271
H	1.609889	0.153393	-2.801220

Vibrational frequencies

-301.9863	16.5829	23.4317
28.2051	33.4241	33.9988
40.8489	47.1104	53.8571
56.1430	66.2356	68.9911
73.4329	75.0720	82.9237
94.6293	96.2888	108.2829

117.2860	120.3963	135.4957
139.7534	148.0700	156.2604
164.8983	171.1307	190.0642
205.1345	207.4556	208.6701
227.4881	231.5452	240.4129
245.3698	250.5555	254.4879
261.8850	273.7221	282.3324
285.1274	293.3590	295.9215
308.3765	316.4579	326.9003
343.4255	349.9405	370.3994
390.5009	413.6151	418.3816
435.4997	447.9126	454.9467
459.1407	468.4145	471.6340
482.9718	501.7603	508.4535
511.9135	516.0199	527.4984
530.0003	532.9181	547.6608
566.0075	580.9029	588.2944
590.5914	599.7471	607.0586
617.5717	623.9868	627.8939
633.9251	649.7627	652.7919
679.2037	701.5050	702.9013
718.5835	729.7991	736.1024
745.3992	755.8190	766.2271
767.8535	775.2966	784.9768
795.1461	796.9016	800.6892
838.5638	839.8375	841.5222
856.7350	866.8786	883.0122
887.5607	898.7812	902.9473
903.5287	906.4377	922.4453
933.5884	960.1252	969.5006

976.3634	977.0949	978.1510
981.1820	996.1475	999.7296
1002.6200	1003.4220	1007.4763
1011.1122	1013.8991	1032.3835
1037.8257	1041.0242	1045.3077
1050.7639	1053.8084	1056.4480
1061.9700	1065.8148	1070.4690
1071.1738	1072.9951	1080.0160
1087.4087	1098.8045	1111.0629
1118.4318	1127.6706	1133.6584
1152.8202	1169.6452	1183.9096
1188.1374	1188.8946	1189.2788
1194.7265	1201.1962	1208.5525
1218.1973	1221.2427	1230.2419
1235.7043	1242.3991	1246.6251
1250.8477	1266.6648	1281.3821
1290.5382	1291.6039	1300.8708
1303.6958	1321.3356	1325.9039
1332.2738	1339.5975	1340.4064
1349.7974	1353.8437	1370.3938
1371.4356	1372.1035	1373.6248
1384.3102	1414.1595	1416.9777
1417.7389	1419.5078	1421.4984
1423.9049	1449.6535	1456.9363
1464.2758	1466.7451	1468.1563
1479.7918	1483.4966	1485.2297
1486.9689	1487.4849	1488.8052
1492.8230	1498.7768	1502.9281
1506.9272	1510.2969	1516.0648
1519.1520	1527.7982	1537.2837

1557.9295	1612.1658	1616.8536
1632.9619	1639.1124	1641.2083
1642.0922	1647.3388	1654.2793
1657.8172	1662.0941	1757.0693
3040.4914	3044.8220	3045.8669
3049.5079	3058.4505	3063.0585
3092.5311	3101.5357	3104.1673
3108.6441	3120.7536	3120.9318
3129.5639	3131.1366	3133.6733
3142.2711	3148.5618	3167.7075
3181.1002	3183.7706	3184.6294
3187.0059	3188.4240	3193.4649
3196.8683	3197.7071	3198.2455
3202.2901	3203.8679	3208.3881
3208.7832	3210.4324	3216.9397
3223.3194	3223.9085	3224.6957

M5R

Zero-point correction= 0.674954

Thermal correction to Energy= 0.716607

Thermal correction to Enthalpy= 0.717551

Thermal correction to Gibbs Free Energy= 0.601113

Sum of electronic and zero-point Energies= -2462.460666

Sum of electronic and thermal Energies= -2462.419014

Sum of electronic and thermal Enthalpies= -2462.418069

Sum of electronic and thermal Free Energies= -2462.534508

Cartesian coordinates

C	1.771627	0.382243	0.085226
C	0.365705	0.524730	-0.404192
H	1.704161	0.196010	1.160058

C	-0.686764	0.176565	0.401886
O	-0.711154	-0.366628	1.555513
C	2.658921	1.615811	-0.091350
C	3.995121	1.565069	0.336057
C	2.165673	2.826886	-0.584971
C	4.818677	2.686676	0.253117
H	4.390552	0.639711	0.742823
C	2.987876	3.954437	-0.669072
H	1.129766	2.901603	-0.889875
C	4.318225	3.889523	-0.255122
H	5.850076	2.623409	0.589258
H	2.581161	4.884236	-1.057892
H	4.958006	4.765117	-0.320988
C	-2.066947	0.570940	-0.095246
C	-4.171508	0.635706	-0.727579
C	-3.051283	-1.619079	-1.013122
H	-2.319588	-1.646669	-1.823120
N	-3.888665	1.863621	-0.386516
N	-2.572723	1.803821	0.011366
N	-3.087730	-0.197964	-0.549378
C	-5.460020	0.135732	-1.299150
H	-5.906517	0.913736	-1.921496
H	-6.167529	-0.098151	-0.492457
C	-4.483794	-2.025907	-1.491021
O	-5.209179	-0.987875	-2.132438
C	-3.974693	-3.260408	0.469997
C	-2.782270	-2.646504	0.062328
C	-1.551724	-3.071459	0.555610
C	-1.523482	-4.108401	1.489883
C	-2.713498	-4.709443	1.916441

C	-3.946497	-4.294382	1.404551
C	-5.158142	-2.683427	-0.261290
H	-0.635332	-2.606624	0.223072
H	-2.677698	-5.517505	2.641756
H	-4.866348	-4.779083	1.719018
H	-5.674198	-1.942963	0.360917
H	-5.897451	-3.431158	-0.559999
C	-1.885756	2.995164	0.440773
C	-1.412186	3.873471	-0.543891
C	-1.727367	3.219201	1.814218
C	-0.721192	5.006771	-0.109732
C	-1.019995	4.364537	2.193828
C	-0.501002	5.258393	1.250538
H	-0.334166	5.700933	-0.851027
H	-0.870064	4.558863	3.252529
C	-2.293601	2.261300	2.830331
H	-1.799475	1.285919	2.758290
H	-3.364519	2.099086	2.660541
H	-2.163648	2.649422	3.843336
C	0.314858	6.450961	1.681498
H	0.085419	6.747499	2.709063
H	0.144171	7.311505	1.027049
H	1.385563	6.214881	1.637167
C	-1.619070	3.590853	-2.009378
H	-2.683852	3.525649	-2.257061
H	-1.161375	2.637647	-2.297094
H	-1.171731	4.375934	-2.623008
H	-4.342166	-2.788174	-2.260672
H	-0.570173	-4.452882	1.878652
H	0.182127	0.971442	-1.372636

C	2.853167	-1.889490	0.510067
C	4.137022	-2.480105	0.512589
C	4.403831	-3.540799	1.393059
C	3.442084	-3.985970	2.291310
C	2.192937	-3.356207	2.325068
C	1.892567	-2.324313	1.437380
H	5.394470	-3.983572	1.366438
H	3.664812	-4.800961	2.973304
H	1.440864	-3.673244	3.041808
H	0.924039	-1.831983	1.483789
C	5.256678	-1.957528	-0.312903
H	5.083753	-0.979924	-0.789997
O	6.333597	-2.524647	-0.417864
N	2.537021	-0.844370	-0.415170
S	2.377948	-1.256399	-2.047738
O	2.201712	0.000523	-2.784760
O	3.483556	-2.161038	-2.399520
C	0.869072	-2.229124	-2.179199
H	0.033144	-1.593602	-1.891092
H	0.783689	-2.554034	-3.218567
H	0.959834	-3.092661	-1.518872

Vibrational frequencies

22.9194	29.1445	32.0270
39.7663	42.1703	45.4399
50.0456	54.1767	64.8605
65.7454	72.0886	76.3949
78.8303	87.9555	96.7324
101.4458	110.8959	130.0316
141.4089	149.3594	160.5365
165.9418	175.5064	184.3998

185.2045	193.2750	200.8359
207.6793	208.3922	213.9442
215.7006	242.1975	248.8435
256.0439	261.7565	273.0550
278.3129	286.9232	291.1280
297.6188	301.1600	324.6915
338.7833	350.2409	352.3449
366.7369	367.4614	389.8281
404.3356	415.5039	421.6703
443.7614	451.7226	465.0535
473.7386	481.3070	486.4930
491.9078	505.4282	508.0283
519.5327	528.7374	531.6698
534.7019	541.1195	565.4725
582.2280	588.9894	595.2939
600.2413	606.4275	628.7021
632.5715	633.9860	640.0892
646.6524	657.2636	688.1572
709.4234	711.6539	716.5369
725.8612	737.0085	741.4041
748.2915	753.4159	770.0474
774.5883	780.7270	789.7644
800.9428	810.7920	837.1975
840.1502	845.7216	868.5527
875.4655	881.4974	887.9027
889.5907	897.4559	905.1369
916.6167	924.7915	947.0602
953.3449	961.9814	963.5575
976.9962	978.6475	983.8009
986.8771	997.4863	1002.7215

1003.4445	1007.5908	1014.9203
1016.2082	1032.6158	1038.6655
1045.1388	1047.2218	1047.3600
1052.8728	1055.2418	1055.9019
1065.6425	1068.8358	1074.1082
1074.8157	1079.1507	1081.5994
1087.3362	1103.0685	1111.2682
1118.6316	1124.4802	1129.6885
1134.5318	1168.6091	1183.6386
1185.6905	1188.4875	1190.5962
1194.1381	1201.6413	1212.2908
1216.4044	1219.4672	1229.9633
1242.2708	1244.8560	1261.1583
1274.0752	1278.8555	1292.0861
1294.9598	1301.0106	1305.8618
1315.2815	1322.5482	1334.9559
1338.8148	1345.2758	1347.6358
1349.7826	1351.1734	1354.4248
1361.6568	1373.1798	1375.1075
1384.5471	1413.0213	1416.2148
1421.7880	1425.4694	1433.7838
1440.6426	1449.0868	1449.2858
1457.6698	1462.8860	1463.7028
1471.2082	1483.6703	1485.8291
1486.3960	1486.5241	1487.6446
1492.3468	1496.4011	1502.8721
1505.1747	1510.3817	1514.9607
1521.3230	1526.6084	1532.7503
1536.1861	1619.4462	1626.7453
1635.9542	1639.2819	1642.2298

1645.7038	1654.1069	1656.9824
1664.6778	1671.1623	1769.9514
3026.9348	3036.2502	3039.1078
3041.5362	3049.3100	3062.3019
3079.4328	3091.4736	3100.5826
3101.9753	3107.9337	3108.3787
3120.5129	3129.2558	3130.7274
3136.5192	3136.7214	3140.8503
3160.8331	3175.8756	3181.8594
3181.9106	3184.1276	3185.7884
3185.8628	3191.9712	3198.1372
3198.6657	3203.6509	3209.8957
3210.2626	3212.2013	3214.4508
3221.1248	3237.2255	3272.2784

M5S

Zero-point correction= 0.673754

Thermal correction to Energy= 0.715949

Thermal correction to Enthalpy= 0.716894

Thermal correction to Gibbs Free Energy= 0.597451

Sum of electronic and zero-point Energies= -2462.464594

Sum of electronic and thermal Energies= -2462.422399

Sum of electronic and thermal Enthalpies= -2462.421454

Sum of electronic and thermal Free Energies= -2462.540898

Cartesian coordinates

C	1.183653	-1.546493	-0.352501
C	0.004944	-0.750526	-0.797179
H	0.969367	-1.881233	0.666024
C	-0.693381	-0.052444	0.154080
O	-0.534471	0.002634	1.416951

C	1.498226	-2.770494	-1.193729
C	1.687351	-4.007922	-0.561356
C	1.612091	-2.709823	-2.591754
C	1.989169	-5.154832	-1.299200
H	1.596248	-4.071557	0.519825
C	1.917633	-3.854264	-3.330419
H	1.475110	-1.760697	-3.097008
C	2.108341	-5.081002	-2.688170
H	2.128686	-6.103663	-0.788436
H	2.003776	-3.788041	-4.411674
H	2.343302	-5.970436	-3.265956
C	-1.851963	0.773161	-0.357399
C	-3.825531	1.508782	-0.978870
C	-3.658895	-1.006534	-0.666313
H	-3.096464	-1.521209	-1.446772
N	-3.071237	2.574835	-0.930164
N	-1.840829	2.094577	-0.534675
N	-3.120448	0.383210	-0.618303
C	-5.262928	1.422675	-1.386210
H	-5.451601	2.117797	-2.207090
H	-5.910993	1.710163	-0.547469
C	-5.188034	-0.931015	-0.971539
O	-5.555285	0.115065	-1.862238
C	-4.897116	-1.684447	1.268012
C	-3.630797	-1.718181	0.667134
C	-2.564599	-2.387210	1.266415
C	-2.777249	-3.012931	2.496749
C	-4.035617	-2.970111	3.108053
C	-5.105993	-2.311750	2.495081
C	-5.887803	-0.939509	0.410376

H	-1.597256	-2.424832	0.780087
H	-4.185102	-3.463331	4.064501
H	-6.085791	-2.295934	2.964107
H	-6.036981	0.077620	0.791078
H	-6.870875	-1.415155	0.361579
C	-0.709084	2.977113	-0.404041
C	0.054938	3.254923	-1.547102
C	-0.427264	3.509365	0.860156
C	1.147117	4.110115	-1.389372
C	0.682078	4.352640	0.963362
C	1.480147	4.656877	-0.143941
H	1.765336	4.334826	-2.254618
H	0.940089	4.755702	1.937065
C	-1.260992	3.143403	2.058094
H	-1.158945	2.070862	2.256145
H	-2.322794	3.354094	1.883744
H	-0.939666	3.699186	2.941284
C	2.714455	5.509722	0.006948
H	2.653898	6.157603	0.886312
H	2.881425	6.137161	-0.874416
H	3.600274	4.873457	0.126252
C	-0.247496	2.607397	-2.872633
H	-1.317836	2.617095	-3.100677
H	0.094944	1.567245	-2.859517
H	0.279355	3.119291	-3.681882
H	-5.442595	-1.851980	-1.501298
H	-1.959021	-3.537819	2.980734
H	-0.220914	-0.638706	-1.849336
C	3.089329	-0.842646	1.169342
C	2.911807	0.107607	2.193397

C	3.544392	-0.096020	3.427384
C	4.325414	-1.225777	3.653739
C	4.486293	-2.172481	2.637495
C	3.873513	-1.978670	1.398797
H	3.401649	0.651253	4.201645
H	4.807130	-1.371378	4.616033
H	5.090960	-3.058717	2.806554
H	3.989760	-2.706091	0.602635
C	2.071652	1.323498	2.003225
H	1.581944	1.430776	1.028695
O	1.937451	2.162086	2.882070
N	2.423094	-0.682133	-0.089011
S	3.192991	0.216542	-1.260159
O	2.266586	0.391584	-2.389233
O	3.780275	1.396367	-0.605334
C	4.564466	-0.796341	-1.843111
H	4.159795	-1.711691	-2.277196
H	5.101317	-0.218148	-2.598604
H	5.220516	-1.018633	-1.000455

Vibrational frequencies

13.3364	22.1392	26.8305
31.3774	36.4245	42.7857
48.0749	48.5571	53.9946
56.4812	62.5909	70.4047
75.4683	79.5864	84.2327
91.4357	109.5175	118.3017
126.8579	141.2370	145.2010
163.0820	169.8992	181.9443
187.1990	193.3727	197.1335
210.1370	210.3977	227.4314

237.1834	243.7059	245.5564
254.2793	265.9724	271.7813
273.7089	284.3179	287.3769
291.6050	300.8840	310.4454
315.6440	318.7072	330.1985
359.6176	371.1042	382.3671
394.5442	412.3495	421.3160
426.4682	452.2686	457.0616
467.7497	473.2680	481.8740
492.6793	505.3182	513.1101
522.8270	527.3650	529.4271
533.4489	541.4153	566.8621
583.0893	586.0554	587.8740
601.5310	606.0119	611.7721
628.5403	632.7555	640.8431
643.2090	652.4923	681.0405
685.3933	697.8171	715.1301
720.4047	731.6344	741.0517
746.3349	748.7643	768.5294
772.3208	778.2096	792.8362
800.0761	807.7560	833.6038
840.2227	842.0395	859.3464
868.1444	882.6802	885.9317
894.4251	896.6523	901.7242
906.7251	933.7742	939.3259
948.3835	963.9865	964.4920
976.5035	978.7017	982.3516
988.1104	989.6602	1002.5981
1003.4701	1007.2234	1007.4849
1008.4549	1014.7926	1015.7228

1041.1219	1042.0397	1050.0950
1051.7164	1054.2860	1056.9715
1061.9397	1069.1325	1071.1155
1075.7251	1077.7409	1080.0517
1088.0658	1102.7255	1108.8669
1117.9087	1125.4388	1131.4226
1133.4209	1164.7396	1182.9748
1187.4575	1188.7348	1190.1023
1192.0368	1200.9262	1216.3502
1217.4548	1220.5997	1222.1618
1230.7625	1249.5074	1251.6452
1272.2353	1282.6801	1289.5577
1293.6607	1297.0333	1298.3359
1305.1099	1320.6174	1337.5468
1339.3221	1346.8258	1347.0900
1348.0763	1352.8078	1360.3683
1366.6887	1371.1630	1378.9981
1402.5086	1413.9162	1416.2838
1419.7087	1423.3940	1428.8958
1434.8250	1451.6285	1454.9147
1460.5381	1467.1197	1467.9300
1475.4941	1482.3137	1482.5498
1486.0186	1486.6855	1494.9679
1495.7151	1496.3939	1499.7377
1502.8561	1511.9633	1519.3187
1520.0640	1524.1899	1537.3205
1538.6234	1619.3706	1625.4993
1634.6495	1639.3482	1642.9431
1644.6395	1654.6127	1656.2714
1660.8386	1662.6356	1766.3923

3036.0299	3037.7053	3040.0381
3049.5906	3059.8159	3073.5066
3075.3099	3097.7588	3101.5055
3101.9524	3107.2615	3118.9287
3119.3206	3126.1869	3127.9814
3134.6119	3134.8478	3142.7677
3177.2773	3177.4122	3182.4079
3183.3816	3184.3899	3190.3631
3190.8429	3193.2426	3195.8254
3201.6950	3202.6033	3205.7838
3206.9924	3210.7317	3218.0259
3223.7928	3228.1135	3232.1251

TS5R(M06-2X)

Zero-point correction= 0.677835

Thermal correction to Energy= 0.718839

Thermal correction to Enthalpy= 0.719783

Thermal correction to Gibbs Free Energy= 0.603706

Sum of electronic and zero-point Energies= -2461.461338

Sum of electronic and thermal Energies= -2461.420334

Sum of electronic and thermal Enthalpies= -2461.419390

Sum of electronic and thermal Free Energies= -2461.535467

Cartesian coordinates

C	-2.186800	-0.479396	-0.942728
C	-1.228563	0.371817	-0.407203
H	-1.872171	-1.152732	-1.735734
C	0.136749	0.125478	-0.674381
O	0.635417	-0.737770	-1.408417
C	-3.626378	-0.157143	-0.912182
C	-4.458370	-0.675967	-1.911150

C	-4.184284	0.655682	0.083999
C	-5.818929	-0.376882	-1.923512
H	-4.030292	-1.329824	-2.665036
C	-5.542887	0.946302	0.074899
H	-3.555139	1.053627	0.875842
C	-6.363883	0.433540	-0.930686
H	-6.453434	-0.780564	-2.706518
H	-5.965725	1.573727	0.853555
H	-7.424730	0.664307	-0.936499
C	1.139462	1.011201	0.041798
C	2.980133	1.699334	0.987019
C	3.132249	-0.611621	0.123272
H	2.406286	-1.421080	0.038132
N	2.174304	2.720178	1.042389
N	1.033872	2.280209	0.441509
N	2.383961	0.632227	0.376913
C	4.333449	1.484906	1.578861
H	4.530402	2.234324	2.345869
H	5.113292	1.546106	0.807743
C	4.155509	-0.875146	1.292132
O	4.284248	0.213393	2.196752
C	5.314729	-0.811787	-0.839448
C	3.991308	-0.475673	-1.114938
C	3.592983	-0.073006	-2.386659
C	4.556579	-0.001959	-3.389569
C	5.887068	-0.334343	-3.120118
C	6.274515	-0.744337	-1.846506
C	5.491062	-1.224200	0.597907
H	2.552183	0.163159	-2.587260
H	6.626558	-0.271792	-3.912699

H	7.309268	-1.001900	-1.639736
H	6.318512	-0.709043	1.096077
H	5.684607	-2.298833	0.673817
C	-0.061022	3.202661	0.271580
C	-0.844545	3.496512	1.393324
C	-0.266358	3.772432	-0.984734
C	-1.883830	4.405106	1.219804
C	-1.323138	4.677012	-1.103524
C	-2.136638	5.003416	-0.019387
H	-2.512350	4.652691	2.071929
H	-1.505905	5.139898	-2.069760
C	0.591747	3.418645	-2.168453
H	0.335359	2.423952	-2.551058
H	1.655712	3.419085	-1.912597
H	0.433893	4.134980	-2.976578
C	-3.278425	5.972301	-0.169968
H	-4.237962	5.457309	-0.057246
H	-3.265002	6.453025	-1.150285
H	-3.234110	6.750417	0.597606
C	-0.596634	2.815084	2.711136
H	0.422518	2.989741	3.068888
H	-0.729970	1.730515	2.615507
H	-1.296209	3.179651	3.465145
H	3.794746	-1.695575	1.912204
H	4.270999	0.309054	-4.389417
H	-1.502458	1.163268	0.277565
C	-1.203633	-2.103375	1.294695
C	0.072057	-2.690009	1.126329
C	1.044700	-2.556288	2.123452
C	0.819194	-1.784166	3.254067

C	-0.411947	-1.136049	3.392254
C	-1.403830	-1.298205	2.432796
H	1.995132	-3.059749	1.966874
H	1.587129	-1.678428	4.013844
H	-0.606085	-0.514278	4.261970
H	-2.374604	-0.824432	2.550130
C	0.474188	-3.345910	-0.144726
H	-0.220361	-3.248032	-0.993095
O	1.550173	-3.895890	-0.287329
N	-2.237057	-2.155980	0.370810
S	-2.722492	-3.537760	-0.304686
O	-2.747947	-3.398243	-1.771131
O	-2.021399	-4.713347	0.237269
C	-4.422441	-3.653334	0.216793
H	-4.946130	-2.758455	-0.124809
H	-4.858916	-4.548521	-0.230540
H	-4.445543	-3.718828	1.305204

Vibrational frequencies

-226.4410	-26.6469	20.0137
26.3060	30.1426	34.0159
42.3265	47.5153	49.6078
51.6109	56.0926	63.1974
67.5222	78.3031	80.6986
90.7456	92.2798	94.4255
108.4059	119.2552	128.8564
137.0673	137.9877	146.9396
159.5746	185.2456	194.7206
205.9629	209.7762	220.4947
231.0067	236.6188	243.3350
250.6504	258.8116	262.7975

265.0933	279.7514	284.5466
287.3837	301.1196	308.8926
326.2545	327.3397	337.8780
349.7023	363.2885	396.7334
397.5185	402.0649	411.0203
414.4988	445.1515	451.1685
458.5311	480.0869	494.4217
497.6935	504.9303	505.6113
515.4983	525.3213	533.0126
535.2210	543.2184	545.5437
547.4165	582.2043	586.1522
589.8530	600.7688	608.6049
616.0376	622.8561	629.9716
640.8671	644.8991	691.7650
706.4926	712.5182	723.0524
726.0662	746.8330	754.2668
758.4810	768.0697	775.5127
790.1947	796.3167	801.8785
805.2293	814.0891	817.7788
838.0713	846.0490	863.0747
866.4672	876.5629	889.3114
895.7785	910.2197	914.5117
924.5886	929.6865	947.9318
956.0319	964.1205	980.6697
982.4897	984.9426	989.2612
996.4392	997.5591	999.9248
1013.5477	1017.3202	1018.9956
1025.8151	1031.0034	1037.5750
1038.1868	1039.3932	1053.1967
1054.0042	1056.7662	1060.3455

1062.0408	1065.3541	1066.9258
1069.1254	1069.9104	1072.0845
1078.1545	1115.9898	1119.4988
1122.5033	1137.8912	1139.3714
1144.2969	1167.5759	1174.0628
1174.8711	1178.1182	1196.5247
1203.2928	1206.1653	1209.4392
1219.5683	1227.5338	1234.1144
1245.2964	1257.8502	1275.5362
1280.5323	1281.5955	1288.2556
1298.2347	1300.9935	1309.8121
1314.2696	1323.3603	1332.4821
1336.8639	1340.2412	1346.7634
1357.9896	1362.7932	1367.8917
1368.5156	1371.6705	1386.9151
1386.9916	1410.4465	1417.6143
1421.6561	1429.5611	1450.3859
1455.4656	1457.7664	1459.3284
1461.1672	1471.7947	1475.5567
1480.2770	1485.3090	1488.8224
1492.7480	1493.2837	1496.3829
1499.4954	1516.7858	1518.1509
1520.1725	1527.3036	1536.6626
1539.9429	1547.6624	1578.5529
1591.5240	1643.8046	1674.8782
1680.4486	1680.9562	1681.1387
1687.4752	1693.8847	1696.9532
1700.4187	1715.6002	1822.3306
3064.5473	3069.8802	3070.9172
3085.2150	3088.7824	3090.4766

3102.0224	3134.9782	3139.6951
3142.8073	3143.4199	3162.5979
3164.0738	3172.9888	3177.7427
3179.4604	3189.2587	3195.4079
3198.2141	3203.7620	3206.3772
3206.5793	3210.2065	3210.8861
3211.4838	3212.2301	3215.0859
3220.3379	3221.0721	3223.9368
3224.3316	3229.8235	3231.9417
3236.2839	3239.8083	3258.9212

TS5R(ωB97X-D)

Zero-point correction= 0.679596

Thermal correction to Energy= 0.721356

Thermal correction to Enthalpy= 0.722300

Thermal correction to Gibbs Free Energy= 0.602925

Sum of electronic and zero-point Energies= -2461.689554

Sum of electronic and thermal Energies= -2461.647794

Sum of electronic and thermal Enthalpies= -2461.646850

Sum of electronic and thermal Free Energies= -2461.766225

Cartesian coordinates

C	-2.139519	-0.483323	-0.980563
C	-1.155996	0.342339	-0.441434
H	-1.857080	-1.126881	-1.807051
C	0.204475	0.143635	-0.732957
O	0.722051	-0.668431	-1.515206
C	-3.566155	-0.100636	-0.926822
C	-4.438833	-0.589040	-1.905274
C	-4.071316	0.756143	0.060542
C	-5.782293	-0.223378	-1.904584

H	-4.058901	-1.274447	-2.656051
C	-5.412096	1.118599	0.062208
H	-3.418337	1.140156	0.838218
C	-6.272497	0.632092	-0.921978
H	-6.446539	-0.608756	-2.671933
H	-5.788381	1.783242	0.833958
H	-7.320199	0.916617	-0.919221
C	1.177178	1.023913	0.034248
C	2.968641	1.713027	1.070054
C	3.202520	-0.550309	0.100224
H	2.494513	-1.368045	-0.024770
N	2.135881	2.709717	1.150767
N	1.025891	2.268625	0.491701
N	2.423532	0.664387	0.385742
C	4.301175	1.505232	1.704360
H	4.443562	2.213523	2.520417
H	5.109889	1.640668	0.974611
C	4.209233	-0.837283	1.278469
O	4.272143	0.200130	2.246683
C	5.407009	-0.667334	-0.827075
C	4.079676	-0.366424	-1.117785
C	3.691066	0.041670	-2.389872
C	4.666616	0.161654	-3.375117
C	6.002018	-0.131128	-3.088442
C	6.380190	-0.551501	-1.815881
C	5.573044	-1.106282	0.601808
H	2.646051	0.240569	-2.602538
H	6.752713	-0.033677	-3.866812
H	7.418990	-0.781030	-1.597978
H	6.370025	-0.570698	1.126813

H	5.812791	-2.172824	0.656113
C	-0.110325	3.136511	0.344813
C	-0.975888	3.272765	1.434264
C	-0.319077	3.754211	-0.888078
C	-2.116235	4.047385	1.245159
C	-1.474608	4.522817	-1.023051
C	-2.387580	4.665641	0.021405
H	-2.818124	4.159081	2.067231
H	-1.668925	5.011171	-1.974161
C	0.636065	3.568117	-2.034986
H	0.502169	2.583496	-2.497259
H	1.678373	3.648165	-1.711917
H	0.459368	4.321573	-2.805215
C	-3.666011	5.434873	-0.173080
H	-4.478484	4.750695	-0.443206
H	-3.573412	6.172479	-0.974260
H	-3.963402	5.953205	0.742619
C	-0.707496	2.559697	2.730207
H	0.220135	2.908634	3.194278
H	-0.604080	1.481364	2.566462
H	-1.524976	2.719168	3.436054
H	3.866216	-1.703351	1.842525
H	4.386696	0.478061	-4.375034
H	-1.425933	1.097417	0.280163
C	-1.195195	-2.119752	1.232175
C	0.091721	-2.681527	1.073451
C	1.047455	-2.542765	2.085454
C	0.787494	-1.798151	3.225160
C	-0.461544	-1.188441	3.362272
C	-1.434955	-1.352573	2.385216

H	2.011555	-3.019622	1.935647
H	1.545264	-1.685387	3.993787
H	-0.682055	-0.591625	4.242759
H	-2.413806	-0.896378	2.497698
C	0.513328	-3.331120	-0.190703
H	-0.180197	-3.245657	-1.040186
O	1.594057	-3.876860	-0.328922
N	-2.200607	-2.160915	0.272342
S	-2.736430	-3.543994	-0.364446
O	-2.769421	-3.435269	-1.831597
O	-2.066761	-4.723780	0.203958
C	-4.437200	-3.601942	0.172379
H	-4.947891	-2.710649	-0.195699
H	-4.900565	-4.501425	-0.238065
H	-4.458084	-3.628412	1.262832

Vibrational frequencies

-276.7630	12.1188	17.8124
26.0921	28.3850	35.0116
39.8988	42.4991	48.0697
53.2461	58.3985	61.8126
69.0674	76.1756	88.0817
89.8919	93.8804	107.8108
114.6702	135.7156	137.8656
143.3031	146.0487	151.6303
162.8295	187.4957	196.0766
200.8625	206.5312	222.5904
223.2317	233.1128	241.8333
250.3912	254.1751	265.5738
275.1397	286.9023	287.8614
288.6897	292.0833	300.4007

310.3147	328.3798	330.2374
344.2259	365.1410	397.3671
399.3982	403.3689	410.3148
418.0300	447.0869	457.2338
461.4348	482.1748	489.4807
498.8532	503.3372	509.1341
520.6434	529.3137	535.6583
538.8635	545.8642	546.7405
550.0139	585.6190	588.2484
591.9572	607.0498	614.6881
618.4212	626.6810	636.4444
646.4857	647.3486	694.5973
709.1538	713.1008	724.2770
728.7755	746.7969	757.1482
762.7790	768.8237	778.0943
782.5016	795.8957	803.8579
808.4298	813.0218	818.8477
840.1638	848.3100	863.1902
873.4371	883.3655	890.7739
893.2231	914.6784	919.6136
926.1044	930.8476	950.4014
959.0756	967.3720	982.2178
984.2941	988.0011	1002.5861
1002.9034	1004.0453	1006.3444
1009.3255	1013.7995	1022.8485
1026.3780	1029.1890	1031.2567
1041.9931	1049.2385	1052.9778
1055.7339	1058.4449	1066.9263
1067.9488	1070.1560	1073.2749
1075.2555	1077.7584	1080.1468

1082.0272	1119.2545	1123.5007
1131.6667	1133.4065	1137.2358
1143.2206	1178.2493	1185.0411
1186.2464	1192.1922	1202.7522
1208.6108	1214.3179	1219.2084
1226.2830	1229.6904	1245.1779
1248.4665	1261.6705	1286.2135
1289.7756	1292.7383	1295.2740
1302.6604	1304.9658	1318.7818
1321.1874	1330.9780	1337.5950
1341.7573	1347.7463	1351.1425
1363.6777	1368.2395	1373.1703
1377.3657	1386.5647	1396.8119
1397.4808	1423.9022	1424.8229
1426.7968	1435.6570	1439.8626
1461.4907	1463.4346	1466.2132
1467.0089	1477.2845	1484.9973
1490.6685	1493.0769	1497.1036
1498.7500	1500.7576	1503.1453
1504.0878	1517.5434	1518.5582
1519.5273	1531.1954	1536.5245
1545.2039	1553.2252	1574.6251
1596.2826	1643.3925	1667.0951
1672.1649	1677.8150	1680.0105
1682.0872	1688.4870	1691.0296
1696.8221	1710.5184	1804.6125
3062.2925	3065.1900	3069.2008
3069.6587	3074.3872	3090.7451
3097.4231	3138.2187	3140.2429
3142.8205	3144.5539	3167.0005

3168.9515	3169.5234	3175.7854
3188.0524	3191.4874	3206.8800
3208.1363	3211.3569	3212.2098
3215.3941	3216.7227	3217.8778
3218.5818	3221.8144	3224.2169
3224.7059	3227.6609	3234.0330
3234.3733	3235.4368	3241.1083
3245.1405	3245.7644	3314.6562

TS5S(M06-2X)

Zero-point correction= 0.678231

Thermal correction to Energy= 0.719081

Thermal correction to Enthalpy= 0.720025

Thermal correction to Gibbs Free Energy= 0.605032

Sum of electronic and zero-point Energies= -2461.450594

Sum of electronic and thermal Energies= -2461.409744

Sum of electronic and thermal Enthalpies= -2461.408800

Sum of electronic and thermal Free Energies= -2461.523793

Cartesian coordinates

C	1.081309	-1.515171	-0.260732
C	-0.058368	-0.858755	-0.734402
H	1.169689	-1.533140	0.823604
C	-0.799823	-0.097046	0.192158
O	-0.598142	0.069310	1.398936
C	1.715444	-2.653344	-0.946140
C	2.507281	-3.527729	-0.191212
C	1.527813	-2.916244	-2.309174
C	3.108902	-4.632221	-0.784461
H	2.643347	-3.335471	0.869360
C	2.128748	-4.019543	-2.901942

H	0.904662	-2.262118	-2.912356
C	2.923901	-4.878144	-2.142919
H	3.718661	-5.301985	-0.186059
H	1.976091	-4.213853	-3.959107
H	3.391419	-5.739793	-2.609524
C	-2.014668	0.634234	-0.363103
C	-3.954099	1.252220	-1.131304
C	-3.694464	-1.241825	-0.756580
H	-3.087831	-1.760584	-1.501328
N	-3.265859	2.353019	-1.019867
N	-2.062848	1.948005	-0.530739
N	-3.218746	0.167107	-0.725449
C	-5.354272	1.090493	-1.632656
H	-5.506292	1.743727	-2.493686
H	-6.064192	1.384154	-0.850089
C	-5.206193	-1.223101	-1.114974
O	-5.551476	-0.237944	-2.065326
C	-4.975744	-1.846882	1.163126
C	-3.693253	-1.890055	0.607448
C	-2.638365	-2.509039	1.271264
C	-2.879830	-3.065986	2.525610
C	-4.154090	-3.009891	3.092462
C	-5.212661	-2.407543	2.413534
C	-5.951945	-1.172457	0.234842
H	-1.652571	-2.568454	0.819644
H	-4.324791	-3.452787	4.068953
H	-6.206865	-2.384051	2.850071
H	-6.141609	-0.142562	0.557335
H	-6.916925	-1.680868	0.177532
C	-0.966204	2.867119	-0.356241

C	-0.185368	3.150999	-1.483006
C	-0.733013	3.408726	0.906722
C	0.893943	4.010244	-1.304370
C	0.364073	4.264108	1.030407
C	1.186745	4.566447	-0.053259
H	1.523395	4.250539	-2.158192
H	0.584112	4.685839	2.006791
C	-1.598086	3.062398	2.084635
H	-1.392216	2.034850	2.397740
H	-2.661047	3.144915	1.834875
H	-1.383615	3.729127	2.921262
C	2.388714	5.456956	0.111057
H	2.364836	5.983724	1.067335
H	2.443363	6.196896	-0.692411
H	3.308968	4.864315	0.073999
C	-0.508736	2.539961	-2.819543
H	-1.511989	2.825434	-3.152623
H	-0.474924	1.445100	-2.766022
H	0.209171	2.866593	-3.574391
H	-5.417972	-2.178953	-1.599386
H	-2.071705	-3.553961	3.060541
H	-0.381437	-0.902231	-1.769010
C	3.320785	-0.309750	1.084073
C	2.793319	0.327119	2.230241
C	3.334060	0.068243	3.494163
C	4.409366	-0.793808	3.645652
C	4.960675	-1.397551	2.510890
C	4.425048	-1.169607	1.250484
H	2.897694	0.580265	4.347064
H	4.828001	-0.986770	4.628103

H	5.812072	-2.064728	2.612941
H	4.839746	-1.662866	0.376466
C	1.744516	1.369222	2.103025
H	1.453088	1.628689	1.071924
O	1.270209	1.954247	3.058224
N	2.668928	-0.116868	-0.140046
S	3.633773	0.087916	-1.436304
O	4.586594	1.183591	-1.191104
O	4.223409	-1.149812	-1.974792
C	2.438585	0.666862	-2.617135
H	1.974575	1.567356	-2.214476
H	2.977921	0.887116	-3.540569
H	1.695417	-0.112051	-2.792089

Vibrational frequencies

-225.9862	-51.5549	23.2053
25.9947	35.4358	40.8961
42.2115	49.1674	54.2401
56.0174	57.9115	58.7005
69.9880	77.1475	79.7702
82.6820	94.6504	114.8644
117.3647	127.4837	140.0443
145.2167	152.0961	171.4223
184.8050	186.8001	192.1692
200.1064	208.6058	211.3646
216.6006	235.1220	236.3625
245.5053	252.7801	257.3961
265.7280	275.7075	282.7440
285.1271	300.7260	304.6991
310.9507	326.0493	332.9904
343.4212	351.2516	377.0559

401.3388	417.2149	419.9173
443.9505	456.1714	458.8371
467.8122	469.8101	484.8169
496.4010	500.2624	506.4189
516.3973	520.9550	523.4072
531.8169	537.0155	545.3784
573.7440	586.5429	590.3342
591.3950	593.7789	606.8059
622.8248	624.2952	629.5278
630.6543	653.5340	661.7650
701.9587	716.5950	718.4704
726.9768	742.2072	747.2258
753.2436	768.6415	786.3455
787.3925	789.0493	803.1886
810.4900	812.9746	814.1068
847.1262	850.3132	852.0523
872.9750	876.9899	888.5795
900.7393	913.9400	916.5721
918.2722	922.0392	943.9568
954.0724	964.8381	979.0262
982.4907	989.5367	996.3175
998.9148	999.3583	1007.1304
1015.7221	1016.6828	1021.6767
1027.7163	1036.3417	1036.8709
1040.7176	1044.2125	1051.5817
1059.6689	1062.5210	1065.9681
1067.3983	1068.8118	1070.5206
1075.0123	1077.1601	1101.8206
1115.0045	1119.5589	1123.1591
1128.4893	1140.2384	1146.1365

1158.9945	1169.5714	1171.9139
1179.4955	1181.0212	1188.7772
1201.8766	1207.8371	1211.4321
1223.1958	1233.5832	1236.3728
1252.0862	1253.9390	1270.9635
1283.6037	1284.7532	1286.9089
1288.8244	1302.2352	1308.5710
1325.5723	1327.4911	1338.2914
1342.8917	1346.3016	1348.0021
1356.5442	1364.1254	1365.2511
1371.2435	1376.9405	1386.3225
1391.9406	1411.1258	1413.2850
1424.7389	1425.0725	1426.9071
1441.7205	1450.6044	1457.6592
1461.7374	1475.1645	1477.1935
1486.3083	1486.7708	1488.8449
1492.4376	1497.7895	1499.5908
1502.2700	1518.5153	1519.3068
1521.7665	1527.3862	1535.5989
1538.1950	1546.5390	1569.2878
1614.7728	1648.4964	1668.7280
1674.7455	1681.0607	1682.2664
1686.3025	1694.7949	1697.3613
1700.6781	1721.1170	1819.5361
3062.5750	3068.5877	3071.1966
3086.6097	3086.9552	3098.6522
3100.3404	3130.5946	3142.3195
3143.7172	3147.8731	3152.2044
3157.3821	3163.1407	3168.0552
3174.3031	3174.9187	3199.3298

3200.1236	3204.1925	3204.3698
3205.2054	3208.1531	3208.6991
3211.3839	3211.7813	3218.1647
3219.7521	3220.0323	3221.0533
3222.4434	3227.9364	3228.8467
3232.4690	3236.8649	3245.5222

TS5S(ωB97X-D)

Zero-point correction= 0.680573

Thermal correction to Energy= 0.721916

Thermal correction to Enthalpy= 0.722860

Thermal correction to Gibbs Free Energy= 0.606595

Sum of electronic and zero-point Energies= -2461.678430

Sum of electronic and thermal Energies= -2461.637088

Sum of electronic and thermal Enthalpies= -2461.636143

Sum of electronic and thermal Free Energies= -2461.752408

Cartesian coordinates

C	1.077040	-1.470943	-0.314956
C	-0.051759	-0.765607	-0.752887
H	1.152919	-1.552359	0.765366
C	-0.796779	-0.055221	0.201061
O	-0.613990	0.045323	1.421926
C	1.658131	-2.610166	-1.046380
C	2.365490	-3.576463	-0.321016
C	1.490764	-2.792110	-2.424570
C	2.905564	-4.688760	-0.956711
H	2.490621	-3.448968	0.749753
C	2.027307	-3.904086	-3.059792
H	0.937882	-2.063541	-3.009222
C	2.739198	-4.854177	-2.328857

H	3.452616	-5.427818	-0.379767
H	1.890575	-4.032485	-4.128991
H	3.159024	-5.722337	-2.827435
C	-2.015738	0.688080	-0.319412
C	-3.986602	1.306007	-1.003219
C	-3.680200	-1.192794	-0.763924
H	-3.094453	-1.651782	-1.561421
N	-3.310418	2.412136	-0.879222
N	-2.083045	2.005293	-0.444382
N	-3.225434	0.217749	-0.660731
C	-5.398612	1.147593	-1.466578
H	-5.587354	1.839566	-2.288721
H	-6.087793	1.398702	-0.650697
C	-5.203160	-1.183212	-1.071425
O	-5.600359	-0.158403	-1.955096
C	-4.885099	-1.950215	1.149520
C	-3.623938	-1.936138	0.547450
C	-2.541933	-2.589843	1.126556
C	-2.729901	-3.233756	2.346840
C	-3.981773	-3.231370	2.962850
C	-5.070191	-2.598621	2.364759
C	-5.901592	-1.229936	0.304838
H	-1.574099	-2.604842	0.636942
H	-4.112594	-3.738906	3.913598
H	-6.047226	-2.619087	2.837757
H	-6.088268	-0.226929	0.703693
H	-6.863416	-1.743888	0.248453
C	-0.994165	2.931543	-0.286333
C	-0.244950	3.243087	-1.426575
C	-0.727849	3.451835	0.979061

C	0.830486	4.108844	-1.261507
C	0.366182	4.311352	1.089992
C	1.155071	4.642277	-0.009618
H	1.435383	4.369086	-2.126397
H	0.609405	4.719013	2.066240
C	-1.555455	3.073873	2.173550
H	-1.353690	2.032622	2.440556
H	-2.625670	3.174619	1.965056
H	-1.308781	3.706331	3.027966
C	2.352305	5.542432	0.135697
H	2.372616	6.028185	1.114024
H	2.357597	6.318466	-0.635542
H	3.278441	4.967741	0.026560
C	-0.584775	2.648424	-2.766144
H	-1.607569	2.898298	-3.065950
H	-0.504094	1.555794	-2.739195
H	0.096703	3.017254	-3.535213
H	-5.412867	-2.114571	-1.601355
H	-1.896247	-3.744083	2.818054
H	-0.367179	-0.749524	-1.790194
C	3.337679	-0.413109	1.066252
C	2.867416	0.202549	2.247408
C	3.414115	-0.147275	3.487041
C	4.436138	-1.078455	3.578822
C	4.929253	-1.663321	2.409586
C	4.386613	-1.345033	1.172682
H	3.024691	0.346164	4.372424
H	4.857250	-1.341481	4.543837
H	5.736493	-2.388161	2.464961
H	4.756021	-1.822243	0.271437

C	1.868192	1.295061	2.188796
H	1.550656	1.592708	1.177100
O	1.455377	1.874833	3.177545
N	2.676828	-0.136173	-0.140580
S	3.630292	0.180574	-1.426032
O	4.575441	1.259832	-1.098345
O	4.221986	-1.005773	-2.066660
C	2.428340	0.847155	-2.554294
H	1.970648	1.720640	-2.091834
H	2.961440	1.130441	-3.463900
H	1.677615	0.091624	-2.783364

Vibrational frequencies

-275.7540	24.7147	27.1250
28.2626	35.9119	40.1446
43.3769	50.6949	54.6787
58.3527	69.9075	73.9319
79.2417	80.5987	91.6296
103.6953	108.9679	112.3377
120.2356	132.0250	136.5798
137.7521	155.0705	161.2926
164.4118	187.4009	198.9139
207.6199	209.4887	221.9442
234.3742	236.0273	246.0519
252.0255	258.5401	263.6808
279.4048	282.3880	287.4219
289.3746	300.8982	310.4851
313.7733	318.3983	328.1467
348.0930	364.9344	374.1212
394.2620	415.7575	428.0164
442.6471	455.8557	460.0210

468.5554	471.5995	486.1720
499.7119	506.1413	512.4992
518.5661	523.7101	531.1659
535.3226	540.6703	550.9241
574.5989	587.7831	593.6609
596.4883	600.8099	610.0045
627.5460	630.7595	633.5301
637.7452	657.5117	663.0801
700.8712	715.1226	721.5801
730.5216	744.7179	750.9649
754.9805	768.3942	784.7312
788.7268	791.7713	803.2585
809.3003	812.2885	814.1718
850.8413	853.1121	853.2795
876.1430	882.8744	892.9326
901.1108	912.6332	915.8785
918.1036	919.7688	946.4676
966.0848	968.6314	976.6614
985.0956	993.9900	995.9633
1013.0569	1015.7834	1018.1292
1022.8856	1024.0721	1024.8291
1032.9628	1039.2447	1044.6607
1047.4444	1051.0744	1060.1901
1064.0368	1065.2012	1069.0525
1070.4700	1072.2777	1075.1075
1076.8142	1083.5030	1099.5801
1119.5164	1125.3575	1127.3425
1128.0484	1135.2587	1144.5066
1167.5830	1174.5329	1185.1545
1190.7363	1193.6513	1193.9409

1206.4968	1210.6927	1218.8527
1224.3102	1239.1918	1241.9981
1255.3165	1257.0454	1273.1274
1283.7783	1286.7881	1292.9809
1293.1548	1303.7228	1310.9799
1330.5037	1334.1057	1341.1847
1344.4179	1349.2090	1355.3834
1363.2599	1367.9547	1380.0237
1380.8281	1387.2883	1399.7524
1401.8457	1421.1684	1423.3087
1424.7530	1430.6771	1433.3171
1454.0154	1462.8005	1472.1296
1476.6761	1481.5444	1486.4486
1488.4186	1490.0480	1496.6984
1497.4899	1499.8299	1501.0141
1503.1786	1516.2006	1519.0585
1522.6658	1525.1848	1537.5361
1539.5831	1549.5112	1571.8254
1608.1283	1645.2737	1658.1011
1670.0066	1674.4497	1678.5984
1680.4897	1688.4920	1691.3006
1697.8307	1708.6926	1809.2850
3065.0020	3072.6001	3073.7610
3078.3476	3079.1176	3093.6147
3110.8293	3136.6339	3145.3653
3145.9945	3154.5900	3157.5243
3162.0432	3170.4910	3170.5134
3172.5021	3179.7061	3206.0166
3209.7468	3216.2086	3217.3107
3217.9924	3221.2131	3223.7973

3227.9990	3231.1835	3231.8701
3232.0912	3234.0005	3238.4955
3241.1536	3242.1396	3244.4485
3247.1663	3249.0907	3250.0757

TS6R

Zero-point correction= 0.674799

Thermal correction to Energy= 0.715534

Thermal correction to Enthalpy= 0.716478

Thermal correction to Gibbs Free Energy= 0.600962

Sum of electronic and zero-point Energies= -2462.457288

Sum of electronic and thermal Energies= -2462.416553

Sum of electronic and thermal Enthalpies= -2462.415608

Sum of electronic and thermal Free Energies= -2462.531124

Cartesian coordinates

C	-1.731099	-1.006133	-0.926957
C	-0.654499	-0.388484	-0.047922
H	-1.229293	-1.549300	-1.728043
C	0.595012	-0.117249	-0.713643
O	1.028126	-0.617935	-1.756118
C	-2.605221	0.083130	-1.532809
C	-2.356927	0.526128	-2.837667
C	-3.621074	0.698520	-0.787044
C	-3.104624	1.570867	-3.387027
H	-1.571278	0.053211	-3.420678
C	-4.373916	1.734703	-1.338445
H	-3.820537	0.364958	0.226702
C	-4.116588	2.177192	-2.639739
H	-2.900727	1.903776	-4.400912
H	-5.157948	2.202670	-0.750187

H	-4.702340	2.985783	-3.067567
C	1.563537	0.747624	0.062935
C	3.387184	1.499788	1.003570
C	3.515398	-0.865747	0.264500
H	2.731333	-1.620231	0.197124
N	2.532075	2.486335	1.102742
N	1.393009	1.997790	0.499200
N	2.832746	0.427303	0.357574
C	4.724399	1.284760	1.629862
H	4.942516	2.075256	2.348839
H	5.517314	1.260553	0.870938
C	4.378843	-1.118826	1.560282
O	4.619806	0.055466	2.348660
C	5.738694	-1.413903	-0.431816
C	4.508439	-0.921242	-0.874783
C	4.302652	-0.561359	-2.205692
C	5.365869	-0.695430	-3.101738
C	6.603117	-1.187100	-2.666091
C	6.796407	-1.553478	-1.331053
C	5.693798	-1.749640	1.038391
H	3.333059	-0.196120	-2.528032
H	7.421478	-1.284370	-3.373897
H	7.757931	-1.933693	-0.997222
H	6.548957	-1.364797	1.602341
H	5.671548	-2.835748	1.187393
C	0.173380	2.764245	0.482888
C	-0.594996	2.769880	1.657756
C	-0.215655	3.401751	-0.702104
C	-1.816444	3.447514	1.609558
C	-1.445036	4.064608	-0.691928

C	-2.256387	4.094691	0.448524
H	-2.444330	3.455272	2.496439
H	-1.783429	4.552773	-1.601313
C	0.630779	3.339423	-1.947530
H	0.573398	2.348348	-2.412769
H	1.684633	3.539966	-1.728991
H	0.287660	4.069662	-2.684020
C	-3.576358	4.822943	0.423976
H	-4.264521	4.432013	1.179083
H	-4.055810	4.739669	-0.555637
H	-3.434892	5.891417	0.629419
C	-0.134790	2.040787	2.894005
H	0.726558	2.547083	3.345434
H	0.178674	1.011891	2.668385
H	-0.934434	2.004840	3.637673
H	3.829101	-1.779733	2.229613
H	5.231891	-0.418587	-4.143365
H	-1.011147	0.443550	0.551709
C	-2.634819	-1.922935	1.261362
C	-1.454180	-1.674617	1.981202
C	-1.521680	-1.501432	3.364009
C	-2.738184	-1.614286	4.038092
C	-3.906463	-1.878303	3.317656
C	-3.861357	-2.013255	1.929107
H	-0.592207	-1.292515	3.883924
H	-2.778063	-1.497266	5.117560
H	-4.859664	-1.964116	3.831514
H	-4.774229	-2.193433	1.373030
C	-0.125470	-1.540858	1.257790
H	0.024200	-2.426930	0.596001

O	0.892569	-1.107861	1.931587
N	-2.523779	-2.010375	-0.159003
S	-3.231241	-3.269695	-1.021686
O	-2.369084	-3.548022	-2.180283
O	-3.549031	-4.338350	-0.068023
C	-4.774076	-2.609511	-1.669280
H	-4.547276	-1.750207	-2.301065
H	-5.241668	-3.403939	-2.255654
H	-5.420040	-2.318944	-0.840140

Vibrational frequencies

-212.9185	18.7786	23.8984
26.5818	33.8182	39.1035
39.5199	48.5598	50.3094
52.7919	68.7850	71.7569
77.4874	81.8925	86.8249
108.7031	115.1771	119.9748
127.8765	138.2937	139.6347
147.6893	167.0652	171.1087
187.0461	200.5802	205.0455
214.0225	223.0976	230.9357
234.5514	238.7061	244.2070
257.7165	261.7990	279.9499
288.5974	294.4450	299.3644
302.4110	315.2034	330.2017
336.0832	348.0096	362.4603
385.7331	388.7604	399.5996
405.9520	413.8755	423.2217
445.3618	448.6128	470.9700
483.5301	489.7679	493.9520
500.5746	513.6536	519.8693

525.0805	526.6851	529.4365
531.8431	563.3226	581.5616
585.8593	595.2854	600.2996
608.5384	612.8490	615.0072
632.3752	637.1180	648.8334
660.5525	701.7251	704.5068
715.9067	719.6999	724.6854
736.6835	743.9791	747.7412
759.7524	766.4682	772.9505
782.6288	791.9426	797.2248
821.9793	837.3950	841.5671
844.7204	863.9949	864.8599
866.9333	879.2711	886.4492
890.8660	898.1897	910.8606
931.0774	944.0616	945.5347
957.3599	962.7507	976.9574
979.9475	981.6164	986.4495
991.1197	996.1828	1000.0897
1003.9433	1009.0189	1014.0135
1031.6640	1037.4508	1041.4832
1044.7722	1048.3127	1053.2046
1055.5480	1056.3764	1063.3237
1065.3796	1071.2893	1073.3209
1083.3678	1086.2664	1089.2717
1097.2440	1106.9027	1112.6969
1113.8727	1117.7006	1125.3001
1172.1585	1183.0972	1185.9474
1186.2279	1188.0264	1193.5210
1198.4564	1202.6293	1205.0271
1210.8031	1212.5348	1217.2450

1229.8812	1246.9753	1252.8918
1265.6331	1285.5778	1292.5785
1293.9553	1298.0129	1302.1449
1310.7973	1321.3084	1330.3860
1333.5516	1335.3419	1344.0325
1345.1357	1354.5126	1358.3861
1364.4530	1369.8158	1378.9981
1382.0566	1412.5771	1414.8118
1420.5308	1425.5791	1432.0313
1438.7779	1446.7748	1450.2153
1452.9490	1458.4208	1462.9902
1468.1187	1470.0793	1487.4953
1490.4872	1491.2533	1493.3721
1493.8388	1499.4078	1503.3956
1505.1408	1505.9095	1515.4375
1519.9115	1523.8405	1526.0113
1534.6345	1550.8498	1629.5618
1630.3612	1636.1911	1641.4564
1641.5120	1648.8901	1653.6650
1655.1535	1659.8110	1699.5366
2801.9680	3011.7388	3040.4705
3044.1677	3051.8262	3056.2091
3078.2347	3082.8398	3103.9496
3104.8590	3106.2274	3128.0282
3132.1576	3132.7269	3138.2616
3139.2040	3146.0263	3153.9312
3179.2237	3180.8778	3182.3492
3182.6189	3183.6061	3184.0418
3186.6554	3190.8509	3194.2178
3194.6716	3196.4472	3198.6640

3201.5346	3205.6088	3209.1090
3210.5420	3219.9247	3229.4542

M6R

Zero-point correction= 0.677016

Thermal correction to Energy= 0.717480

Thermal correction to Enthalpy= 0.718424

Thermal correction to Gibbs Free Energy= 0.603366

Sum of electronic and zero-point Energies= -2462.458162

Sum of electronic and thermal Energies= -2462.417699

Sum of electronic and thermal Enthalpies= -2462.416754

Sum of electronic and thermal Free Energies= -2462.531813

Cartesian coordinates

C	-1.981825	-0.366538	-0.286615
C	-0.819279	-0.056945	0.653471
H	-1.646212	-0.038273	-1.270797
C	0.573568	-0.260869	-0.061562
O	0.664401	-0.471123	-1.323497
C	-3.263435	0.364217	0.077257
C	-3.845201	1.231376	-0.855493
C	-3.889044	0.187482	1.320390
C	-5.031669	1.907462	-0.558300
H	-3.365601	1.371594	-1.819363
C	-5.073878	0.860411	1.618647
H	-3.446442	-0.478410	2.055213
C	-5.649279	1.722858	0.680036
H	-5.470287	2.575909	-1.293395
H	-5.548577	0.714509	2.585017
H	-6.571686	2.246853	0.913903
C	1.628643	0.803979	0.339628

C	3.558308	1.810089	0.680949
C	3.692008	-0.672580	0.723954
H	2.975912	-1.419296	1.068806
N	2.714975	2.785955	0.491268
N	1.510305	2.138188	0.265357
N	2.937710	0.587149	0.597400
C	4.992785	1.820544	1.095412
H	5.268379	2.796001	1.498823
H	5.650259	1.592831	0.245571
C	4.886091	-0.496916	1.744187
O	5.115194	0.859810	2.143786
C	5.718159	-1.315614	-0.392125
C	4.356053	-1.068689	-0.578209
C	3.749561	-1.201845	-1.827804
C	4.548076	-1.582804	-2.909079
C	5.916666	-1.827540	-2.734800
C	6.509802	-1.699787	-1.475745
C	6.121050	-1.127738	1.048163
H	2.682578	-1.012370	-1.935296
H	6.523543	-2.120932	-3.586989
H	7.571101	-1.892402	-1.343598
H	6.994971	-0.479858	1.173591
H	6.367118	-2.087577	1.516696
C	0.323968	2.911233	0.005267
C	-0.367204	3.449964	1.102790
C	-0.082827	3.095336	-1.321982
C	-1.539547	4.158081	0.838146
C	-1.267412	3.812582	-1.531138
C	-2.009505	4.339381	-0.469956
H	-2.105691	4.568760	1.670016

H	-1.615276	3.957324	-2.550394
C	0.718908	2.537048	-2.467237
H	0.749376	1.442692	-2.407396
H	1.753508	2.898173	-2.430719
H	0.286194	2.834298	-3.425631
C	-3.288216	5.100363	-0.714173
H	-4.090050	4.737228	-0.063303
H	-3.621246	5.006115	-1.751317
H	-3.155542	6.167982	-0.500644
C	0.129427	3.240504	2.510022
H	1.144524	3.632236	2.634364
H	0.164807	2.174941	2.765605
H	-0.522892	3.737877	3.231329
H	4.646143	-1.006923	2.677691
H	4.102543	-1.692174	-3.893755
H	-0.984788	0.919212	1.103019
C	-2.156606	-2.693760	0.712726
C	-1.294735	-2.329910	1.771455
C	-1.260592	-3.102699	2.934646
C	-2.037624	-4.251186	3.071417
C	-2.861351	-4.627340	2.011778
C	-2.932255	-3.858158	0.850617
H	-0.597575	-2.793642	3.739226
H	-1.995065	-4.842934	3.980461
H	-3.470790	-5.523678	2.082699
H	-3.572666	-4.200753	0.051277
C	-0.388111	-1.147788	1.633861
O	0.815183	-1.445470	0.868948
N	-2.201982	-1.841788	-0.426296
S	-2.909800	-2.341891	-1.886717

O	-2.571574	-1.335311	-2.898353
O	-2.546284	-3.746962	-2.103440
C	-4.692080	-2.241844	-1.634155
H	-4.956265	-1.194073	-1.491149
H	-5.161585	-2.636391	-2.538187
H	-4.984250	-2.831491	-0.765295
H	-0.132450	-0.761340	2.629050

Vibrational frequencies

12.1572	24.2167	31.8200
33.0229	39.0953	40.3769
46.3273	48.4418	55.1806
66.7805	76.9752	81.0505
83.6516	101.1815	107.0055
117.4090	118.6995	122.7678
131.5836	148.5465	158.8949
174.9466	184.7813	192.8952
198.5847	207.1093	213.0916
216.0319	220.9435	235.3966
250.8552	252.2189	257.0148
261.2204	267.8444	288.2191
295.4874	306.0194	320.8177
322.2259	330.6266	349.9417
357.1763	385.0987	389.5833
397.5009	401.5378	418.7638
429.3147	446.5170	449.2894
461.4072	470.1624	485.4527
493.7114	500.9261	510.5556
515.9747	520.3381	527.7789
531.9665	541.3699	546.3116
579.7821	582.5560	592.9841

595.8826 602.8060 609.2396

613.4105 618.3347 633.3577

634.4853 652.3290 672.0936

701.7615 718.2871 719.9326

726.6412 729.7543 744.6980

750.6902 755.6760 766.9564

767.6758 775.8529 783.6259

794.2161 799.9726 815.4382

825.2105 841.4868 848.8301

866.8804 871.0715 872.6741

874.9730 879.1525 901.2200

908.5978 914.4476 930.8311

937.9963 949.4123 953.4113

959.5386 961.5900 973.0445

982.7711 983.2469 984.1128

985.9532 986.0313 989.7768

995.8087 999.9178 1006.6445

1015.4095 1026.1795 1029.1288

1033.3794 1043.4520 1044.4000

1050.8609 1055.5477 1058.4664

1062.8421 1064.0156 1069.9039

1075.6588 1079.5299 1088.4661

1089.5874 1099.4658 1113.7446

1116.9574 1121.0135 1145.4083

1153.7481 1182.6224 1187.4106

1190.2322 1198.1384 1200.5041

1203.4879 1210.2468 1215.4242

1220.5728 1225.8672 1234.0271

1244.8761 1253.7404 1255.1337

1272.5092 1288.5346 1293.3878

1297.0214	1302.8512	1305.4781
1309.1713	1320.1384	1324.4603
1328.5859	1336.0318	1345.6060
1346.1520	1350.2516	1358.5558
1366.0875	1369.8123	1370.0287
1379.5863	1380.9908	1391.4901
1409.9568	1417.8134	1418.9689
1426.0936	1428.2617	1436.4767
1438.4067	1448.7366	1449.9824
1455.7493	1472.1891	1473.2716
1476.8506	1479.6271	1484.3761
1491.0312	1495.1729	1496.9588
1498.6191	1501.5615	1502.8510
1509.2717	1517.6095	1530.3862
1533.2599	1534.9348	1538.7876
1631.2444	1637.1757	1639.1442
1640.5164	1644.1386	1654.8406
1655.6984	1657.6592	1658.6364
3025.0294	3027.4281	3041.1672
3042.6937	3044.4165	3055.3644
3079.0592	3094.2859	3096.2649
3101.9757	3103.1986	3123.6408
3126.8413	3130.8119	3131.8215
3132.9012	3140.7908	3147.6218
3150.9750	3162.2942	3176.2911
3179.9422	3180.8240	3182.8840
3183.7069	3185.5859	3188.7692
3189.9740	3190.7781	3197.2658
3197.5970	3203.4253	3204.2369
3207.8343	3210.0385	3260.2655

TS6S

Zero-point correction= 0.674246

Thermal correction to Energy= 0.714891

Thermal correction to Enthalpy= 0.715835

Thermal correction to Gibbs Free Energy= 0.601012

Sum of electronic and zero-point Energies= -2462.450049

Sum of electronic and thermal Energies= -2462.409404

Sum of electronic and thermal Enthalpies= -2462.408459

Sum of electronic and thermal Free Energies= -2462.523283

Cartesian coordinates

C	1.853811	-1.056533	-1.001766
C	0.836462	-0.281695	-0.173614
H	1.295429	-1.546330	-1.802047
C	-0.342809	0.093695	-0.926872
O	-0.733576	-0.407724	-1.984156
C	2.932743	-0.229978	-1.686167
C	3.432966	-0.681502	-2.916359
C	3.463551	0.942807	-1.135705
C	4.440108	0.018059	-3.580953
H	3.030713	-1.593181	-3.350810
C	4.469025	1.647831	-1.800500
H	3.114886	1.297859	-0.175894
C	4.962448	1.188383	-3.023219
H	4.813450	-0.346751	-4.533699
H	4.868093	2.555028	-1.355343
H	5.745594	1.737063	-3.538754
C	-1.277316	1.112965	-0.301779
C	-3.087830	2.265562	0.154935
C	-3.545932	0.274741	-1.215324

H	-2.952890	-0.307285	-1.918899
N	-2.115952	2.932687	0.720923
N	-0.991422	2.196060	0.435714
N	-2.613793	1.157097	-0.493882
C	-4.531243	2.597778	-0.029380
H	-4.715220	3.640778	0.232766
H	-5.163982	1.956871	0.597182
C	-4.619086	1.134772	-1.977926
O	-4.806964	2.446233	-1.422903
C	-5.706251	-0.604380	-0.697327
C	-4.368860	-0.599775	-0.291055
C	-3.926144	-1.329172	0.809781
C	-4.869305	-2.092112	1.506040
C	-6.210152	-2.117661	1.102144
C	-6.638967	-1.372824	-0.001603
C	-5.906689	0.280926	-1.903174
H	-2.879497	-1.279709	1.117041
H	-6.928415	-2.714460	1.657641
H	-7.682535	-1.383856	-0.304036
H	-6.787442	0.926442	-1.838224
H	-6.007090	-0.318319	-2.816788
C	0.290354	2.703835	0.865835
C	1.093443	3.365674	-0.073999
C	0.648249	2.538654	2.212787
C	2.324690	3.853270	0.371974
C	1.898822	3.031588	2.597006
C	2.749463	3.681313	1.694681
H	2.970763	4.364141	-0.336783
H	2.214598	2.902084	3.628586
C	-0.270654	1.850270	3.184640

H	-0.583243	0.867707	2.797975
H	-1.179280	2.443984	3.341539
H	0.220532	1.720221	4.152163
C	4.115243	4.151505	2.127083
H	4.144011	4.371969	3.198115
H	4.423335	5.048053	1.580459
H	4.865373	3.374658	1.932191
C	0.678128	3.507338	-1.515555
H	-0.371445	3.803149	-1.610474
H	0.806894	2.561499	-2.055186
H	1.291524	4.257257	-2.020171
H	-4.302992	1.318030	-3.006197
H	-4.558274	-2.667379	2.373755
H	1.253358	0.531885	0.405515
C	1.388765	-3.184001	0.062133
C	0.220569	-2.705690	0.677085
C	-0.840624	-3.593425	0.869722
C	-0.732272	-4.928214	0.473503
C	0.442329	-5.392480	-0.125642
C	1.503991	-4.511868	-0.344098
H	-1.737119	-3.221827	1.353132
H	-1.562530	-5.610042	0.637066
H	0.528137	-6.430956	-0.432119
H	2.417019	-4.838248	-0.832707
C	0.151437	-1.279034	1.200429
H	1.024812	-1.120899	1.866606
O	-0.989724	-0.837066	1.640866
N	2.431290	-2.241617	-0.268648
S	3.611504	-1.969342	0.937683
O	3.495578	-0.610315	1.500222

O	3.572361	-3.126599	1.843082
C	5.144668	-2.049828	0.005239
H	5.178105	-1.230236	-0.711164
H	5.955695	-1.955364	0.731053
H	5.190513	-3.014957	-0.500053

Vibrational frequencies

-262.3954	10.8195	23.2302
34.9694	35.3889	44.9112
48.3735	51.2296	59.6060
70.2432	73.4004	80.3772
85.3459	87.1774	96.0223
98.3830	103.1174	108.3635
120.6676	131.6599	147.2822
167.3945	174.1459	180.1862
187.5200	193.5319	200.0506
201.2022	216.5660	228.3122
235.8941	242.1879	244.9515
253.1453	261.1354	275.2063
280.8230	286.6859	296.2030
297.9869	306.0758	331.8625
346.2765	359.3360	370.7237
378.4737	397.2669	407.8300
416.1035	422.5889	427.8591
436.4146	450.9441	462.1782
481.8168	491.3557	492.7498
500.9023	509.7921	513.3324
515.5649	529.9964	534.7437
548.8153	569.6150	580.3512
583.2132	590.7136	595.6472
613.7126	618.4025	622.9748

632.8365 639.3167 652.7342

659.2057 670.6338 702.7630

712.8769 715.3064 732.4213

741.8997 744.4237 752.7801

753.4673 765.6271 776.0419

780.1842 791.6579 797.4948

821.3779 828.9675 838.6314

844.6739 862.6418 865.0440

871.3978 873.5889 890.5654

891.4067 901.9731 915.6705

932.4014 945.8425 956.4301

961.2884 962.4672 973.5083

982.3046 984.3839 986.2850

988.3417 992.5849 993.7669

996.6396 1004.2824 1017.1400

1022.0748 1025.8863 1044.2655

1046.0350 1047.4100 1054.8126

1055.7669 1056.8116 1061.0486

1062.6460 1065.8827 1069.8873

1074.6626 1083.8122 1087.2883

1090.4219 1101.5880 1107.3346

1113.5028 1115.1723 1117.0448

1149.8686 1178.5945 1182.7558

1184.2003 1189.2299 1193.3824

1198.4696 1203.2381 1213.7245

1218.7335 1225.7883 1227.8438

1234.0713 1236.9490 1253.7295

1266.5641 1284.1113 1287.0772

1288.9901 1292.1034 1293.7701

1305.5733 1320.6805 1329.9459

1336.6644	1340.3595	1342.4022
1345.6462	1352.0797	1356.6836
1365.3918	1370.5340	1371.6225
1376.9128	1391.8886	1407.3762
1419.3466	1423.3758	1432.5469
1437.1467	1443.2201	1446.1479
1446.9040	1452.2170	1456.3991
1465.6553	1468.2473	1488.9798
1489.0557	1490.0123	1490.5312
1491.9954	1492.9578	1495.7562
1498.7643	1500.0383	1505.4751
1510.0510	1524.8470	1531.6735
1533.4279	1538.7796	1627.0674
1631.8171	1637.7913	1638.3482
1639.8991	1650.5547	1651.3155
1657.8760	1660.3449	1704.9902
2876.9448	2972.6635	3039.3460
3047.0932	3048.6856	3055.9652
3073.2808	3083.3247	3092.9463
3096.2314	3102.5672	3107.4005
3108.5579	3118.8678	3128.2787
3130.9297	3140.0401	3152.3429
3154.8362	3178.5880	3181.0201
3181.1620	3184.3346	3185.4715
3185.5451	3187.2489	3191.3364
3194.0959	3195.2023	3203.5187
3207.1604	3207.4162	3209.2332
3218.6270	3223.9222	3255.2055

M6S

Zero-point correction= 0.676416

Thermal correction to Energy= 0.717042

Thermal correction to Enthalpy= 0.717987

Thermal correction to Gibbs Free Energy= 0.602456

Sum of electronic and zero-point Energies= -2462.453389

Sum of electronic and thermal Energies= -2462.412762

Sum of electronic and thermal Enthalpies= -2462.411818

Sum of electronic and thermal Free Energies= -2462.527349

Cartesian coordinates

C	-2.129179	-0.440699	-0.636732
C	-0.937643	0.007221	0.226600
H	-2.471991	0.426051	-1.200092
C	0.534604	-0.264567	-0.252703
O	0.864046	-0.634216	-1.426253
C	-2.026338	-1.594645	-1.629070
C	-2.899873	-1.561021	-2.724810
C	-1.200309	-2.712915	-1.462279
C	-2.947563	-2.612577	-3.640723
H	-3.556379	-0.704046	-2.855401
C	-1.249813	-3.767910	-2.375065
H	-0.499444	-2.748753	-0.639082
C	-2.120719	-3.724239	-3.465977
H	-3.629051	-2.563035	-4.485599
H	-0.599005	-4.626545	-2.233025
H	-2.152440	-4.547003	-4.175128
C	1.513504	0.860497	0.194939
C	3.387919	1.930212	0.637422
C	3.533981	-0.529958	0.948101
H	2.786575	-1.260979	1.259590
N	2.557248	2.869489	0.279089

N	1.389618	2.181615	-0.008229
N	2.790774	0.692560	0.601119
C	4.768457	1.999287	1.200376
H	5.003443	3.016373	1.517239
H	5.512094	1.677963	0.459029
C	4.563726	-0.230324	2.108527
O	4.766240	1.166449	2.360498
C	5.702286	-1.256329	0.220844
C	4.389523	-1.028087	-0.198393
C	3.988990	-1.260030	-1.514308
C	4.944942	-1.723984	-2.421508
C	6.265190	-1.952942	-2.012358
C	6.651791	-1.724324	-0.688736
C	5.870897	-0.950227	1.687501
H	2.954574	-1.082483	-1.800998
H	6.996636	-2.312203	-2.730995
H	7.676794	-1.902495	-0.374888
H	6.736519	-0.316384	1.905363
H	5.994971	-1.872175	2.267752
C	0.207523	2.893787	-0.416992
C	-0.132935	2.911882	-1.775450
C	-0.587597	3.479013	0.581670
C	-1.358821	3.495557	-2.117343
C	-1.796249	4.052978	0.185615
C	-2.209847	4.045920	-1.153929
H	-1.659356	3.503141	-3.161528
H	-2.441664	4.492364	0.941519
C	-0.188804	3.410985	2.033406
H	0.824825	3.791595	2.192524
H	-0.202857	2.374786	2.393862

H	-0.876068	3.991086	2.653512
C	-3.572554	4.566129	-1.529534
H	-3.633679	4.812773	-2.593306
H	-3.838964	5.456715	-0.951271
H	-4.324145	3.796279	-1.317187
C	0.768851	2.299077	-2.814021
H	0.828744	1.213944	-2.670095
H	1.786749	2.697566	-2.734446
H	0.396929	2.505146	-3.820524
H	4.176844	-0.613226	3.053611
H	4.661152	-1.910622	-3.453401
H	-1.126438	1.045184	0.486623
C	-2.946490	-1.846404	1.228457
C	-1.642809	-1.947909	1.747658
C	-1.318946	-3.038562	2.560250
C	-2.278399	-3.998676	2.876838
C	-3.577995	-3.877311	2.373421
C	-3.910142	-2.813105	1.538142
H	-0.305657	-3.127119	2.941913
H	-2.015877	-4.840948	3.510229
H	-4.328082	-4.624913	2.613569
H	-4.902099	-2.718424	1.113530
C	-0.633974	-0.875115	1.437705
O	0.623733	-1.336986	0.894307
N	-3.251298	-0.792118	0.300759
S	-4.320318	0.422786	0.791933
O	-4.422688	1.369288	-0.328991
O	-5.528122	-0.238308	1.302115
C	-3.552265	1.266883	2.188000
H	-2.663487	1.794169	1.843225

H	-4.285175	1.974933	2.580549
H	-3.303236	0.522570	2.946313
H	-0.464250	-0.281890	2.350294

Vibrational frequencies

12.3042	20.1840	28.3165
31.4379	41.9443	43.3170
46.9593	53.0545	55.4628
69.7709	77.6425	79.0953
83.0917	89.3439	101.4766
108.7648	120.4004	125.6517
133.9243	152.7570	163.6824
167.8969	177.5765	183.9460
194.1933	198.4736	212.5520
218.4555	230.8759	234.2593
236.5526	256.1279	261.7193
269.7270	276.9436	285.6221
290.0530	292.6042	302.5392
317.5998	325.4882	344.2831
370.3354	380.4417	393.8166
402.0537	418.5918	424.2161
424.5885	440.5655	447.6441
449.1257	468.7340	482.0762
490.0109	493.3191	501.6329
507.2486	517.9576	530.2069
530.3830	534.8033	538.9075
578.0338	581.3624	590.1257
595.5101	600.7969	605.7346
617.2348	623.7894	630.3836
633.2647	662.2413	674.1086
683.6455	707.6668	717.3612

719.9792	726.9260	730.7908
741.8062	751.3623	758.5518
767.1491	772.4300	774.8930
781.6263	794.9843	812.6683
823.7240	838.5368	845.9901
863.8390	869.9734	871.8349
880.7645	887.1136	902.8568
908.4923	920.9137	936.7152
940.4961	949.5052	951.5270
961.8883	964.3803	977.6800
980.6171	983.1103	983.2800
987.0448	990.8312	995.5514
997.8421	1002.7405	1017.6940
1017.7861	1021.1281	1028.5444
1031.5767	1044.6741	1045.5615
1048.8902	1054.2398	1057.6323
1059.9468	1063.0240	1066.6345
1068.6912	1074.6888	1077.7724
1088.0356	1097.1070	1114.8375
1116.1401	1119.9138	1137.4050
1144.1578	1183.0395	1187.2636
1187.7916	1188.1351	1196.1547
1203.7134	1207.5979	1220.5753
1225.3094	1234.3643	1236.2165
1244.2604	1254.1954	1265.2967
1266.0806	1279.0361	1288.1927
1293.5345	1303.8771	1305.5947
1315.2386	1316.6053	1318.7331
1328.2418	1335.5708	1341.8373
1344.6433	1348.9428	1356.9112

1362.3583	1367.1996	1370.0739
1375.0957	1377.5893	1385.7763
1406.4923	1412.4535	1421.0478
1425.6880	1430.3731	1436.4696
1444.1840	1450.7032	1452.2439
1462.9704	1469.8211	1472.4052
1482.0637	1485.4904	1487.6756
1490.7650	1493.9165	1496.3901
1497.4783	1498.7390	1499.7567
1509.9734	1511.6196	1520.2340
1528.0865	1533.0756	1542.3220
1625.6240	1638.0715	1639.1532
1641.1361	1642.2174	1653.2550
1657.0840	1658.3100	1659.7056
2978.7680	3031.4439	3036.4038
3041.6934	3045.7114	3052.4898
3080.9333	3097.6793	3100.0823
3101.3269	3107.6206	3122.1492
3128.8854	3129.9499	3134.0075
3135.5806	3140.4049	3153.9045
3163.4769	3172.8647	3179.7787
3180.3568	3181.3053	3181.7086
3184.2122	3185.0531	3187.2709
3190.2989	3192.5596	3194.8575
3202.8226	3203.5288	3204.4244
3207.5962	3234.1658	3244.4561

TS7R

Zero-point correction= 0.675310

Thermal correction to Energy= 0.715724

Thermal correction to Enthalpy= 0.716669

Thermal correction to Gibbs Free Energy= 0.602337

Sum of electronic and zero-point Energies= -2462.425059

Sum of electronic and thermal Energies= -2462.384645

Sum of electronic and thermal Enthalpies= -2462.383701

Sum of electronic and thermal Free Energies= -2462.498033

Cartesian coordinates

C	0.960822	1.455778	-0.186900
C	0.752459	0.570030	-1.392428
H	0.555294	0.957316	0.694093
C	-0.350735	-0.426039	-1.845942
C	0.372545	2.845008	-0.284817
C	-0.580148	3.258011	0.652595
C	0.775265	3.734281	-1.290687
C	-1.138245	4.537337	0.577417
H	-0.878086	2.579243	1.446562
C	0.222046	5.011726	-1.364294
H	1.532285	3.427195	-2.006762
C	-0.739026	5.415680	-0.431394
H	-1.874985	4.848341	1.312595
H	0.540373	5.693723	-2.147545
H	-1.167984	6.411876	-0.488748
C	-1.060563	-1.020453	-0.006384
C	-2.412765	-0.889408	1.762879
C	-3.044729	0.586561	-0.127208
H	-2.454684	1.138785	-0.858477
N	-1.571341	-1.831536	2.079312
N	-0.745603	-1.900329	0.958005
N	-2.142127	-0.382757	0.512472
C	-3.477377	-0.216956	2.566019

H	-3.308550	-0.370001	3.633246
H	-4.473917	-0.601879	2.309681
C	-3.680812	1.549450	0.952406
O	-3.364411	1.183310	2.299918
C	-5.439464	0.428188	-0.302076
C	-4.234106	-0.101533	-0.768183
C	-4.210469	-1.142023	-1.697518
C	-5.426275	-1.656577	-2.152791
C	-6.639426	-1.132876	-1.686307
C	-6.653672	-0.084734	-0.762996
C	-5.207784	1.550508	0.675586
H	-3.262719	-1.518476	-2.067363
H	-7.577754	-1.544208	-2.047961
H	-7.595663	0.320622	-0.403519
H	-5.763185	1.428997	1.611634
H	-5.513349	2.513189	0.249940
C	0.307122	-2.875222	0.920765
C	1.396254	-2.721144	1.795736
C	0.217883	-3.930849	0.002457
C	2.424244	-3.663416	1.720572
C	1.276876	-4.845253	-0.033795
C	2.382981	-4.729907	0.813567
H	3.282533	-3.554440	2.378753
H	1.232913	-5.666976	-0.743949
C	-0.951486	-4.067856	-0.939169
H	-0.858971	-3.348888	-1.759101
H	-1.903977	-3.879156	-0.434044
H	-0.985772	-5.073199	-1.367024
C	3.505030	-5.737258	0.767918
H	3.412840	-6.465725	1.583321

H	4.479809	-5.251313	0.879725
H	3.506866	-6.295022	-0.172976
C	1.473408	-1.561032	2.753514
H	2.467299	-1.493470	3.202292
H	0.737245	-1.658063	3.558424
H	1.272305	-0.609243	2.254629
H	-3.257083	2.546592	0.843104
H	-5.431540	-2.466695	-2.876489
H	1.009266	1.112288	-2.309439
C	3.398647	0.893827	-0.956590
C	3.006063	-0.280111	-1.651856
C	3.851391	-0.867440	-2.583830
C	5.116545	-0.320634	-2.821334
C	5.511935	0.827434	-2.135279
C	4.654431	1.445921	-1.220465
H	3.515106	-1.750739	-3.118194
H	5.783330	-0.785000	-3.541537
H	6.489903	1.262393	-2.318696
H	4.977792	2.346571	-0.713255
C	1.616918	-0.666188	-1.290789
H	1.612973	-1.073560	-0.272505
O	0.695379	-1.420544	-2.114189
N	2.478055	1.491035	-0.018695
S	3.024865	1.999077	1.505823
O	1.913364	1.802764	2.449330
O	4.324780	1.371210	1.766967
C	3.268495	3.772178	1.345483
H	2.308680	4.232293	1.110693
H	3.640810	4.130403	2.308169
H	3.995225	3.969960	0.556807

O -1.324240 -0.287229 -2.569552

Vibrational frequencies

-198.9456	21.1464	25.1146
27.1129	33.8504	36.9078
44.6911	52.0289	56.1093
62.4221	68.4092	77.1331
82.8133	85.9671	91.1353
97.3758	116.4073	128.7208
132.2961	136.5364	150.5249
155.9248	157.9448	171.9594
180.1637	189.7716	197.1615
201.3116	220.5967	224.7626
232.9965	235.0475	243.8448
255.9627	277.7511	283.0411
290.7190	296.3763	301.3703
306.7152	324.2035	332.2440
350.9513	362.4841	365.8818
385.3042	400.3817	421.6956
426.8489	440.9180	445.3751
450.2653	460.1662	482.3662
490.6679	495.9989	500.1273
503.9263	515.1545	519.9837
520.8911	531.6989	535.0270
562.9352	576.3906	584.3054
589.6030	598.8163	607.3752
613.2293	625.6243	630.6616
634.1794	641.3992	660.2908
692.9625	694.6011	699.7866
704.0054	717.6257	721.5346
738.9080	745.0153	750.6349

755.4525	762.7560	766.3011
787.9079	792.6592	803.9868
822.6988	844.4671	852.1065
870.6933	872.0832	873.1739
876.7558	877.4148	896.4608
901.1385	904.6883	912.7219
943.9448	947.4994	949.2193
960.0423	966.7718	968.9851
974.5351	980.7076	984.7048
985.9268	990.5301	995.9447
996.8186	1002.2203	1007.6287
1008.3284	1016.3227	1038.7732
1039.0984	1041.6304	1046.1093
1054.1135	1054.9960	1056.8696
1057.4141	1061.1541	1065.6156
1068.7331	1070.8118	1073.4570
1097.8945	1106.5975	1114.9903
1117.1777	1118.3403	1141.5853
1172.0878	1181.2248	1186.4715
1186.9445	1188.7563	1194.6822
1200.1787	1201.2310	1211.9915
1214.4630	1219.9486	1225.3196
1237.1969	1244.0818	1260.1109
1267.5702	1276.5676	1288.5588
1292.4204	1294.1148	1305.9458
1310.0847	1313.9256	1318.2240
1325.2931	1327.9251	1339.0403
1341.4084	1345.8466	1360.7650
1364.2079	1369.6539	1371.6143
1381.7820	1393.1669	1399.0908

1412.6243	1415.5520	1418.2320
1419.9267	1427.9804	1435.2903
1437.0460	1444.5927	1449.2617
1449.5278	1451.7898	1476.4442
1477.2325	1486.6329	1488.7734
1490.1000	1492.7360	1494.6427
1497.8269	1498.4390	1499.3138
1507.7624	1512.4534	1523.9191
1530.6545	1538.0333	1624.8119
1637.8953	1639.8095	1641.2473
1645.9738	1656.1700	1657.7905
1658.3193	1661.8000	1736.3300
3039.5178	3039.5823	3051.6537
3054.8182	3055.7544	3058.0096
3069.3146	3076.9639	3094.6201
3100.3341	3121.0337	3121.9958
3128.2442	3128.6521	3132.9170
3138.1601	3145.1771	3145.4100
3151.5848	3179.4387	3180.2062
3181.5021	3182.6914	3183.0529
3187.9435	3188.5846	3191.5848
3196.0202	3197.2296	3198.1878
3202.2621	3203.7800	3210.3806
3210.5723	3217.3865	3231.9957

TS7S

Zero-point correction= 0.674795

Thermal correction to Energy= 0.715252

Thermal correction to Enthalpy= 0.716196

Thermal correction to Gibbs Free Energy= 0.600368

Sum of electronic and zero-point Energies= -2462.423741

Sum of electronic and thermal Energies= -2462.383284

Sum of electronic and thermal Enthalpies= -2462.382339

Sum of electronic and thermal Free Energies= -2462.498168

Cartesian coordinates

C	-1.609548	1.560135	-0.665506
C	-0.834326	0.307046	-1.006657
H	-1.425072	2.318576	-1.428595
C	0.492688	0.117024	-1.757765
O	1.267742	0.909502	-2.254956
C	-1.268412	2.122564	0.700297
C	-0.260508	3.089599	0.805579
C	-1.888115	1.652843	1.864124
C	0.121453	3.580399	2.056033
H	0.222546	3.459613	-0.095049
C	-1.515849	2.153213	3.112954
H	-2.664903	0.898988	1.787353
C	-0.507989	3.115589	3.213400
H	0.899717	4.335134	2.124018
H	-2.009253	1.786238	4.008504
H	-0.217407	3.502426	4.185763
C	1.713589	-1.061825	-0.410002
C	3.599045	-1.921576	0.433257
C	3.929513	-0.209083	-1.333272
H	3.388538	-0.015375	-2.258904
N	2.657591	-2.482510	1.137968
N	1.498734	-1.923243	0.597697
N	3.070975	-1.069212	-0.507865
C	5.078526	-2.117929	0.444827
H	5.340575	-3.078455	0.891733

H	5.571422	-1.320270	1.018856
C	5.324738	-0.897823	-1.609605
O	5.510034	-2.135849	-0.915499
C	5.654788	1.269033	-0.540398
C	4.273948	1.075755	-0.608417
C	3.383910	1.984828	-0.036006
C	3.901799	3.100090	0.624678
C	5.286915	3.299859	0.699983
C	6.170816	2.389526	0.114709
C	6.400592	0.161744	-1.240529
H	2.313759	1.827834	-0.117551
H	5.677530	4.171410	1.217956
H	7.244178	2.548292	0.174973
H	7.179372	-0.291820	-0.617915
H	6.895567	0.530638	-2.146037
C	0.228695	-2.231691	1.190479
C	-0.149890	-1.530896	2.346651
C	-0.584727	-3.199994	0.589500
C	-1.412552	-1.801004	2.879844
C	-1.837110	-3.438609	1.165120
C	-2.273269	-2.739239	2.294756
H	-1.733052	-1.262433	3.767928
H	-2.491910	-4.173696	0.707549
C	-0.130512	-3.927314	-0.649185
H	0.853509	-4.385614	-0.500311
H	-0.042082	-3.231125	-1.489614
H	-0.837872	-4.714373	-0.920857
C	-3.657351	-2.959255	2.852921
H	-4.338488	-2.170088	2.512011
H	-3.657068	-2.939745	3.947707

H	-4.076243	-3.915279	2.525910
C	0.770650	-0.513954	2.970598
H	0.963240	0.320245	2.287940
H	1.740219	-0.959207	3.216354
H	0.336720	-0.102994	3.883920
H	5.388628	-1.177663	-2.661722
H	3.226019	3.817038	1.081984
H	-0.868614	-0.388525	-0.169054
C	-3.459407	-0.241619	-0.983207
C	-2.653996	-1.093633	-1.781953
C	-3.025771	-2.413062	-2.002011
C	-4.208266	-2.907832	-1.442269
C	-4.997081	-2.079070	-0.644537
C	-4.620034	-0.754727	-0.402001
H	-2.385694	-3.050542	-2.603166
H	-4.501798	-3.938257	-1.618379
H	-5.908525	-2.461497	-0.195130
H	-5.236054	-0.127574	0.231811
C	-1.418828	-0.388627	-2.226150
H	-1.673641	0.335210	-3.015713
O	-0.132530	-0.989792	-2.534544
N	-3.059149	1.132310	-0.778765
S	-4.165870	2.370184	-1.166739
O	-3.395694	3.486064	-1.735546
O	-5.269209	1.778526	-1.931570
C	-4.807644	2.921860	0.417331
H	-3.975110	3.272978	1.027269
H	-5.502761	3.738558	0.208961
H	-5.324742	2.095320	0.905579

Vibrational frequencies

-150.4428	9.3224	17.4243
20.3151	28.5395	41.2726
44.2784	48.3883	54.3113
57.7438	65.2831	72.5303
76.3463	79.4337	95.1318
100.7200	103.3506	120.4994
129.2596	150.8538	154.6461
167.3466	173.2167	184.9421
199.2614	203.4714	210.4198
214.2182	228.4426	231.6956
240.8409	242.1123	251.6781
258.2505	272.3660	281.4940
282.0502	290.6780	292.3958
308.1098	322.5710	329.9897
355.1807	364.9676	371.9688
374.3859	383.9710	402.4409
420.0643	433.2951	446.1324
451.0825	458.3695	480.9057
484.1988	495.3599	498.5533
503.6580	512.0389	516.2871
529.1739	531.7716	550.2329
563.9034	574.7695	575.4607
581.1712	597.1777	604.4132
610.5246	615.0428	622.5327
629.4621	635.7006	667.3689
684.4913	694.0584	698.0980
700.2055	713.2057	717.5255
734.2982	748.2322	751.8195
753.8350	759.8417	770.0081
787.9765	790.0579	801.1499

822.5834 843.4674 845.9856

867.0557 867.7663 870.8176

873.0533 880.0625 885.2034

897.9832 898.2100 903.5827

936.2451 945.7526 952.0650

958.8964 966.1596 970.0566

977.6920 982.2529 986.4944

986.9998 992.9883 994.3044

994.3323 995.5042 1005.3416

1014.7335 1019.6164 1033.9052

1035.9171 1039.9478 1042.9513

1047.4077 1052.1070 1054.0811

1055.5228 1064.7058 1066.7101

1069.0352 1071.0057 1074.0618

1091.4093 1101.2540 1110.9343

1117.1585 1118.2058 1140.2238

1170.4409 1180.8835 1183.5181

1188.2411 1189.2540 1190.7174

1199.4792 1200.7811 1208.5142

1219.0014 1220.8334 1228.8818

1232.2018 1243.1896 1253.1406

1267.2686 1277.7129 1286.4666

1291.0766 1296.9847 1305.9079

1309.4126 1312.0338 1316.6282

1323.7292 1328.8945 1330.1811

1340.0739 1344.9378 1359.5822

1362.3145 1368.4808 1378.8239

1379.2782 1389.3523 1396.2365

1403.8968 1408.6695 1419.7306

1420.4615 1426.1681 1435.9485

1437.7193	1447.3535	1449.9311
1456.1355	1463.5382	1472.6679
1478.8965	1483.4732	1484.8364
1489.9029	1491.7930	1494.4941
1495.2843	1495.8185	1496.7934
1509.0661	1512.0921	1522.3707
1534.1446	1535.9099	1624.5084
1637.9326	1638.1352	1640.8879
1641.1835	1656.2383	1657.1300
1657.5841	1660.6744	1761.7349
2998.1681	3031.9228	3039.7042
3044.1367	3053.0924	3055.0691
3080.5255	3093.4562	3100.7326
3108.8044	3109.4736	3112.4157
3123.9657	3127.2550	3135.9412
3142.2852	3143.1212	3143.8410
3146.7996	3179.8549	3180.5338
3181.4586	3183.8258	3185.4579
3189.9555	3190.4647	3194.0570
3195.4453	3199.9464	3202.7646
3202.9645	3205.8353	3211.4492
3213.0957	3220.0439	3231.8190

M7R

Zero-point correction= 0.293209

Thermal correction to Energy= 0.312222

Thermal correction to Enthalpy= 0.313166

Thermal correction to Gibbs Free Energy= 0.244466

Sum of electronic and zero-point Energies= -1410.373598

Sum of electronic and thermal Energies= -1410.354586

Sum of electronic and thermal Enthalpies= -1410.353641

Sum of electronic and thermal Free Energies= -1410.422341

Cartesian coordinates

C	-0.616268	0.567369	-0.586167
C	0.276406	1.731915	-0.210344
H	-0.831661	0.596507	-1.654777
C	0.464598	3.179302	-0.657262
O	-0.166868	4.179529	-0.829428
C	-1.909192	0.474335	0.197124
C	-3.133875	0.626510	-0.459533
C	-1.895594	0.227085	1.577183
C	-4.332548	0.546455	0.254205
H	-3.149450	0.802430	-1.531608
C	-3.090764	0.143756	2.289192
H	-0.946776	0.082279	2.086819
C	-4.313244	0.305148	1.628573
H	-5.278464	0.665559	-0.266121
H	-3.070784	-0.050714	3.357653
H	-5.244678	0.237393	2.183131
H	0.358963	1.783854	0.882709
C	1.569462	-0.557686	0.313800
C	2.387015	0.583144	0.094949
C	3.619212	0.709463	0.721536
C	4.078990	-0.312985	1.557463
C	3.287138	-1.441189	1.770705
C	2.031549	-1.560885	1.168255
H	4.212158	1.603696	0.555989
H	5.045109	-0.222683	2.044068
H	3.636333	-2.234597	2.424564
H	1.425562	-2.437520	1.361158

C	1.675082	1.557910	-0.770965
H	1.664964	1.227799	-1.815923
O	1.843268	3.025600	-0.771095
N	0.283978	-0.638028	-0.337734
S	-0.159031	-2.059680	-1.163972
O	-0.951829	-1.647970	-2.331000
O	1.047577	-2.872668	-1.345987
C	-1.265417	-2.919585	-0.040961
H	-2.130999	-2.284169	0.146288
H	-1.567590	-3.843082	-0.540503
H	-0.738514	-3.141971	0.887791

Vibrational frequencies

17.7477	28.2939	54.1845
67.5911	69.1274	86.5790
129.8988	151.9862	179.7200
194.5631	214.7156	229.8442
249.6411	262.3503	288.3819
302.2119	311.8474	339.7136
366.0659	376.2268	414.8277
445.1527	455.3052	480.1496
503.7532	518.9427	548.9064
585.8785	608.3300	631.5296
637.9711	646.7760	689.1523
697.1653	714.9860	727.4434
750.1794	753.7146	768.4223
798.6181	832.1894	861.7283
866.1828	876.0213	891.8550
931.4531	937.3478	949.4324
971.3663	985.4626	990.2194
992.3550	998.0859	1007.7672

1008.9089	1015.8158	1056.9387
1068.1557	1085.8891	1100.1921
1114.5131	1118.4248	1143.2405
1181.2140	1188.6744	1190.4594
1202.3514	1211.8458	1223.9636
1237.1329	1255.9761	1294.6192
1306.8247	1312.9553	1324.1157
1331.4909	1361.0857	1364.8155
1375.9129	1394.8468	1412.1540
1437.6409	1439.3234	1461.0749
1492.9530	1498.3535	1512.7117
1538.4772	1624.6483	1641.2637
1659.1063	1664.2079	1922.2380
3054.0836	3069.5008	3079.4450
3127.1574	3183.1138	3183.3489
3187.1202	3193.0973	3194.2625
3199.3758	3202.9122	3203.1333
3212.5587	3214.8183	3236.0919

M07R

Zero-point correction= 0.690241

Thermal correction to Energy= 0.731184

Thermal correction to Enthalpy= 0.732128

Thermal correction to Gibbs Free Energy= 0.616840

Sum of electronic and zero-point Energies= -2462.954568

Sum of electronic and thermal Energies= -2462.913624

Sum of electronic and thermal Enthalpies= -2462.912680

Sum of electronic and thermal Free Energies= -2463.027968

Cartesian coordinates

C	2.152265	-0.156115	0.307874

C	2.052344	0.146070	1.804768
H	1.325778	-0.812466	0.030045
C	0.789562	0.848061	2.291866
O	-0.381700	0.589526	2.430914
C	3.468056	-0.815433	-0.103837
C	3.647539	-1.151619	-1.453550
C	4.505581	-1.078664	0.795301
C	4.831662	-1.736244	-1.893897
H	2.854572	-0.948482	-2.165141
C	5.697517	-1.665498	0.355711
H	4.408816	-0.824755	1.845286
C	5.865102	-1.995055	-0.987869
H	4.948871	-1.992120	-2.942894
H	6.493832	-1.856856	1.068821
H	6.790419	-2.449412	-1.329107
C	-2.390558	-0.960307	0.739097
C	-4.199301	-1.892055	-0.044087
C	-4.526528	0.364802	1.090186
H	-4.480670	0.348763	2.180273
N	-3.234441	-2.731708	-0.326625
N	-2.103328	-2.122323	0.169131
N	-3.713109	-0.789698	0.616775
C	-5.658933	-2.000516	-0.363448
H	-6.001012	-3.023192	-0.191175
H	-5.819145	-1.768349	-1.424947
C	-5.977852	0.200959	0.548323
O	-6.414562	-1.153553	0.491658
C	-4.914690	2.016027	-0.592048
C	-4.064285	1.653533	0.460843
C	-2.942748	2.411463	0.790662

C	-2.673428	3.558418	0.040634
C	-3.523340	3.933852	-1.006277
C	-4.650089	3.170058	-1.327800
C	-6.026557	1.010970	-0.772345
H	-2.281596	2.113805	1.598956
H	-3.303281	4.830819	-1.578208
H	-5.304401	3.468935	-2.141824
H	-5.829556	0.375337	-1.643600
H	-7.008344	1.467004	-0.924550
C	-0.803302	-2.725632	0.045641
C	-0.253324	-2.849964	-1.238867
C	-0.140311	-3.142289	1.210592
C	1.011794	-3.436683	-1.336595
C	1.126005	-3.711906	1.052465
C	1.712202	-3.877868	-0.208072
H	1.462163	-3.547082	-2.318946
H	1.660643	-4.048963	1.936693
C	-0.748717	-2.973974	2.580581
H	-0.712482	-1.927085	2.902848
H	-0.202610	-3.568390	3.316577
H	-1.796655	-3.290888	2.598014
C	3.079394	-4.498646	-0.329697
H	3.126506	-5.448982	0.213067
H	3.840500	-3.838778	0.099528
H	3.346725	-4.685147	-1.372425
C	-0.983731	-2.350214	-2.457995
H	-1.305840	-1.313699	-2.316572
H	-1.877837	-2.948578	-2.660185
H	-0.339671	-2.396608	-3.339374
H	-6.637965	0.673267	1.278612

H	-1.792153	4.150068	0.261695
H	2.287651	-0.732633	2.408345
C	2.932016	2.147089	-0.165247
C	3.371947	2.286908	1.163715
C	4.364201	3.224555	1.463410
C	4.892177	4.041532	0.465337
C	4.433019	3.910651	-0.847438
C	3.469808	2.955073	-1.168499
H	4.710264	3.316550	2.489187
H	5.657137	4.772194	0.707685
H	4.841523	4.539484	-1.632534
H	3.143580	2.835916	-2.194698
C	2.752220	1.459180	2.238903
O	1.401221	1.997646	2.646015
N	1.989285	1.112860	-0.453774
S	0.533308	1.463451	-1.242470
O	-0.470148	0.523546	-0.716442
O	0.317838	2.910157	-1.166330
C	0.800459	1.013516	-2.959924
H	0.977550	-0.060607	-3.014954
H	-0.113230	1.274072	-3.499443
H	1.649242	1.571769	-3.355317
H	3.372902	1.394062	3.132211
H	-1.678213	-0.290892	1.202006

Vibrational frequencies

14.3758	27.8851	33.5317
36.7333	44.4098	49.8999
51.0546	56.7664	62.6291
70.1496	73.8143	78.1974
80.4034	84.7347	96.9530

99.9638	115.2460	122.4477
136.4352	144.9334	154.1224
170.5903	174.0817	177.3842
190.6835	206.3928	212.7509
214.1883	227.3079	230.1990
236.4869	237.2986	246.0697
255.5433	260.2110	292.0076
292.1958	296.3423	304.2730
322.3911	338.2439	344.4763
351.9461	353.3692	374.8128
390.8492	396.8320	411.7057
413.6588	417.1914	443.5679
448.7704	461.3359	477.5082
491.0835	492.3080	494.9541
512.4680	514.6066	520.3234
523.2817	526.2629	540.1051
567.7943	582.1454	591.1373
595.0102	597.4423	602.0503
612.2401	618.4022	626.0010
635.1430	650.6535	667.6666
692.3285	698.1915	708.1098
710.9599	722.6223	725.2615
738.8077	745.0559	763.2221
769.2833	773.5413	784.4324
789.2552	811.1276	816.4015
836.9232	837.7346	844.9668
855.2331	873.4400	876.3846
879.3599	882.4105	889.9715
901.8595	906.9257	922.3339
931.4493	937.2164	960.1230

963.1644 965.2711 971.5820

975.8576 978.0302 980.2638

985.2271 995.8545 997.3494

998.1070 1003.8477 1005.3976

1007.2280 1009.5976 1019.6966

1036.8630 1038.7559 1048.1623

1049.9414 1055.4235 1057.7087

1061.6075 1065.2150 1067.4770

1072.3292 1072.8790 1074.0962

1076.3864 1097.7836 1113.9807

1125.4798 1130.1568 1133.4011

1149.5191 1168.8251 1178.5421

1183.2026 1188.7997 1193.6273

1193.6935 1198.2125 1199.1720

1215.1976 1220.5614 1223.5582

1230.5004 1231.3284 1252.4373

1252.8112 1254.6914 1272.8698

1278.8810 1291.6466 1294.3989

1296.3467 1308.6317 1311.2325

1319.8702 1322.3724 1334.1450

1334.6289 1341.0980 1345.7474

1347.6324 1350.8309 1358.0661

1363.9152 1370.5164 1376.4109

1378.4311 1391.3480 1404.8500

1410.7650 1411.9493 1420.4609

1425.2264 1430.0359 1449.5590

1451.4142 1458.8677 1479.5939

1481.5779 1482.5593 1485.0449

1488.3179 1490.7532 1494.2347

1495.7966 1497.7955 1501.0132

1505.6843	1509.3274	1523.8380
1527.0583	1532.1024	1541.0618
1572.5299	1624.4829	1634.8345
1639.7867	1640.7558	1641.2011
1652.1453	1658.4531	1659.8871
1663.9940	1866.0697	3038.9407
3045.2763	3050.0787	3053.5089
3058.7710	3079.3527	3108.0161
3109.5033	3113.7372	3119.2606
3121.2620	3129.4445	3132.4255
3133.0428	3135.1236	3139.5898
3139.7609	3140.7952	3149.3460
3181.3594	3182.6766	3187.2479
3187.7388	3188.4306	3190.6058
3194.8864	3198.5078	3200.4402
3201.7285	3204.5941	3208.0683
3215.3076	3216.8803	3227.1558
3235.9272	3249.0455	3250.6846

M07R'

Zero-point correction= 0.940646

Thermal correction to Energy= 0.992120

Thermal correction to Enthalpy= 0.993064

Thermal correction to Gibbs Free Energy= 0.855576

Sum of electronic and zero-point Energies= -2924.892418

Sum of electronic and thermal Energies= -2924.840943

Sum of electronic and thermal Enthalpies= -2924.839999

Sum of electronic and thermal Free Energies= -2924.977487

Cartesian coordinates

C	2.076303	-0.746528	-0.095861

C	1.463359	0.392968	-0.907733
H	1.876305	-0.502176	0.946928
C	0.101449	0.897897	-0.305028
O	-0.328157	0.468497	0.846764
C	3.576606	-0.887581	-0.294983
C	4.426283	-0.741761	0.808432
C	4.136685	-1.165125	-1.550986
C	5.809957	-0.875844	0.665748
H	3.999493	-0.524088	1.782850
C	5.517508	-1.300616	-1.694318
H	3.492938	-1.275643	-2.417917
C	6.358507	-1.156746	-0.586692
H	6.454494	-0.761905	1.532136
H	5.938657	-1.516094	-2.672190
H	7.433411	-1.262381	-0.701017
C	-0.073744	2.430581	-0.318746
C	-0.993640	4.427895	-0.303373
C	-2.481044	2.646587	-1.191354
H	-2.259412	1.750681	-1.770688
N	0.192304	4.610842	0.207409
N	0.753493	3.345597	0.202291
N	-1.194573	3.110723	-0.641035
C	-2.063029	5.399800	-0.680140
H	-1.661077	6.413072	-0.721229
H	-2.887425	5.374871	0.045441
C	-3.128368	3.764886	-2.099420
O	-2.487950	5.041318	-1.994420
C	-4.709180	3.040321	-0.395310
C	-3.507138	2.389818	-0.107418
C	-3.350840	1.616138	1.042788

C	-4.437787	1.495480	1.911904
C	-5.648902	2.141138	1.630478
C	-5.792193	2.916995	0.476770
C	-4.624199	3.807252	-1.690186
H	-2.399573	1.134170	1.248229
H	-6.483862	2.042891	2.318519
H	-6.730492	3.422696	0.266010
H	-4.960927	4.845082	-1.601522
H	-5.239201	3.337700	-2.466551
C	2.086345	3.150949	0.714794
C	2.241926	2.716145	2.037317
C	3.168243	3.427135	-0.137259
C	3.550823	2.501966	2.486420
C	4.450521	3.197081	0.361591
C	4.660003	2.725607	1.664765
H	3.700667	2.153415	3.504625
H	5.306382	3.384642	-0.281568
C	2.947158	3.935172	-1.538703
H	3.899880	4.146034	-2.029398
H	2.350100	4.852899	-1.538537
H	2.410710	3.202070	-2.152691
C	6.062254	2.481736	2.161795
H	6.643456	1.915267	1.427352
H	6.066114	1.926751	3.103822
H	6.587893	3.429521	2.329745
C	1.052880	2.496566	2.934909
H	0.412294	1.704961	2.531923
H	0.447027	3.407392	3.007101
H	1.373802	2.219471	3.941936
H	-3.007095	3.497803	-3.149650

H	-4.340758	0.900271	2.815485
H	2.220438	1.157574	-1.061936
C	1.037510	-2.429075	-1.678094
C	0.721560	-1.409349	-2.601874
C	0.418412	-1.740432	-3.924962
C	0.398304	-3.065163	-4.356179
C	0.700702	-4.070613	-3.439037
C	1.028770	-3.762275	-2.119315
H	0.186457	-0.935782	-4.617982
H	0.153981	-3.307466	-5.385446
H	0.693334	-5.112207	-3.746087
H	1.233053	-4.578194	-1.441905
C	0.672013	0.018403	-2.164129
O	-0.597030	0.370628	-1.521604
N	1.345416	-2.033489	-0.342342
S	1.392355	-3.158713	0.928007
O	1.483032	-2.386415	2.173157
O	0.274519	-4.093162	0.734851
C	2.935496	-4.074078	0.766912
H	3.760597	-3.385972	0.950841
H	2.909243	-4.857600	1.527828
H	3.013551	-4.509257	-0.229494
H	0.858982	0.680959	-3.016053
C	-2.406907	-3.097553	-1.384466
C	-3.528893	-4.120933	-1.589571
C	-3.999081	-4.823302	-0.310182
C	-2.773608	-1.910330	-0.466405
C	-4.512160	-3.857254	0.764878
C	-2.666503	-2.247732	0.995991
H	-1.515851	-3.587319	-0.981680

H	-4.390914	-3.616371	-2.048699
H	-3.187974	-5.425355	0.118632
H	-5.159676	-3.094188	0.320474
H	-3.790249	-1.559385	-0.682000
H	-2.120341	-2.683344	-2.356690
H	-3.190739	-4.876207	-2.308987
H	-4.813653	-5.513775	-0.558717
H	-2.096717	-1.078543	-0.665828
H	-5.116164	-4.392076	1.499759
C	-3.238535	-3.658039	2.920604
H	-3.396038	-4.739868	2.931916
H	-4.008247	-3.199934	3.553514
C	-1.838938	-3.318272	3.419629
H	-1.775543	-3.520960	4.491719
H	-1.102700	-3.940167	2.902416
C	-1.534535	-1.853863	3.129385
H	-0.491696	-1.614153	3.336078
H	-2.173702	-1.192757	3.728185
N	-1.765428	-1.600108	1.709061
N	-3.436799	-3.198003	1.530715
H	-1.159250	-0.889795	1.239906

Vibrational frequencies

15.9072	24.9017	26.3498
32.6560	37.6357	41.3554
43.2814	48.1117	49.2735
51.9861	57.1298	62.0030
68.4317	72.3823	80.3363
83.3951	86.3750	88.5778
89.8787	105.2047	108.1396
117.4284	123.6590	128.6735

133.1265	138.0679	152.3881
156.0719	169.9833	176.0155
183.7492	186.9131	189.7023
202.3465	209.0220	214.7411
220.1221	233.7247	235.3686
239.4234	243.0395	253.0046
259.9641	264.6124	272.2194
278.9509	288.5603	300.4132
309.1787	318.3820	319.9998
327.4512	332.9545	348.9749
357.5346	363.2130	376.3992
384.0815	393.8202	402.5625
405.5665	413.0347	419.1573
427.8479	428.5957	449.8605
455.2533	470.8499	476.4165
487.3277	489.0316	495.9434
500.7891	511.7934	516.1657
520.5793	522.4265	526.6290
528.2306	531.1187	544.1093
548.0688	580.9437	582.3669
593.1791	596.6736	603.8590
610.7970	613.8651	620.1480
633.2718	638.4123	648.8400
655.6069	672.2117	703.2564
705.6612	713.4466	717.2085
720.4416	727.5363	732.6422
747.8227	755.2154	765.5215
768.3265	770.6280	782.6714
793.3678	799.6158	800.1518
808.6953	824.8227	830.2270

843.1456	849.0096	852.4613
862.4309	865.7633	870.1311
872.7467	877.8861	880.3262
883.0282	900.1450	906.7302
909.1436	913.7513	921.5024
932.6093	935.3129	939.2581
944.5824	953.4312	954.8908
960.0118	963.4775	972.7923
982.2443	983.3758	984.0427
985.3910	987.7035	991.5756
993.2478	999.9143	1003.6373
1005.3929	1005.8376	1015.6029
1016.8533	1023.2181	1025.5902
1028.4660	1034.7768	1040.8747
1044.5041	1052.2952	1055.6162
1058.3025	1064.5790	1066.5364
1071.5417	1073.6888	1078.8184
1088.2758	1091.6896	1095.7359
1100.9757	1105.1848	1112.9097
1116.0080	1116.9362	1117.9576
1133.1818	1138.7484	1148.5172
1154.8079	1183.3583	1185.9008
1187.1289	1187.2128	1196.3700
1202.7462	1205.9728	1212.7827
1217.5062	1221.4745	1221.8415
1225.2646	1233.9132	1237.6020
1249.2264	1250.3982	1253.3569
1253.9053	1263.0712	1271.3606
1272.1531	1291.9398	1292.6623
1295.2390	1302.3001	1305.2247

1306.9130	1308.0463	1314.6179
1315.6958	1322.2837	1324.5917
1327.8518	1337.2050	1342.6596
1344.5541	1349.5632	1351.8747
1359.2366	1359.6884	1367.6250
1369.3099	1370.2661	1373.1586
1378.8844	1382.3276	1382.5983
1394.1082	1400.5449	1401.3705
1407.4417	1408.5221	1410.7218
1418.6236	1419.6000	1420.9316
1426.6056	1429.3619	1436.4014
1448.8755	1451.9264	1459.9968
1462.3336	1469.6435	1470.7136
1478.0982	1479.5089	1482.4804
1486.5203	1488.6840	1489.7247
1490.7965	1493.6984	1495.9199
1497.2432	1498.0639	1500.0790
1501.8516	1504.1787	1504.2266
1511.2793	1519.1764	1519.5553
1524.5958	1526.9887	1534.7013
1535.9826	1537.5712	1632.0064
1636.7437	1638.1816	1640.3520
1641.7749	1653.1881	1656.2394
1656.9520	1657.6219	1658.3578
1696.3037	2974.6157	3021.1050
3035.7630	3039.1545	3041.8717
3042.3994	3043.4507	3045.2524
3048.9366	3054.7448	3057.3776
3061.3890	3065.0491	3069.2301
3076.0125	3082.8180	3083.4596

3088.1511	3101.7563	3102.1767
3102.3319	3104.2080	3111.0718
3122.5658	3129.0420	3130.5383
3134.9653	3136.1341	3136.7022
3137.9173	3139.5771	3140.9554
3141.2667	3154.9926	3155.1576
3171.2677	3181.9408	3182.8023
3183.2920	3183.3164	3185.0382
3187.5869	3189.2126	3190.0690
3195.6288	3196.0373	3198.6371
3202.3756	3205.8088	3206.0177
3211.4425	3213.8841	3259.5351

M07R''

Zero-point correction= 0.557123

Thermal correction to Energy= 0.587337

Thermal correction to Enthalpy= 0.588281

Thermal correction to Gibbs Free Energy= 0.495263

Sum of electronic and zero-point Energies= -1872.807261

Sum of electronic and thermal Energies= -1872.777047

Sum of electronic and thermal Enthalpies= -1872.776103

Sum of electronic and thermal Free Energies= -1872.869120

Cartesian coordinates

C	0.903843	0.101677	-0.359838
C	0.814402	-1.274211	-1.030286
H	-0.043309	0.274432	0.152274
C	0.419607	-2.410838	-0.097816
O	-0.554131	-2.743627	0.537561
C	1.142843	1.256478	-1.319998
C	0.518145	2.483905	-1.059671

C	1.982306	1.149727	-2.436563
C	0.735948	3.586562	-1.886168
H	-0.148327	2.572159	-0.206862
C	2.203911	2.253109	-3.263015
H	2.471433	0.210326	-2.670072
C	1.584077	3.474152	-2.989881
H	0.240217	4.528741	-1.670998
H	2.860433	2.155796	-4.122590
H	1.756868	4.330112	-3.635458
H	0.216627	-1.232266	-1.942974
C	3.263610	-0.363675	0.327345
C	3.376135	-1.389733	-0.631487
C	4.638399	-1.774959	-1.091519
C	5.791223	-1.180218	-0.583747
C	5.674210	-0.181609	0.384990
C	4.421073	0.239468	0.828698
H	4.707411	-2.555671	-1.844127
H	6.768652	-1.490432	-0.938587
H	6.563690	0.291987	0.789077
H	4.357071	1.027512	1.567647
C	2.147626	-2.055000	-1.146355
O	1.591273	-3.069132	-0.171737
N	1.949392	0.040668	0.702380
S	1.543860	0.405260	2.304013
O	0.107919	0.122631	2.447983
O	2.520163	-0.263447	3.165648
C	1.745829	2.183436	2.459305
H	1.070220	2.671625	1.756595
H	1.486086	2.445817	3.487577
H	2.780052	2.454244	2.245662

H	2.310812	-2.560640	-2.097904
C	-2.536748	1.395360	0.965145
C	-3.645198	2.440819	1.131649
C	-4.920781	2.166103	0.327514
C	-2.923260	-0.031452	1.412279
C	-5.578815	0.820731	0.655533
C	-3.731017	-0.776215	0.385069
H	-2.195634	1.367184	-0.077424
H	-3.908228	2.502569	2.196308
H	-4.716579	2.205297	-0.749888
H	-5.604027	0.654202	1.736995
H	-3.488194	0.009635	2.350694
H	-1.673678	1.687756	1.570141
H	-3.249761	3.423957	0.851177
H	-5.651751	2.954170	0.540580
H	-2.018332	-0.606321	1.615926
H	-6.613197	0.809615	0.310075
C	-5.677414	-0.995357	-1.086462
H	-6.204276	-0.214516	-1.639992
H	-6.427557	-1.655683	-0.636560
C	-4.744650	-1.767921	-2.011899
H	-5.337595	-2.363732	-2.709636
H	-4.138432	-1.066160	-2.594360
C	-3.832738	-2.668064	-1.187734
H	-3.047357	-3.119101	-1.797879
H	-4.401901	-3.475978	-0.714221
N	-3.186014	-1.858060	-0.154218
N	-4.924689	-0.333815	0.001658
H	-2.251203	-2.127417	0.159690

Vibrational frequencies

20.5619	28.6211	37.3050
44.2698	48.6537	59.2386
65.5140	71.4124	80.4189
86.3474	88.1721	97.4379
113.1846	121.3071	145.8267
154.8569	171.0506	185.6723
217.2065	218.7083	227.1256
238.6067	258.7946	265.2239
274.0011	281.6583	302.4490
317.7861	346.2612	346.9931
351.4192	373.5665	389.1627
408.0812	411.4229	419.6779
422.6084	438.2786	476.1138
484.7578	486.8171	508.3251
515.5180	515.9634	524.9879
538.8140	594.0280	599.1197
615.0993	633.8191	642.6569
664.3603	697.7091	702.1042
714.4141	722.1191	727.3251
743.9165	765.1333	771.2575
776.7121	787.7138	809.7827
814.7759	832.9925	842.5030
849.0996	865.2182	871.6019
875.4464	878.8379	890.4030
903.7311	910.4896	932.7782
935.7558	946.8811	966.7007
977.4520	983.7031	988.7638
990.9431	993.5529	997.2923
1002.0039	1002.5680	1010.9392
1014.3394	1018.4403	1027.9406

1032.1107	1058.1482	1079.7733
1095.4744	1103.8448	1105.8425
1115.6281	1118.0372	1122.6435
1128.6638	1135.4563	1153.6865
1184.9723	1186.0662	1189.3269
1192.8709	1201.1939	1216.3648
1216.9455	1222.4271	1232.4728
1235.6041	1250.5736	1257.8368
1258.9381	1271.9394	1299.3127
1302.7544	1313.9314	1314.8765
1321.4791	1322.0475	1325.2272
1341.2173	1351.5653	1355.5077
1364.2343	1364.9414	1370.9796
1377.6266	1379.1426	1386.9071
1395.7317	1400.6731	1403.3326
1405.1853	1409.6433	1420.6697
1444.4984	1455.2372	1458.6228
1474.8531	1480.4758	1491.8989
1492.8697	1493.6935	1499.2540
1502.4255	1510.5957	1512.5002
1519.2398	1534.2825	1539.1455
1634.6200	1639.0932	1639.8862
1657.6861	1658.9250	1685.5251
1862.6980	3031.4057	3043.0723
3049.4604	3059.1351	3063.2383
3063.8911	3072.5600	3078.2327
3081.6138	3084.0143	3093.5259
3110.2678	3119.2341	3128.2190
3129.6552	3136.1822	3136.8696
3140.0681	3141.8364	3145.4154

3187.1506	3188.1138	3193.1633
3196.2933	3200.8376	3205.1660
3208.4332	3216.9433	3219.2076
3222.2088	3244.1878	3404.4782

NHC

Zero-point correction= 0.413569

Thermal correction to Energy= 0.434531

Thermal correction to Enthalpy= 0.435475

Thermal correction to Gibbs Free Energy= 0.364738

Sum of electronic and zero-point Energies= -940.716083

Sum of electronic and thermal Energies= -940.695121

Sum of electronic and thermal Enthalpies= -940.694177

Sum of electronic and thermal Free Energies= -940.764914

Cartesian coordinates

C	-0.013016	-0.866644	0.907155
C	1.132742	-1.464456	-1.024241
N	-0.203607	-1.405020	-0.359071
H	1.524311	-2.476890	-0.702306
C	-2.613049	-1.336883	-0.037192
C	-1.173698	-0.842195	1.855754
C	-1.448322	-1.068625	-1.035391
H	-1.052224	-0.045567	2.594316
H	-1.584818	-1.785786	-1.855693
H	-1.243485	-1.799121	2.398052
C	3.301488	-0.571723	0.004351
C	3.808060	0.703207	0.705782
H	4.896906	0.674323	0.835750
H	3.551495	1.589112	0.114649
H	3.344902	0.813898	1.689417

C	3.923980	-0.641489	-1.399509
H	5.017723	-0.599358	-1.329172
H	3.646480	-1.561492	-1.919459
H	3.587780	0.200984	-2.012814
C	3.743664	-1.808704	0.823553
H	3.342379	-1.754652	1.840565
H	3.377295	-2.734302	0.368417
H	4.836592	-1.871040	0.885713
N	1.841347	-0.474139	-0.140455
N	1.169079	-0.406482	1.137743
O	-2.408916	-0.577635	1.176667
C	-3.971088	-0.875087	-0.565225
H	-4.187592	-1.346628	-1.529082
H	-4.758210	-1.158579	0.140683
H	-4.013646	0.206897	-0.696413
C	-2.696624	-2.842560	0.279453
H	-3.397945	-3.007319	1.103982
H	-3.058360	-3.394457	-0.594421
H	-1.723461	-3.253830	0.552708
C	-1.419373	0.332414	-1.727182
H	-0.677989	0.221724	-2.525397
H	-2.385911	0.507905	-2.213503
C	-1.025814	1.531280	-0.891023
C	-1.920338	2.170648	-0.017579
C	0.275166	2.048174	-0.990911
C	-1.527947	3.275655	0.737647
H	-2.927460	1.787040	0.091122
C	0.676502	3.148718	-0.230127
H	0.985106	1.556153	-1.644823
C	-0.222222	3.768144	0.638420

H	-2.239779	3.750045	1.408780
H	1.695589	3.517334	-0.315806
H	0.087255	4.624930	1.231461

Vibrational frequencies

9.7777	52.2310	65.8779
68.8515	84.8666	123.2812
147.6069	164.0491	185.8837
199.3240	212.9904	231.1254
246.6407	257.0880	264.2836
274.3545	286.5160	300.9278
310.3737	326.4374	343.6213
355.2943	388.2669	407.0294
415.0474	422.6570	430.3236
458.6681	471.7818	494.0552
503.2635	528.1912	552.3612
570.9351	600.9954	636.9170
640.9806	658.1373	703.9602
710.3932	755.7915	764.4151
774.9266	795.5059	811.7969
841.7633	852.3478	878.7637
907.4281	912.4437	926.9597
935.2929	939.9016	945.7297
953.8559	961.3842	961.9505
982.1396	989.3352	1012.5062
1018.3678	1030.9958	1042.7406
1045.5685	1057.2742	1058.9544
1068.5290	1089.9467	1110.8389
1142.6363	1171.4937	1182.9428
1210.2515	1212.6493	1221.2775
1230.8016	1234.9707	1243.2979

1249.1661	1258.9395	1266.3253
1279.2222	1303.0872	1324.7575
1352.9516	1360.2964	1365.7424
1383.6672	1389.3820	1394.7101
1397.5608	1402.1754	1417.1359
1422.9412	1425.2440	1472.7219
1481.6090	1484.7018	1487.0710
1489.3956	1489.5443	1493.5074
1493.8717	1498.1596	1499.1476
1508.3311	1519.5024	1523.5734
1537.0388	1632.0030	1654.8421
1674.8663	2558.5402	2979.2928
3023.4380	3029.8473	3032.0408
3039.6455	3046.3680	3047.8504
3056.6170	3089.7183	3098.0292
3101.8789	3101.8913	3106.3810
3114.4613	3117.1430	3122.5788
3128.3018	3132.4797	3150.0800
3153.5626	3167.2728	3177.1459
3192.2855	3225.3972	3227.2166

NHC'

Zero-point correction= 0.407440

Thermal correction to Energy= 0.427828

Thermal correction to Enthalpy= 0.428772

Thermal correction to Gibbs Free Energy= 0.359310

Sum of electronic and zero-point Energies= -940.113370

Sum of electronic and thermal Energies= -940.092982

Sum of electronic and thermal Enthalpies= -940.092038

Sum of electronic and thermal Free Energies= -940.161500

Cartesian coordinates

C	0.440532	-0.591496	0.904916
C	1.526786	-0.651715	-1.079698
N	0.344025	-0.916307	-0.425348
C	-1.759795	-2.049840	0.047643
C	-0.692591	-0.831792	1.857773
C	-0.917972	-1.335644	-1.046155
H	-0.895254	0.074961	2.434564
H	-0.669434	-2.073685	-1.813600
H	-0.404371	-1.621493	2.567171
C	3.677974	0.297977	-0.102398
C	4.513251	-0.596010	0.828076
H	5.558117	-0.270882	0.818471
H	4.144440	-0.544523	1.855680
H	4.472842	-1.638869	0.496871
C	3.704702	1.758376	0.376858
H	4.731757	2.135622	0.361902
H	3.095546	2.390156	-0.278042
H	3.319291	1.844705	1.395812
C	4.203442	0.204992	-1.537520
H	4.185289	-0.822962	-1.907554
H	3.615841	0.823241	-2.220613
H	5.238563	0.559779	-1.553184
N	2.269232	-0.176161	-0.059988
N	1.628777	-0.132531	1.178222
O	-1.897784	-1.163099	1.180386
C	-3.188637	-2.322944	-0.414663
H	-3.190298	-2.873852	-1.359832
H	-3.706432	-2.925838	0.336640
H	-3.747457	-1.396393	-0.545944

C	-1.099368	-3.378265	0.455087
H	-1.626202	-3.796392	1.317684
H	-1.164619	-4.095193	-0.368930
H	-0.043123	-3.271248	0.713623
C	-1.575796	-0.126254	-1.764975
H	-0.879808	0.154042	-2.562947
H	-2.490795	-0.472339	-2.253227
C	-1.861099	1.092424	-0.910851
C	-3.158924	1.396047	-0.477864
C	-0.821041	1.959383	-0.540113
C	-3.408796	2.510410	0.324208
H	-3.985655	0.756856	-0.773754
C	-1.063666	3.070230	0.269651
H	0.187080	1.763504	-0.891293
C	-2.359379	3.347789	0.710345
H	-4.423895	2.724532	0.647413
H	-0.239562	3.720756	0.549665
H	-2.551577	4.213294	1.338216

Vibrational frequencies

27.2371	33.9886	45.8861
69.0698	107.5451	120.5770
137.9550	153.4286	199.1391
203.7522	228.7422	246.9385
253.3005	254.4723	273.8573
296.2289	303.9101	310.9887
327.3700	335.4412	344.0279
373.3294	384.8931	407.1273
417.8683	426.0177	457.7632
470.1986	489.6334	508.0316
518.2960	541.3888	588.7992

599.0468	636.3181	655.3392
675.6694	695.2574	716.6180
725.3459	768.7858	773.7627
799.9290	845.1968	854.6241
870.1603	887.8483	933.2371
941.1455	951.1156	954.3112
966.0576	968.9536	972.7833
981.8521	987.3370	1004.5731
1010.7561	1016.4622	1031.8652
1045.2172	1058.7050	1060.5109
1063.6789	1106.8164	1114.5825
1133.4352	1166.6682	1187.6707
1195.4443	1212.3896	1220.6537
1226.8703	1238.9707	1248.0760
1255.9947	1258.7950	1278.1183
1291.3997	1296.1527	1310.2605
1347.4249	1361.4867	1371.3741
1391.0793	1396.8587	1408.1517
1410.0335	1413.0125	1416.8275
1427.6906	1437.5078	1450.6751
1479.3920	1484.7867	1487.4688
1488.8185	1492.0383	1494.5469
1495.8487	1501.9680	1502.8737
1503.6819	1504.8508	1518.5305
1523.9743	1538.2054	1632.1311
1636.4307	1659.7466	3014.2830
3048.3131	3051.4848	3056.6629
3060.2870	3062.5062	3065.7153
3092.3856	3107.9167	3115.7877
3123.3439	3124.6349	3129.4093

3133.5418	3134.6483	3137.0053
3139.0807	3141.1209	3143.8589
3169.8472	3177.6305	3184.3356
3194.0772	3200.7138	3207.6989

TS8R

Zero-point correction= 0.686909

Thermal correction to Energy= 0.728412

Thermal correction to Enthalpy= 0.729357

Thermal correction to Gibbs Free Energy= 0.610339

Sum of electronic and zero-point Energies= -2462.929064

Sum of electronic and thermal Energies= -2462.887560

Sum of electronic and thermal Enthalpies= -2462.886616

Sum of electronic and thermal Free Energies= -2463.005633

Cartesian coordinates

C	2.728412	1.168376	-0.761739
C	2.190667	0.467360	-2.012243
H	2.026141	1.981246	-0.575207
C	0.645628	0.291283	-1.974900
O	-0.086260	1.237608	-1.646287
C	4.122626	1.757910	-0.924843
C	4.225538	3.045113	-1.469314
C	5.293310	1.067543	-0.586965
C	5.474154	3.628809	-1.683220
H	3.320901	3.592543	-1.721687
C	6.543458	1.654186	-0.796071
H	5.240800	0.074378	-0.153295
C	6.638113	2.933525	-1.347157
H	5.536780	4.629123	-2.101411
H	7.443312	1.108535	-0.527396

H	7.611188	3.388669	-1.506307
C	-2.675456	0.099643	-0.771388
C	-4.171640	-1.317228	-0.044634
C	-2.171000	-2.377825	-1.085018
H	-1.514528	-2.062814	-1.898101
N	-4.625766	-0.142869	0.307695
N	-3.665042	0.735403	-0.150153
N	-2.972619	-1.204053	-0.705186
C	-4.757850	-2.688855	0.054290
H	-5.839039	-2.636152	0.189342
H	-4.324674	-3.235350	0.902921
C	-3.118557	-3.571462	-1.489454
O	-4.500527	-3.330253	-1.193917
C	-1.608021	-4.260048	0.290752
C	-1.385809	-2.894239	0.101185
C	-0.551594	-2.165896	0.948112
C	0.053718	-2.829619	2.016707
C	-0.156995	-4.200848	2.209387
C	-0.983430	-4.925827	1.346595
C	-2.551498	-4.811327	-0.748638
H	-0.381990	-1.104519	0.793048
H	0.322568	-4.705037	3.043653
H	-1.149778	-5.987748	1.504819
H	-3.368896	-5.401986	-0.322646
H	-2.023540	-5.461225	-1.455949
C	-3.755338	2.147811	0.106736
C	-4.822846	2.861747	-0.456987
C	-2.765434	2.743457	0.907745
C	-4.882498	4.233465	-0.193560
C	-2.875842	4.117673	1.133261

C	-3.922331	4.876584	0.594923
H	-5.696592	4.811464	-0.622227
H	-2.125028	4.606033	1.749053
C	-1.611336	1.960753	1.485190
H	-1.923160	0.976534	1.849288
H	-1.161969	2.501880	2.319954
H	-0.824599	1.810429	0.738048
C	-3.997602	6.359375	0.859734
H	-4.902022	6.800474	0.432412
H	-3.132474	6.877586	0.429756
H	-3.992544	6.567562	1.935567
C	-5.863687	2.190016	-1.316258
H	-6.473608	2.935576	-1.831421
H	-6.528892	1.561710	-0.714979
H	-5.405916	1.541306	-2.070839
H	-3.103518	-3.706169	-2.571148
H	0.688558	-2.271890	2.694599
H	2.458714	1.058307	-2.892647
C	2.940618	-1.099835	0.284075
C	2.989288	-1.688997	-1.036110
C	3.348433	-3.061511	-1.193130
C	3.641406	-3.846003	-0.106887
C	3.570368	-3.266493	1.176310
C	3.228693	-1.937571	1.378282
H	3.373326	-3.463451	-2.201167
H	3.915345	-4.888198	-0.223638
H	3.794780	-3.874049	2.047806
H	3.176669	-1.571588	2.391457
C	2.600656	-0.949773	-2.147490
O	0.319168	-0.895447	-2.289629

N	2.623533	0.245914	0.402102
S	2.300171	1.010473	1.937243
O	1.747220	2.323317	1.608147
O	1.516412	0.062069	2.732498
C	3.918178	1.242724	2.679320
H	4.494804	1.906039	2.034076
H	3.742051	1.704080	3.654398
H	4.414979	0.279437	2.797175
H	2.651840	-1.402858	-3.130442
H	-1.778570	0.549460	-1.210052

Vibrational frequencies

-123.6371	14.1361	20.3806
25.8781	29.5652	31.8509
38.4934	41.6394	50.2356
51.3790	56.8671	60.6813
65.6982	71.8533	80.1722
83.8956	86.0826	100.1793
112.9407	127.1436	140.5999
153.6760	164.0378	169.4828
183.1403	186.1520	195.1791
197.6402	203.8830	220.1754
226.0031	230.0725	237.2609
242.1479	253.7689	264.9315
278.0853	287.0795	291.9079
294.1444	300.8188	321.4248
333.1151	336.1438	356.9190
377.2562	380.4422	402.9785
405.8716	417.1591	427.0588
447.3492	461.5026	469.5411
478.6762	482.2958	493.6266

501.9056 505.3413 513.8122

522.2435 524.8330 528.5084

534.8903 554.1282 567.4696

579.4556 593.1922 597.6777

603.5631 612.4846 619.1396

620.9188 632.2000 635.7737

669.1706 695.5066 704.9053

716.2146 718.9121 728.0784

738.3022 742.5217 746.0985

763.0156 766.5477 769.8035

781.0532 794.1208 796.1175

819.5581 826.8219 837.2580

847.2855 864.0751 869.5355

872.3820 875.4449 882.2806

891.3242 904.7889 907.9291

932.5941 940.6797 947.3533

959.6207 967.5821 968.1010

972.5104 975.4686 985.2017

986.5334 993.4525 996.3171

996.9661 1001.2774 1011.0848

1014.3935 1014.8022 1023.5137

1026.6485 1033.0091 1037.8472

1039.3248 1046.4312 1049.5576

1055.6082 1058.1584 1061.3061

1064.9422 1069.2024 1070.0080

1071.3251 1075.7371 1099.2419

1116.2715 1119.9071 1125.8292

1148.1075 1169.5167 1186.4967

1189.0272 1189.6819 1195.0774

1195.5676 1202.0931 1206.7042

1215.6569	1217.5012	1220.6978
1230.6587	1248.4834	1250.1092
1269.0513	1269.8786	1273.5895
1276.7132	1294.6137	1299.6337
1306.5001	1307.6379	1320.3086
1331.2907	1333.7991	1336.5582
1342.7936	1345.2817	1352.1269
1365.0229	1366.4325	1371.2305
1374.0613	1376.8531	1379.6501
1409.3221	1410.2945	1419.6860
1421.9531	1426.9886	1428.0916
1444.5402	1446.3714	1447.8599
1451.4129	1451.7341	1457.5037
1470.8054	1481.3726	1483.0047
1485.6146	1489.6488	1490.5368
1494.8837	1499.1416	1499.7512
1502.8280	1506.9762	1521.7363
1523.8935	1538.1991	1560.1012
1572.4158	1587.3950	1637.7660
1639.1810	1641.6347	1643.0895
1653.4072	1657.8453	1658.4984
1660.0719	1719.8736	3028.2138
3040.6537	3043.7372	3049.1834
3050.5572	3057.4609	3081.3482
3101.3291	3102.1570	3102.5799
3111.3347	3113.6799	3123.1379
3129.8761	3132.0386	3134.2672
3141.0209	3143.6684	3150.5634
3181.9874	3182.7815	3184.5855
3186.9452	3188.8768	3189.6595

3195.1010	3197.9118	3200.1788
3204.5484	3206.7776	3207.7609
3212.2201	3213.7210	3232.3176
3236.5094	3239.9473	3280.5895

TS8R'

Zero-point correction= 0.936519

Thermal correction to Energy= 0.988713

Thermal correction to Enthalpy= 0.989657

Thermal correction to Gibbs Free Energy= 0.849213

Sum of electronic and zero-point Energies= -2924.838814

Sum of electronic and thermal Energies= -2924.786620

Sum of electronic and thermal Enthalpies= -2924.785676

Sum of electronic and thermal Free Energies= -2924.926120

Cartesian coordinates

C	1.277900	1.530013	-0.826238
C	-0.103810	1.244954	-1.360644
H	1.211850	1.583723	0.265076
C	-0.977528	0.000708	0.116188
O	-0.357438	0.036058	1.204334
C	1.863649	2.838175	-1.342061
C	2.276031	3.824854	-0.440062
C	2.016699	3.061793	-2.717437
C	2.826506	5.023545	-0.903780
H	2.168379	3.648448	0.625132
C	2.575399	4.251677	-3.181644
H	1.692523	2.298297	-3.419310
C	2.979984	5.237608	-2.274677
H	3.138285	5.784844	-0.194234
H	2.691868	4.415013	-4.249385

H	3.410040	6.166806	-2.637319
C	-2.291323	0.741851	0.088757
C	-4.356995	1.363402	-0.339308
C	-3.767666	-0.915398	-1.212671
H	-2.896527	-1.189275	-1.802389
N	-3.869641	2.321321	0.399946
N	-2.583948	1.912624	0.682976
N	-3.430028	0.370456	-0.551350
C	-5.691812	1.265964	-1.001036
H	-6.077043	2.265291	-1.212008
H	-6.411035	0.752359	-0.348905
C	-5.060519	-0.753425	-2.107390
O	-5.512876	0.593893	-2.242309
C	-5.441872	-2.430463	-0.385728
C	-4.126562	-1.991967	-0.211832
C	-3.304575	-2.540201	0.774504
C	-3.828949	-3.529762	1.607564
C	-5.149796	-3.967770	1.444482
C	-5.960714	-3.426017	0.444835
C	-6.127605	-1.720052	-1.522864
H	-2.277247	-2.208545	0.879977
H	-5.545526	-4.739084	2.099091
H	-6.982119	-3.773333	0.316029
H	-7.014442	-1.169088	-1.190666
H	-6.470421	-2.420084	-2.291483
C	-1.737577	2.734491	1.508178
C	-1.559631	2.351479	2.851885
C	-1.167683	3.892914	0.968047
C	-0.714997	3.133371	3.636168
C	-0.322285	4.639715	1.802162

C	-0.072439	4.271123	3.123557
H	-0.555057	2.855209	4.674930
H	0.144941	5.533392	1.397098
C	-1.424379	4.383231	-0.434932
H	-0.493157	4.404510	-1.009775
H	-1.808888	5.408256	-0.404954
H	-2.151506	3.777429	-0.975316
C	0.844302	5.084969	4.002194
H	1.329179	5.889684	3.442888
H	1.626880	4.457092	4.442700
H	0.291693	5.537902	4.833847
C	-2.263519	1.147977	3.421685
H	-1.835054	0.229710	3.010157
H	-3.331533	1.157187	3.177415
H	-2.164676	1.121955	4.509632
H	-4.798673	-1.045002	-3.124877
H	-3.206997	-3.967268	2.383058
H	-0.691446	2.124866	-1.584202
C	2.061920	-0.459110	-2.229156
C	0.750791	-0.665089	-2.724375
C	0.539067	-1.521205	-3.813333
C	1.597999	-2.173902	-4.434655
C	2.891495	-1.954736	-3.956703
C	3.127758	-1.104869	-2.876860
H	-0.478374	-1.661045	-4.168831
H	1.422602	-2.834309	-5.277557
H	3.737560	-2.444772	-4.429256
H	4.144568	-0.990229	-2.531399
C	-0.360354	0.072426	-2.134748
O	-0.886350	-1.053831	-0.731585

N	2.214548	0.377778	-1.095981
S	3.621536	0.338660	-0.144874
O	3.300505	1.029225	1.109939
O	4.098846	-1.050685	-0.098848
C	4.854090	1.329280	-1.006159
H	4.526918	2.368451	-0.997523
H	5.787262	1.210508	-0.450798
H	4.968247	0.966972	-2.027878
H	-1.281597	0.056720	-2.710380
C	1.923397	-3.750610	-0.781744
C	2.640028	-5.104192	-0.740162
C	3.603874	-5.283025	0.439183
C	1.023261	-3.450874	0.436944
C	2.928976	-5.133360	1.808113
C	1.791838	-2.960797	1.635164
H	2.651513	-2.941879	-0.885172
H	1.888569	-5.905599	-0.702637
H	4.429327	-4.563014	0.374515
H	1.971147	-5.663852	1.826646
H	0.456070	-4.346300	0.720416
H	1.287459	-3.711544	-1.672363
H	3.192529	-5.239680	-1.677722
H	4.047862	-6.284313	0.390871
H	0.302360	-2.677493	0.161773
H	3.549190	-5.578454	2.588057
C	3.587074	-3.215364	3.289945
H	4.584015	-3.633908	3.128731
H	3.214518	-3.593578	4.249397
C	3.643895	-1.692279	3.278900
H	4.151007	-1.341529	4.181233

H	4.207896	-1.351671	2.407145
C	2.232164	-1.124806	3.203033
H	2.243863	-0.048721	3.030654
H	1.672979	-1.330085	4.124406
N	1.542517	-1.737790	2.068668
N	2.715164	-3.730184	2.213108
H	0.848811	-1.153709	1.571926

Vibrational frequencies

-795.7187	10.4337	21.5405
24.6322	26.9404	31.5905
35.2807	37.8804	39.3517
46.6738	52.1605	56.4840
58.3162	64.5169	68.2811
71.7948	79.2288	85.3491
88.7490	91.0893	94.4641
101.5301	110.8631	118.9628
125.7627	128.5372	138.3514
142.4537	161.8932	170.9043
175.5342	187.7848	190.9847
194.3504	202.4658	206.5199
213.1573	217.8620	225.3679
230.8632	233.7320	246.2003
249.6179	255.5268	258.4150
270.7436	273.8066	288.6037
294.5164	304.4836	315.1997
317.0962	327.5588	336.1735
337.8934	349.8368	355.7450
363.4799	372.2955	375.7154
388.0572	400.3393	406.7387
408.6617	416.9441	425.5152

434.8897	447.5321	450.4785
461.2732	483.2761	484.7413
486.6739	494.8043	508.5301
510.8244	515.0908	517.6146
522.0278	524.5233	528.5733
538.1176	546.6754	562.7065
572.4997	575.3178	583.1151
588.0678	598.1580	607.4896
615.7338	621.1914	632.1645
637.8337	648.0875	658.2983
668.3653	687.0736	699.6059
702.8251	710.6790	714.4924
721.8670	726.5841	741.0403
746.2005	756.8279	758.0580
769.1884	769.8385	779.7975
790.6689	795.7992	806.7726
807.5282	824.2623	837.5151
849.9293	854.2419	858.8043
861.5105	863.3110	867.7019
873.2791	876.3745	876.6597
878.0688	881.4462	901.4359
903.4116	907.8317	915.4995
932.8726	935.3818	943.2814
953.3293	954.7440	962.2998
969.5648	977.1173	980.2443
983.1295	984.8309	990.0408
993.7536	996.6338	1001.2119
1002.2102	1002.6082	1010.0342
1016.2251	1016.8491	1018.0369
1027.4648	1037.7211	1040.4441

1044.8825	1047.4205	1055.2558
1056.4905	1056.8594	1058.7196
1060.3045	1066.7296	1069.2390
1073.1975	1087.2663	1096.6574
1106.3349	1107.0710	1111.5884
1116.2889	1116.4478	1117.1915
1126.1223	1129.8815	1139.0013
1154.2607	1159.7076	1179.0029
1186.3883	1186.9372	1187.9638
1192.7743	1198.1190	1201.0805
1209.9315	1213.4173	1218.0177
1219.2466	1222.5390	1226.3952
1237.9999	1238.5672	1243.7577
1250.5713	1253.9609	1262.4292
1272.7325	1274.5088	1290.9972
1292.3136	1295.7144	1300.1778
1304.4449	1307.4885	1317.0992
1317.4875	1321.1031	1325.6661
1328.2574	1336.6880	1343.5237
1357.9990	1358.3482	1359.2034
1363.3416	1366.4256	1368.3852
1370.0657	1378.1091	1381.3791
1383.5008	1395.1845	1397.8015
1398.4981	1403.3203	1406.1450
1408.4477	1413.7375	1416.7592
1417.6071	1421.5564	1423.1586
1428.9115	1441.3596	1447.4833
1450.7551	1453.3904	1456.8661
1460.0016	1475.6645	1476.6653
1477.6840	1482.1306	1486.1115

1488.1523	1491.1453	1492.5028
1494.7520	1495.3963	1496.4304
1498.1082	1500.6868	1501.9724
1503.0094	1505.8065	1507.8051
1516.9344	1518.3246	1520.7477
1524.2635	1529.8161	1531.7196
1535.2985	1576.6804	1624.2669
1633.9690	1638.5060	1639.8140
1640.5359	1647.7217	1653.9969
1655.6464	1655.9794	1657.3455
1692.9026	3020.8324	3040.8677
3041.2635	3041.3347	3047.8093
3048.0883	3050.7473	3052.1216
3057.0964	3062.6828	3063.4863
3065.8157	3068.0815	3075.4828
3082.7158	3089.5614	3091.2044
3097.0788	3099.8367	3112.9494
3113.0605	3113.9718	3119.1657
3126.1594	3129.0425	3130.0035
3131.7437	3139.5149	3144.4132
3147.2437	3155.4136	3169.8821
3170.3353	3179.1315	3180.4558
3181.0675	3183.0579	3183.4475
3183.7008	3186.1258	3187.3419
3187.4453	3192.9143	3196.0259
3197.1431	3204.7754	3205.0016
3205.9515	3211.5073	3214.6984
3218.9479	3239.7806	3263.5586

TS8R''

Zero-point correction= 0.554249

Thermal correction to Energy= 0.584692

Thermal correction to Enthalpy= 0.585636

Thermal correction to Gibbs Free Energy= 0.491390

Sum of electronic and zero-point Energies= -1872.783275

Sum of electronic and thermal Energies= -1872.752832

Sum of electronic and thermal Enthalpies= -1872.751888

Sum of electronic and thermal Free Energies= -1872.846134

Cartesian coordinates

C	1.097815	0.127351	0.166844
C	0.556325	-0.870179	-0.860541
H	0.475002	-0.009194	1.050631
C	0.065586	-2.204821	-0.206599
O	-0.685397	-2.153647	0.789075
C	1.019008	1.588121	-0.247226
C	0.233904	2.458405	0.519728
C	1.700717	2.093441	-1.364154
C	0.115181	3.805734	0.170584
H	-0.275676	2.079235	1.399672
C	1.586723	3.439527	-1.710383
H	2.322463	1.438586	-1.966680
C	0.790955	4.298747	-0.946460
H	-0.498804	4.467072	0.774792
H	2.117805	3.818287	-2.578744
H	0.703024	5.346080	-1.219688
H	-0.295216	-0.411748	-1.372049
C	3.387996	-0.827726	-0.294925
C	2.907185	-1.354457	-1.556138
C	3.828180	-1.896941	-2.505062
C	5.171502	-1.944662	-2.240938

C	5.625399	-1.462575	-0.994185
C	4.773320	-0.927113	-0.041476
H	3.424329	-2.275599	-3.438953
H	5.872829	-2.351650	-2.960237
H	6.685815	-1.503979	-0.763584
H	5.195844	-0.599604	0.895652
C	1.546316	-1.395778	-1.822573
O	0.530340	-3.212890	-0.798853
N	2.483453	-0.259846	0.582644
S	2.949543	0.329301	2.166843
O	1.692693	0.641647	2.846027
O	3.873875	-0.643835	2.749137
C	3.817385	1.856731	1.802485
H	3.102331	2.555666	1.368306
H	4.199065	2.230800	2.755354
H	4.639069	1.652433	1.114719
H	1.204118	-1.778784	-2.776673
C	-2.758835	1.173258	-1.127748
C	-3.824075	2.251528	-1.359755
C	-5.274360	1.779264	-1.197403
C	-2.769690	0.568712	0.293629
C	-5.587075	1.196185	0.185903
C	-3.824588	-0.488895	0.486952
H	-2.861534	0.368142	-1.865956
H	-3.641037	3.074761	-0.655403
H	-5.525002	1.030047	-1.959220
H	-5.162804	1.822994	0.976913
H	-2.913365	1.362590	1.035551
H	-1.771324	1.618999	-1.281451
H	-3.694041	2.668409	-2.365063

H	-5.944513	2.631493	-1.358030
H	-1.809222	0.104065	0.514826
H	-6.665319	1.169412	0.350188
C	-6.153678	-1.246205	0.421481
H	-6.932923	-0.975112	-0.294763
H	-6.598047	-1.240889	1.423366
C	-5.572269	-2.614807	0.083822
H	-6.318842	-3.386098	0.286809
H	-5.321296	-2.657231	-0.981278
C	-4.315724	-2.858255	0.911337
H	-3.783646	-3.755730	0.589312
H	-4.561064	-2.970890	1.973870
N	-3.412105	-1.720863	0.739131
N	-5.116616	-0.193257	0.363713
H	-2.395142	-1.891362	0.773619

Vibrational frequencies

-141.6142	21.9437	24.8810
33.6039	40.1755	46.4477
50.1185	54.4237	68.0637
74.3053	77.6611	82.4307
98.5698	112.2466	114.5497
150.0151	170.4295	181.7150
188.1427	204.3679	206.7633
226.6223	232.4747	253.7272
265.9123	268.1322	269.6148
290.9127	315.0816	320.6228
348.4300	349.9003	367.0623
367.8367	404.9346	408.3208
417.6561	429.7878	459.5682
473.3920	486.7957	487.3164

508.0916	513.5177	518.2109
522.6736	532.0199	554.6326
592.3319	620.0587	632.0919
638.7906	646.0098	660.5104
703.0503	705.6722	719.2003
728.9938	743.2199	761.1405
776.1168	785.0904	790.1333
806.1286	822.7371	837.7453
842.7454	846.7669	863.6682
869.7952	877.5563	881.1180
891.9733	904.2959	913.2094
931.5681	932.1229	942.9039
957.8193	974.9420	984.1327
990.6098	991.3412	998.6010
1000.9132	1008.4993	1013.1008
1014.2131	1016.3055	1024.9372
1029.7375	1034.7234	1058.6777
1078.4762	1092.8489	1102.2090
1114.7659	1118.9920	1126.7593
1130.5128	1133.7640	1158.3893
1173.0677	1178.9163	1182.7974
1190.7634	1211.3858	1217.1680
1218.4020	1222.8254	1232.6360
1245.8251	1254.0844	1255.2458
1268.4391	1287.6247	1297.9389
1312.0930	1313.7265	1318.2313
1322.3496	1342.8494	1353.9519
1361.0860	1363.7191	1369.0282
1374.7264	1375.7455	1376.0558
1389.1784	1393.3684	1398.3547

1398.6433	1406.3562	1416.7033
1418.2908	1439.0547	1442.6195
1450.1946	1453.0056	1456.7910
1475.7211	1486.0931	1488.1028
1493.8257	1496.8011	1498.3667
1503.7109	1508.5051	1514.0691
1516.3003	1538.3166	1568.2800
1585.7943	1638.5108	1645.0715
1656.4474	1661.1772	1686.7404
1714.5819	3028.3781	3039.0845
3046.0624	3056.0037	3060.0243
3068.9057	3073.4717	3075.3240
3081.4561	3081.6193	3091.3299
3101.7597	3103.7192	3119.0932
3129.8460	3130.2801	3135.6975
3137.7937	3154.5468	3187.5856
3187.9990	3194.5690	3202.6298
3204.8094	3206.1040	3210.1306
3210.4221	3215.7072	3223.3853
3232.6459	3240.0056	3281.2081

TS8R'''

Zero-point correction= 0.290642

Thermal correction to Energy= 0.309514

Thermal correction to Enthalpy= 0.310458

Thermal correction to Gibbs Free Energy= 0.243156

Sum of electronic and zero-point Energies= -1410.337544

Sum of electronic and thermal Energies= -1410.318671

Sum of electronic and thermal Enthalpies= -1410.317727

Sum of electronic and thermal Free Energies= -1410.385030

Cartesian coordinates

C	-0.535100	0.368399	-0.583150
C	-0.047810	1.738455	-0.128343
H	-0.579809	0.314203	-1.673467
C	-0.662907	3.131343	-0.282400
O	-1.828016	3.445208	-0.483124
C	-1.903731	0.067788	0.000498
C	-3.024614	0.063626	-0.833361
C	-2.068006	-0.148929	1.374209
C	-4.296779	-0.155208	-0.303055
H	-2.898549	0.226866	-1.899504
C	-3.338747	-0.375913	1.904385
H	-1.198165	-0.157909	2.025116
C	-4.456851	-0.377675	1.066267
H	-5.161053	-0.157047	-0.960743
H	-3.455052	-0.550486	2.970141
H	-5.446262	-0.553529	1.478360
H	0.032552	1.663963	0.965530
C	1.815236	-0.181004	0.267081
C	2.299336	1.130097	-0.100198
C	3.663905	1.458495	0.060498
C	4.533287	0.572545	0.667311
C	4.040895	-0.666287	1.107543
C	2.716763	-1.043404	0.909373
H	3.989780	2.448533	-0.243063
H	5.573590	0.836338	0.823203
H	4.707513	-1.360179	1.610548
H	2.398411	-2.022323	1.239914
C	1.328159	2.024555	-0.607917
H	1.528978	2.647899	-1.467724

O	0.366148	3.899330	-0.072348
N	0.516471	-0.603922	-0.090302
S	0.301896	-2.227854	-0.716305
O	-0.730448	-2.129789	-1.751618
O	1.615036	-2.785440	-1.051474
C	-0.368321	-3.112588	0.689140
H	-1.322025	-2.658536	0.957896
H	-0.505925	-4.148965	0.371454
H	0.340337	-3.055974	1.516555

Vibrational frequencies

-210.2124	32.5288	41.2206
61.5470	70.8281	83.6822
98.7400	121.1416	157.0366
188.0967	195.2165	209.1395
235.0772	251.7661	273.8031
283.2033	293.6445	311.9837
347.8907	361.2015	379.2961
418.6722	431.5379	471.5305
497.2414	506.9414	525.3214
547.6028	557.3259	593.0413
631.2188	638.4330	642.5039
650.9881	704.0858	716.3113
735.2327	746.3149	754.4147
770.5080	783.1220	793.7935
830.7527	862.2835	871.2132
889.1111	921.7653	934.1042
968.4272	971.7534	981.5660
990.9989	995.5516	1004.5466
1006.7869	1010.5102	1015.8142
1055.3850	1078.0220	1109.1218

1124.0455	1126.4560	1153.5891
1178.6233	1186.4592	1190.1118
1206.0556	1217.3962	1223.5099
1237.7862	1276.6635	1295.6710
1300.1659	1319.1701	1326.5679
1335.0335	1354.1081	1360.0826
1371.2202	1390.7500	1400.0571
1429.6398	1442.2119	1448.5752
1488.3319	1494.6568	1515.5519
1535.7023	1592.0266	1641.3997
1648.8503	1657.1859	1788.2502
3020.2565	3078.8206	3099.4927
3180.4079	3183.1554	3186.2765
3193.6363	3201.2000	3203.0749
3204.0151	3209.4578	3209.7750
3226.1273	3254.2205	3260.2883

TS8R''''

Zero-point correction= 0.674487

Thermal correction to Energy= 0.714888

Thermal correction to Enthalpy= 0.715832

Thermal correction to Gibbs Free Energy= 0.603210

Sum of electronic and zero-point Energies= -2462.436504

Sum of electronic and thermal Energies= -2462.396102

Sum of electronic and thermal Enthalpies= -2462.395158

Sum of electronic and thermal Free Energies= -2462.507780

Cartesian coordinates

C	-1.604102	0.429606	-0.237400
C	-0.195197	0.417582	-0.864654
H	-1.690449	-0.422755	0.429545

C	1.108945	0.379025	1.400356
O	1.212012	-0.207479	2.480928
C	-2.731978	0.336605	-1.256614
C	-3.834067	-0.479455	-0.966771
C	-2.722608	1.057701	-2.458317
C	-4.908238	-0.570783	-1.853159
H	-3.838844	-1.058930	-0.049278
C	-3.797632	0.970043	-3.344860
H	-1.874079	1.685390	-2.709223
C	-4.893092	0.156435	-3.045179
H	-5.749440	-1.215570	-1.615346
H	-3.776485	1.534121	-4.272878
H	-5.725289	0.085419	-3.739537
C	0.942678	-0.520326	0.067664
C	2.481316	-1.891217	-0.931887
C	3.326958	0.364062	-0.662657
H	2.922027	1.363816	-0.517052
N	1.537831	-2.707441	-0.600240
N	0.613151	-1.921074	0.114763
N	2.236807	-0.601190	-0.552246
C	3.725088	-2.142102	-1.722471
H	3.621554	-3.058638	-2.306393
H	4.596448	-2.248119	-1.062973
C	4.000200	0.250426	-2.073233
O	3.882120	-1.061792	-2.646445
C	5.704040	0.323706	-0.369285
C	4.488071	0.145158	0.300127
C	4.451687	-0.170190	1.657048
C	5.663666	-0.301439	2.342883
C	6.882569	-0.115140	1.681054

C	6.909978	0.198578	0.318424
C	5.473857	0.642102	-1.827431
H	3.507404	-0.325399	2.168657
H	7.815204	-0.223482	2.227785
H	7.856712	0.330590	-0.198667
H	6.136280	0.099817	-2.508617
H	5.611801	1.714112	-2.019320
C	-0.680474	-2.546842	0.244688
C	-1.155823	-2.905277	1.523126
C	-1.409810	-2.903159	-0.917168
C	-2.398840	-3.545619	1.617769
C	-2.629501	-3.565714	-0.761686
C	-3.154320	-3.880482	0.494620
H	-2.770017	-3.807720	2.605448
H	-3.194055	-3.826436	-1.654196
C	-0.980334	-2.580049	-2.331023
H	-1.540638	-1.717246	-2.709799
H	-1.207972	-3.421902	-2.992339
H	0.083319	-2.370200	-2.421799
C	-4.485981	-4.579284	0.615866
H	-4.435800	-5.599452	0.216250
H	-5.261140	-4.051796	0.047987
H	-4.814042	-4.643685	1.657134
C	-0.388231	-2.637888	2.788069
H	-0.600037	-1.632041	3.155633
H	0.688541	-2.681772	2.626666
H	-0.673687	-3.361587	3.558014
H	3.513005	0.912007	-2.793953
H	5.656492	-0.552782	3.399645
H	-0.181935	-0.165706	-1.783317

C	-1.398272	2.895287	0.184910
C	-0.297224	2.931658	-0.715668
C	0.158710	4.168938	-1.215820
C	-0.457796	5.354273	-0.848763
C	-1.530863	5.310160	0.049721
C	-2.000514	4.101024	0.562282
H	1.005645	4.171672	-1.896297
H	-0.107101	6.303375	-1.240251
H	-2.016923	6.230935	0.357934
H	-2.812862	4.119437	1.274817
C	0.357057	1.720307	-1.066975
O	1.251461	1.589736	1.099787
N	-1.786896	1.625510	0.644599
S	-2.615788	1.411717	2.118443
O	-2.498030	-0.011353	2.454628
O	-2.141303	2.438868	3.047766
C	-4.345742	1.734542	1.747749
H	-4.690291	0.998070	1.022349
H	-4.892454	1.634589	2.688362
H	-4.455852	2.743293	1.349487
H	1.246140	1.803106	-1.683017

Vibrational frequencies

-221.1205	20.8733	21.2057
37.8615	41.3720	45.6513
51.8867	55.3479	71.2595
75.7412	80.1659	86.3186
90.8027	101.2106	117.0595
118.0320	120.6306	127.9770
132.9153	148.1185	151.0519
155.7475	174.3068	179.6763

185.0262	190.2330	201.8129
205.0070	213.6446	215.2294
229.1221	235.0624	239.3188
249.6087	258.5867	263.8516
275.4158	292.5476	307.9431
312.2945	319.2211	333.8554
342.2974	361.0760	378.3002
386.1569	397.7123	399.0457
424.7383	425.3788	434.4109
440.0846	446.4959	467.9214
484.6866	487.8038	492.6247
497.4644	505.1718	516.1671
520.9944	536.4270	542.0488
550.6242	557.5063	576.0876
577.1607	579.1792	591.9610
596.6190	606.6083	617.7963
627.2916	633.6538	642.7372
669.2191	681.6753	702.4211
723.4160	725.1557	729.2536
737.8616	749.0784	751.0383
760.7604	763.9899	773.9538
779.9237	791.2969	803.2575
820.6054	826.2723	839.2591
841.3771	860.4586	867.2537
870.0205	874.8180	875.8045
889.5110	902.5608	910.3942
924.8385	942.8248	946.3798
954.9202	959.4500	960.4264
969.6235	975.8325	976.7871
980.4421	987.9147	991.9695

992.5068	995.5196	1002.5421
1005.4541	1010.8558	1016.2981
1025.4802	1035.9853	1039.4162
1041.2963	1044.3728	1050.4415
1053.1063	1056.6726	1059.8398
1063.4121	1065.0330	1071.1524
1080.8428	1082.4673	1094.2746
1114.4909	1117.8615	1122.3547
1142.0296	1151.3340	1167.6810
1181.8594	1189.8360	1190.8369
1193.1537	1202.5549	1204.8813
1209.1818	1218.4302	1225.9966
1232.6075	1240.6735	1253.0329
1263.4386	1269.9334	1271.5425
1284.6890	1290.8090	1298.7851
1310.4911	1312.6040	1316.0612
1320.0779	1327.6486	1337.9815
1339.0993	1339.3413	1357.3960
1367.7323	1369.5640	1371.7511
1372.3584	1378.6753	1387.5244
1397.1254	1409.4736	1409.9553
1415.2927	1420.0988	1425.4017
1449.0823	1454.5538	1455.2259
1459.9191	1463.3147	1467.2453
1480.6105	1483.0824	1485.5224
1490.1258	1498.1929	1498.3885
1500.0248	1502.4336	1505.8708
1517.5562	1520.5459	1521.5224
1537.9560	1540.2823	1614.5001
1623.6762	1638.7823	1639.4990

1649.2609	1655.9576	1657.8564
1659.1478	1682.3891	1773.8345
3036.8782	3039.7536	3044.1216
3050.1848	3059.7772	3082.4147
3093.3985	3097.0265	3105.4513
3105.9537	3124.9775	3140.0325
3142.0741	3154.5883	3159.4983
3165.5320	3169.4333	3170.5767
3175.8528	3180.6716	3181.4379
3183.6265	3185.7037	3190.4417
3191.8759	3192.0122	3199.3418
3201.5498	3203.8007	3204.2214
3208.8564	3213.3241	3213.8635
3215.0019	3218.4061	3257.4719

TS9

Zero-point correction= 0.799578

Thermal correction to Energy= 0.842175

Thermal correction to Enthalpy= 0.843120

Thermal correction to Gibbs Free Energy= 0.723022

Sum of electronic and zero-point Energies= -1978.472686

Sum of electronic and thermal Energies= -1978.430089

Sum of electronic and thermal Enthalpies= -1978.429145

Sum of electronic and thermal Free Energies= -1978.549242

Cartesian coordinates

C	3.908230	-3.792656	-1.336982
C	4.875287	-2.649218	-1.019919
C	4.468496	-1.306012	-1.654043
C	2.955787	-0.908666	-1.396928
C	2.048644	-2.140785	-1.701380

C	2.479629	-3.399731	-0.948376
H	5.113348	-0.509399	-1.281840
H	4.955228	-2.534777	0.063195
H	5.882447	-2.883896	-1.383915
H	3.937830	-4.023878	-2.410711
H	4.218133	-4.699399	-0.805937
H	1.017109	-1.861448	-1.476947
H	2.091350	-2.337312	-2.779666
H	2.421112	-3.231510	0.135264
H	1.776191	-4.207034	-1.181738
H	4.610650	-1.373509	-2.739025
C	2.641724	-0.224737	-0.013680
C	2.750402	1.331192	-0.255331
C	2.319695	1.418995	-1.726762
C	2.666739	0.179447	-2.346839
H	1.587186	-0.427576	0.183440
H	1.994265	1.816965	0.366614
H	2.545422	2.338824	-2.267616
C	3.403754	-0.713290	1.196716
O	4.595781	-0.600374	1.387845
O	2.560920	-1.290031	2.083239
C	3.162862	-1.792141	3.296287
H	3.660512	-0.985051	3.839154
H	2.340028	-2.196923	3.884678
H	3.887249	-2.577071	3.065874
C	4.081191	2.003360	0.033983
C	4.303885	2.531854	1.313495
C	5.088207	2.147937	-0.929503
C	5.502953	3.168424	1.629663
H	3.527954	2.437902	2.069532

C	6.292276	2.782994	-0.617184
H	4.939403	1.768103	-1.936113
C	6.504554	3.294628	0.663551
H	5.654018	3.569853	2.627701
H	7.060452	2.882093	-1.378861
H	7.438198	3.794150	0.905275
C	0.660616	1.225249	-1.855389
O	0.007625	1.975172	-1.134759
O	0.335850	0.320511	-2.656410
H	2.738181	0.027366	-3.418460
C	-3.628639	0.240840	1.497479
C	-2.742322	1.490783	-0.053073
N	-2.544388	0.376286	0.670853
C	-1.411665	-1.428749	1.841249
C	-3.691626	-0.878526	2.493676
C	-1.503008	-0.657926	0.492911
H	-4.676031	-1.351137	2.456331
H	-0.564554	-0.122725	0.344265
H	-3.554414	-0.460598	3.500889
C	-4.612192	3.223314	-0.151905
C	-4.758452	4.180152	1.037291
H	-5.295869	5.074529	0.711004
H	-5.322046	3.714148	1.849029
H	-3.777677	4.483921	1.415566
C	-5.977261	2.763310	-0.680893
H	-6.516231	3.629142	-1.074221
H	-5.856312	2.031216	-1.485153
H	-6.576285	2.312330	0.113559
C	-3.775715	3.852495	-1.267690
H	-2.785846	4.158353	-0.915290

H	-3.660246	3.174206	-2.118754
H	-4.295765	4.746185	-1.619998
N	-3.899297	1.999126	0.343094
N	-4.469874	1.230185	1.322859
O	-2.733621	-1.884075	2.209120
C	-0.579830	-2.700473	1.707049
H	0.411789	-2.468672	1.311024
H	-0.456182	-3.152466	2.694662
H	-1.065177	-3.432502	1.059371
C	-0.796938	-0.530807	2.927680
H	-0.882411	-1.029014	3.897230
H	0.263900	-0.371502	2.715270
H	-1.274604	0.450054	3.002180
C	-1.821894	-1.461774	-0.800578
H	-1.472163	-0.847663	-1.635239
H	-1.201973	-2.361020	-0.800277
C	-3.281446	-1.808773	-1.003552
C	-3.873778	-2.920019	-0.387345
C	-4.084466	-0.982711	-1.804146
C	-5.234370	-3.184197	-0.550041
H	-3.270815	-3.568461	0.237987
C	-5.447851	-1.239469	-1.964202
H	-3.633344	-0.132490	-2.309619
C	-6.028036	-2.340811	-1.332457
H	-5.676175	-4.049699	-0.064209
H	-6.051892	-0.586340	-2.587732
H	-7.087629	-2.546086	-1.454511
H	-2.048499	1.870024	-0.790187

Vibrational frequencies

-452.8997	15.2291	16.1518

22.8411	30.5366	38.3256
44.8202	47.0669	50.5342
55.0321	62.9954	68.6402
70.2592	73.0733	83.8125
96.5229	105.1625	108.6333
117.8161	126.2752	129.2386
132.5635	135.6817	156.6733
164.4967	173.9721	195.2479
200.7063	206.9928	218.4376
224.7031	225.9785	250.3542
252.3772	256.4719	259.7764
262.5852	270.1486	282.3761
297.6946	305.2704	308.7449
313.7315	329.5597	334.6755
342.6066	352.4457	353.6975
372.7566	384.6539	387.3485
397.7677	412.3012	418.7376
423.1321	429.9295	439.6978
450.5151	453.1896	473.6464
487.4785	490.9228	506.2520
511.8942	514.0655	538.4379
546.6751	547.2626	579.5408
587.1895	602.1444	622.6466
634.0839	635.1660	653.0095
656.2481	690.2953	705.8942
709.5799	714.4263	718.7345
722.6412	741.4754	748.1286
771.3497	775.5089	776.5215
783.7734	796.3770	802.3561
825.3340	826.4782	835.8192

850.1477	852.8447	864.3246
866.9182	867.6043	884.2869
896.1568	918.3315	924.5921
933.6040	936.3736	941.0934
949.1885	953.2457	954.0433
956.4714	961.5962	972.6053
976.0133	978.2139	982.4084
986.6602	990.9223	993.1183
1005.0432	1006.1658	1006.6825
1015.1573	1017.2764	1018.8369
1021.8462	1032.9095	1045.5590
1045.9615	1058.7395	1059.5027
1061.9947	1066.8066	1067.2171
1067.7492	1074.4365	1089.7041
1095.7962	1105.5377	1114.2745
1115.6542	1126.6808	1145.1612
1168.9867	1176.8940	1182.0198
1188.9909	1189.6211	1190.1819
1195.5868	1203.0140	1207.7094
1214.3767	1217.7589	1218.6246
1222.4870	1224.3433	1224.5695
1236.4419	1239.1602	1254.8464
1261.9166	1264.9207	1269.3926
1279.6108	1289.3009	1291.3995
1298.2660	1300.3687	1313.4577
1322.6471	1326.1290	1341.3298
1352.7310	1354.8748	1356.9837
1359.3266	1367.8376	1369.5244
1380.3995	1386.5996	1393.3340
1394.9240	1396.9023	1402.1180

1403.8721	1415.4955	1419.4881
1420.3215	1423.4279	1434.3907
1443.0543	1453.2058	1456.7658
1471.5290	1476.7625	1479.5766
1481.6856	1482.2400	1484.4566
1486.1991	1487.9009	1488.4823
1491.5689	1492.9242	1493.3054
1493.5288	1493.9326	1496.3491
1497.2162	1502.8728	1506.8310
1508.6645	1511.1758	1516.4410
1521.1735	1521.7312	1539.3786
1541.1373	1574.0575	1618.4098
1636.8796	1638.5052	1658.5975
1659.1438	1782.6434	1812.7346
3029.0727	3032.4895	3036.6573
3051.3995	3054.1873	3054.3427
3056.8428	3057.6975	3061.6329
3062.1095	3069.0594	3070.1934
3082.0049	3082.5879	3085.9781
3097.6876	3122.0894	3123.1768
3128.9824	3129.8320	3131.0140
3131.7591	3136.9851	3138.0258
3140.1614	3141.2753	3142.8212
3146.7555	3147.6456	3149.1571
3150.7265	3153.4080	3153.4439
3161.6045	3164.8234	3172.0233
3175.8408	3184.0892	3184.4366
3185.0666	3191.8808	3194.0159
3199.9900	3206.2490	3209.9757
3222.1377	3236.2168	3259.0139

TS9'

Zero-point correction= 0.376673

Thermal correction to Energy= 0.396976

Thermal correction to Enthalpy= 0.397920

Thermal correction to Gibbs Free Energy= 0.327264

Sum of electronic and zero-point Energies= -1037.854363

Sum of electronic and thermal Energies= -1037.834060

Sum of electronic and thermal Enthalpies= -1037.833116

Sum of electronic and thermal Free Energies= -1037.903773

Cartesian coordinates

C	-3.216074	-1.825531	-1.502238
C	-1.720836	-1.922723	-1.815622
C	-1.010935	-0.555565	-1.850868
C	-1.313326	0.364858	-0.603163
C	-2.846942	0.369639	-0.334191
C	-3.436960	-1.035409	-0.208328
H	0.066071	-0.704190	-1.936374
H	-1.240031	-2.567240	-1.076646
H	-1.562060	-2.398393	-2.790999
H	-3.740473	-1.318827	-2.324649
H	-3.645770	-2.830653	-1.422304
H	-3.032567	0.974040	0.557038
H	-3.336444	0.886220	-1.169271
H	-2.976285	-1.562405	0.638093
H	-4.506406	-0.951945	0.016778
H	-1.345931	-0.014367	-2.744201
C	-0.455238	0.081237	0.690800
C	0.798174	1.039154	0.608820
C	0.214130	2.213671	-0.181095

C	-0.848273	1.718701	-0.988381
H	-1.051431	0.432317	1.536397
H	1.026292	1.371614	1.625365
H	0.907636	2.934173	-0.614016
C	-0.101081	-1.361198	0.973448
O	0.617177	-2.064714	0.291917
O	-0.679211	-1.785011	2.116382
C	-0.408911	-3.155048	2.479600
H	0.665415	-3.319948	2.593229
H	-0.920096	-3.313823	3.429080
H	-0.799931	-3.837508	1.720131
C	2.076458	0.472954	0.014792
C	3.010884	-0.129992	0.869088
C	2.376361	0.543602	-1.351834
C	4.198751	-0.665533	0.373634
H	2.798323	-0.183984	1.934082
C	3.564442	0.007654	-1.853899
H	1.682784	1.021661	-2.037136
C	4.479441	-0.601128	-0.993669
H	4.907025	-1.129184	1.054639
H	3.775416	0.071449	-2.917794
H	5.405365	-1.014762	-1.382916
C	-0.830408	3.124716	0.808520
O	-0.355125	3.486628	1.866732
O	-1.957616	3.253688	0.269134
H	-1.256652	2.226673	-1.854346

Vibrational frequencies

-583.7462	32.1263	36.3244
50.6733	68.8567	76.1154
98.3486	107.3191	120.8407

130.5938	134.5636	166.0202
191.1444	215.9807	224.0270
244.4637	255.6374	260.3739
311.3476	335.3697	354.7773
385.0639	401.1163	422.2871
437.8228	453.2737	474.2583
510.5172	544.9981	550.0654
599.1124	623.9336	634.2670
646.8440	705.8344	716.9283
739.5049	746.2242	775.9385
784.8065	800.1365	823.2199
828.2479	855.1770	862.9782
866.5104	899.3592	928.6531
932.8663	939.3620	957.2051
958.8608	976.9426	980.7038
998.3395	1002.0286	1014.4027
1019.7962	1049.5313	1058.4959
1061.9686	1063.5549	1076.2929
1089.5597	1096.5283	1108.6909
1123.2647	1168.6597	1181.2498
1189.5980	1191.7082	1196.4622
1205.1350	1217.1081	1224.2211
1227.0337	1256.5579	1274.8707
1291.9609	1296.8686	1313.9961
1326.0285	1338.8098	1355.1957
1358.3262	1369.9386	1379.2935
1387.0582	1394.3531	1396.8383
1401.1498	1415.3263	1459.1220
1476.4551	1478.6631	1483.9975
1489.2746	1494.3814	1495.1722

1497.1320	1501.7959	1513.9974
1541.1671	1638.1858	1659.1333
1804.1911	1837.4476	3023.9780
3034.4921	3044.2673	3046.6717
3056.0946	3063.9810	3077.4184
3083.3567	3087.5283	3098.6823
3116.5251	3124.8909	3145.6673
3147.0423	3149.4591	3174.5085
3177.8196	3180.9074	3189.6941
3197.2053	3207.6097	3244.3397

P0'

Zero-point correction= 0.804565

Thermal correction to Energy= 0.846406

Thermal correction to Enthalpy= 0.847351

Thermal correction to Gibbs Free Energy= 0.730060

Sum of electronic and zero-point Energies= -1978.510655

Sum of electronic and thermal Energies= -1978.468814

Sum of electronic and thermal Enthalpies= -1978.467869

Sum of electronic and thermal Free Energies= -1978.585160

Cartesian coordinates

C	4.014138	-3.642060	-1.452878
C	4.918518	-2.433375	-1.193312
C	4.339956	-1.124167	-1.761646
C	2.852280	-0.837758	-1.405513
C	2.010173	-2.122345	-1.599557
C	2.599432	-3.369102	-0.931096
H	4.970727	-0.288736	-1.454032
H	5.082982	-2.332018	-0.118256
H	5.905613	-2.591744	-1.643476

H	3.963692	-3.846032	-2.532030
H	4.435049	-4.536981	-0.979853
H	0.991547	-1.939946	-1.248022
H	1.934396	-2.313740	-2.678689
H	2.625312	-3.237753	0.158451
H	1.941949	-4.224516	-1.125195
H	4.396962	-1.178816	-2.856926
C	2.603655	-0.161669	-0.004386
C	2.821145	1.391760	-0.173635
C	2.330674	1.620882	-1.619607
C	2.334676	0.261870	-2.348382
H	1.535489	-0.282491	0.189567
H	2.131356	1.884295	0.519558
H	2.764173	2.486711	-2.119353
C	3.303091	-0.759653	1.194229
O	4.489684	-0.712724	1.438622
O	2.406283	-1.366022	2.009403
C	2.948067	-1.993486	3.190506
H	3.445315	-1.253446	3.822260
H	2.093745	-2.425334	3.711209
H	3.661736	-2.774118	2.916387
C	4.200186	1.964924	0.115051
C	4.514572	2.315232	1.436000
C	5.161122	2.193255	-0.878230
C	5.755575	2.859626	1.761106
H	3.777959	2.151065	2.218442
C	6.407336	2.737407	-0.557391
H	4.947831	1.950896	-1.914640
C	6.710512	3.070277	0.763111
H	5.976386	3.121905	2.791892

H	7.138011	2.903228	-1.343896
H	7.678216	3.495826	1.012318
C	0.823563	1.516415	-1.771016
O	-0.141650	2.170754	-1.462462
O	0.831365	0.315197	-2.401991
H	2.713984	0.206382	-3.368132
C	-3.661921	0.166004	1.524025
C	-2.762280	1.483703	0.039248
N	-2.566273	0.339360	0.718374
C	-1.464340	-1.540660	1.810615
C	-3.737469	-0.991872	2.472766
C	-1.526710	-0.693440	0.504817
H	-4.729134	-1.447329	2.423211
H	-0.575477	-0.167512	0.409690
H	-3.588155	-0.617002	3.495163
C	-4.651323	3.203656	-0.018305
C	-4.799497	4.125079	1.198301
H	-5.347289	5.023009	0.900307
H	-5.354619	3.631674	1.999670
H	-3.819612	4.427749	1.579680
C	-6.014553	2.746306	-0.554626
H	-6.556920	3.616965	-0.932063
H	-5.889561	2.029030	-1.371451
H	-6.611614	2.278686	0.231455
C	-3.826743	3.871240	-1.119788
H	-2.842108	4.186326	-0.761369
H	-3.700928	3.214658	-1.986220
H	-4.361954	4.764041	-1.450879
N	-3.927522	1.969373	0.439813
N	-4.504974	1.158042	1.379276

O	-2.796311	-1.996993	2.136544
C	-0.648008	-2.814609	1.614559
H	0.346034	-2.577400	1.228669
H	-0.531720	-3.316165	2.578796
H	-1.143760	-3.508645	0.933385
C	-0.852915	-0.712746	2.952561
H	-0.941384	-1.270557	3.888674
H	0.207394	-0.541103	2.750543
H	-1.330409	0.261750	3.087791
C	-1.820620	-1.424885	-0.837425
H	-1.433575	-0.780618	-1.632196
H	-1.218964	-2.335206	-0.863565
C	-3.279389	-1.727783	-1.107524
C	-3.922935	-2.839874	-0.546047
C	-4.027632	-0.860658	-1.917058
C	-5.281851	-3.064066	-0.771330
H	-3.363748	-3.520064	0.086026
C	-5.388889	-1.078759	-2.140425
H	-3.535876	-0.009137	-2.380869
C	-6.021317	-2.180915	-1.562726
H	-5.764244	-3.930291	-0.327425
H	-5.949984	-0.394812	-2.770877
H	-7.079437	-2.356095	-1.734005
H	-2.080631	1.891745	-0.692842

Vibrational frequencies

19.3122	22.9567	26.1403
39.6266	43.6698	46.2403
48.6147	52.4725	54.1840
64.3809	71.2254	72.0877
78.4194	84.1538	91.3835

110.7118	119.2803	129.7002
134.6071	139.3240	142.2417
145.9115	161.5767	164.9369
193.1866	202.6227	206.6504
211.8001	218.3504	239.3391
250.4969	252.2266	264.5216
265.9313	270.0936	276.6392
293.2199	295.8428	300.9997
307.6404	318.5623	331.0344
337.0568	340.9937	348.9027
354.7724	356.6399	374.8217
381.9562	389.4779	414.0304
422.3241	424.9715	425.1882
430.1799	449.1706	452.1205
460.1287	473.5303	489.6363
507.2363	509.2618	511.9362
516.5903	548.9353	563.5937
577.0011	580.5959	586.7665
628.6670	634.1341	635.1839
656.7292	688.0699	690.2423
710.4400	714.5868	718.0206
720.4276	723.2742	740.2375
761.3155	769.8079	776.7805
786.2979	788.0995	798.5692
799.0648	826.0749	834.8415
838.6412	851.1135	853.2456
860.3590	867.5930	867.7646
868.2290	888.9223	902.1955
911.0564	930.0260	936.3783
940.7321	945.6489	949.5084

953.6407 954.5267 959.6308

966.3856 974.1999 980.1088

982.1377 985.5866 988.5945

989.0679 995.6713 1004.0959

1008.5472 1012.4949 1015.2432

1017.1472 1021.1474 1036.9794

1037.0791 1050.3155 1058.1632

1059.5342 1060.0460 1062.2846

1067.3608 1068.3986 1068.5097

1088.1970 1104.9182 1107.1994

1117.1752 1117.8109 1119.3103

1146.2448 1165.9125 1176.6923

1179.8877 1183.1673 1187.7871

1188.4118 1189.6745 1191.5180

1195.8142 1204.1100 1210.6745

1212.7926 1215.3907 1221.3241

1227.2923 1228.7335 1232.5852

1236.9795 1239.1538 1254.8708

1265.0139 1265.8761 1269.3955

1283.9483 1293.0928 1298.0985

1298.2871 1299.9237 1310.7872

1318.3879 1320.4227 1325.3403

1345.4006 1355.3028 1360.3404

1363.9895 1367.9102 1370.2118

1373.6050 1385.7611 1393.4347

1398.3912 1399.0684 1400.6723

1404.7616 1410.0838 1415.6227

1420.1882 1425.7810 1433.0333

1436.2511 1443.4044 1448.7913

1464.7177 1474.5433 1482.3547

1483.3432	1485.6961	1486.7933
1488.0480	1489.5981	1492.7748
1493.5823	1493.9666	1495.3728
1497.8444	1499.6677	1502.3429
1503.0559	1504.9269	1506.9172
1510.8377	1518.1260	1523.9084
1525.2206	1531.4493	1540.8063
1541.4482	1573.6027	1620.4361
1637.4999	1638.9273	1659.1432
1659.8400	1812.2753	1876.2155
3020.2352	3029.3135	3033.5331
3034.7338	3037.5552	3053.8204
3054.5111	3058.1161	3062.2435
3062.4973	3067.8360	3069.5427
3071.3309	3072.2127	3079.3358
3079.7377	3101.0698	3122.6841
3125.5984	3125.8087	3130.3550
3135.6552	3136.9682	3137.7056
3138.8030	3141.7113	3146.6986
3147.8129	3148.7177	3148.9703
3150.6300	3151.1461	3154.1458
3155.4992	3161.1152	3167.2904
3175.7685	3176.7665	3181.5992
3184.3672	3186.4497	3193.2264
3195.6248	3201.2362	3207.3826
3210.2508	3227.7582	3268.9884

P'

Zero-point correction= 0.380742

Thermal correction to Energy= 0.400441

Thermal correction to Enthalpy= 0.401385

Thermal correction to Gibbs Free Energy= 0.332648

Sum of electronic and zero-point Energies= -1037.898186

Sum of electronic and thermal Energies= -1037.878487

Sum of electronic and thermal Enthalpies= -1037.877543

Sum of electronic and thermal Free Energies= -1037.946280

Cartesian coordinates

C	-3.075655	-1.681144	-1.764662
C	-1.559816	-1.720533	-1.982329
C	-0.903903	-0.333650	-1.842990
C	-1.298453	0.476324	-0.574252
C	-2.830038	0.395827	-0.358419
C	-3.401882	-1.025049	-0.419082
H	0.180173	-0.444712	-1.898818
H	-1.113727	-2.417723	-1.269046
H	-1.326056	-2.109123	-2.980862
H	-3.553397	-1.103502	-2.569234
H	-3.490907	-2.694971	-1.812550
H	-3.088645	0.877890	0.588550
H	-3.308053	0.992202	-1.148136
H	-2.989906	-1.629105	0.399298
H	-4.486113	-0.983432	-0.261159
H	-1.207396	0.267682	-2.710680
C	-0.481068	0.128233	0.730473
C	0.858412	0.964222	0.693423
C	0.407337	2.251548	-0.022441
C	-0.893718	1.948559	-0.789492
H	-1.058925	0.539636	1.563095
H	1.110813	1.200479	1.732291
H	1.203466	2.787683	-0.539031

C	-0.280713	-1.337896	1.040232
O	0.448701	-2.103083	0.441818
O	-1.024730	-1.713470	2.103670
C	-0.924167	-3.105047	2.468984
H	0.100933	-3.353894	2.756188
H	-1.597368	-3.237925	3.315851
H	-1.228338	-3.746166	1.637391
C	2.098068	0.326080	0.084266
C	2.936227	-0.437423	0.909419
C	2.471777	0.503505	-1.254454
C	4.099844	-1.022006	0.412540
H	2.668659	-0.576670	1.953762
C	3.635546	-0.082317	-1.758746
H	1.857752	1.104694	-1.917751
C	4.453469	-0.849123	-0.928142
H	4.732668	-1.608961	1.072415
H	3.903212	0.067907	-2.800963
H	5.360830	-1.301106	-1.318521
C	-0.487137	3.161333	0.810374
O	-0.372926	3.894365	1.754244
O	-1.628275	2.885159	0.112447
H	-0.996618	2.296694	-1.817750

Vibrational frequencies

34.7236	41.1454	62.6000
75.5633	79.8594	100.4896
128.4834	130.8220	157.0352
179.8924	194.1798	207.4822
218.7246	235.0621	249.9762
260.3515	296.2895	306.5604
341.6159	357.5517	382.8399

419.6473	421.7412	445.5110
457.5453	502.1765	508.1190
561.7058	572.8180	627.3521
633.9136	685.5246	714.5677
717.5177	739.8527	758.8450
785.2640	788.0171	798.7493
824.9614	836.9022	859.0503
860.5233	862.0646	877.3221
910.4363	930.4326	936.5926
946.6602	954.4236	967.2853
973.2768	980.3333	994.2217
1001.6022	1014.7673	1031.8268
1056.2040	1060.7229	1062.0701
1064.8048	1087.3621	1106.2438
1114.6767	1115.4606	1160.5273
1162.5000	1180.8476	1188.0705
1189.0896	1191.1086	1195.4574
1209.1275	1218.2517	1219.5605
1232.5587	1265.4040	1282.9036
1291.4506	1297.1445	1308.7203
1317.7653	1324.1567	1348.9340
1361.5431	1364.3791	1364.8464
1385.6328	1391.7409	1394.1456
1402.7558	1408.3693	1422.2402
1483.5943	1484.6912	1486.4121
1492.2521	1492.8203	1497.3015
1500.1554	1505.3657	1518.3823
1538.2527	1637.1155	1658.7050
1801.9238	1905.5364	3016.0981
3021.9658	3026.5980	3038.8014

3050.3655	3063.2383	3066.9548
3068.7882	3080.5107	3084.1099
3100.3106	3121.7928	3134.9892
3137.3629	3143.4540	3145.7923
3174.7484	3177.7294	3182.3046
3191.1057	3199.2043	3208.2918

P''

Zero-point correction= 0.363860

Thermal correction to Energy= 0.381570

Thermal correction to Enthalpy= 0.382514

Thermal correction to Gibbs Free Energy= 0.317653

Sum of electronic and zero-point Energies= -849.344085

Sum of electronic and thermal Energies= -849.326376

Sum of electronic and thermal Enthalpies= -849.325431

Sum of electronic and thermal Free Energies= -849.390292

Cartesian coordinates

C	-4.266157	0.595232	-0.738010
C	-3.369560	1.266017	0.312119
C	-2.677717	0.218869	1.196567
C	-1.819073	-0.774623	0.382584
C	-2.733128	-1.433007	-0.694299
C	-3.470951	-0.413562	-1.576601
H	-2.070643	0.697689	1.967317
H	-2.612199	1.882538	-0.193117
H	-3.957574	1.949050	0.936740
H	-5.085423	0.072051	-0.224269
H	-4.729761	1.347861	-1.387214
H	-2.137487	-2.112969	-1.315272
H	-3.471900	-2.055440	-0.171282

H	-2.747168	0.129332	-2.199038
H	-4.135475	-0.943561	-2.269818
H	-3.448287	-0.366516	1.717674
C	-0.546886	-0.170236	-0.318038
C	0.514632	-1.343735	-0.285464
C	0.036368	-2.175724	0.885116
C	-1.209006	-1.865243	1.243129
H	-0.748490	0.112185	-1.351218
H	0.369755	-1.923147	-1.208004
H	0.644824	-2.965755	1.314667
C	0.033063	1.048083	0.373263
O	0.204115	1.187427	1.568978
O	0.403822	1.978652	-0.532089
C	1.093388	3.125052	0.004150
H	2.016858	2.815989	0.501080
H	1.319126	3.761484	-0.851938
H	0.461417	3.659744	0.718123
C	1.965482	-0.901327	-0.264861
C	2.643913	-0.675709	-1.470850
C	2.643675	-0.665203	0.939314
C	3.964004	-0.223958	-1.477542
H	2.128783	-0.853856	-2.411936
C	3.966446	-0.218174	0.936813
H	2.123557	-0.816540	1.879623
C	4.630648	0.006275	-0.271285
H	4.473022	-0.054944	-2.422566
H	4.477393	-0.043070	1.879705
H	5.659816	0.354155	-0.273125
H	-1.788484	-2.369084	2.012129

Vibrational frequencies

27.1819	36.1472	45.6305
69.0635	102.5802	128.2493
147.4619	151.0332	162.5859
204.5728	225.9125	240.2132
255.1461	268.7508	334.2438
347.5753	358.2589	385.1476
389.4601	417.7259	440.9041
460.4956	489.8266	536.4037
545.5231	608.8682	630.5099
633.7500	707.7226	714.8776
724.7814	754.0232	777.0388
807.8144	822.8272	835.8308
844.5472	862.6428	864.0290
867.2229	910.8284	925.5215
931.0882	950.1332	957.3135
969.8587	972.8988	979.3406
992.3965	1002.8304	1014.9274
1024.8352	1049.2896	1056.5530
1066.1060	1083.6821	1097.2495
1110.8554	1124.0486	1129.9034
1168.3768	1180.2950	1187.9132
1195.3349	1199.8189	1210.1177
1214.7804	1217.0955	1228.2346
1235.1601	1284.4231	1292.1835
1301.5746	1306.0924	1317.5794
1353.1615	1360.8083	1367.2179
1375.3361	1382.4401	1391.1741
1392.8384	1396.7147	1404.6828
1478.5594	1483.8820	1488.1994
1491.9094	1492.6161	1497.1662

1498.2121	1503.5069	1515.6212
1536.5472	1636.1817	1658.5665
1698.6468	1798.4547	3017.4606
3018.1464	3019.4920	3024.3916
3027.3969	3029.0078	3061.2058
3066.0441	3066.3924	3069.8029
3075.2787	3122.1525	3130.1219
3142.4948	3172.9112	3172.9844
3182.1569	3184.9655	3191.6116
3203.0123	3209.7751	3211.5899

P

Zero-point correction= 0.277916

Thermal correction to Energy= 0.294513

Thermal correction to Enthalpy= 0.295458

Thermal correction to Gibbs Free Energy= 0.233346

Sum of electronic and zero-point Energies= -1221.855378

Sum of electronic and thermal Energies= -1221.838780

Sum of electronic and thermal Enthalpies= -1221.837836

Sum of electronic and thermal Free Energies= -1221.899947

Cartesian coordinates

C	-0.590024	-0.196534	1.334982
C	0.090177	-1.281980	2.125689
H	-1.035456	0.505583	2.040478
C	-1.702846	-0.730615	0.436193
C	-2.987359	-0.179869	0.514570
C	-1.447162	-1.736620	-0.506317
C	-4.002337	-0.622699	-0.338130
H	-3.186783	0.608838	1.234467
C	-2.456870	-2.173729	-1.362721

H	-0.455833	-2.174834	-0.567997
C	-3.737612	-1.617705	-1.280716
H	-4.995249	-0.187838	-0.267174
H	-2.247223	-2.951142	-2.091964
H	-4.523957	-1.960847	-1.946928
H	-0.478778	-1.689599	2.955540
C	1.575776	-0.050927	0.010323
C	2.036615	-1.226030	0.658564
C	3.178401	-1.877282	0.174960
C	3.870004	-1.399868	-0.935686
C	3.408265	-0.248802	-1.572112
C	2.271871	0.419892	-1.111275
H	3.516205	-2.773750	0.688150
H	4.753924	-1.916039	-1.296842
H	3.929483	0.144286	-2.439946
H	1.968370	1.324063	-1.618510
C	1.300657	-1.750051	1.803038
H	1.756361	-2.554387	2.374448
N	0.431240	0.588392	0.567918
S	-0.017250	2.173722	0.145508
O	-1.014014	2.597411	1.136789
O	1.206691	2.961885	-0.033767
C	-0.849299	2.037496	-1.443962
H	-1.768299	1.468377	-1.304281
H	-1.072974	3.055350	-1.771737
H	-0.193430	1.541203	-2.159838

Vibrational frequencies

31.0181	46.0725	54.2494
70.8329	122.9242	162.1720
166.5648	192.0402	209.9067

247.7770	253.3033	259.3674
303.0443	324.9648	357.4243
374.4246	394.4676	416.9296
442.9397	477.1413	484.3612
503.0569	540.0425	541.2930
556.5159	592.2353	631.2438
643.0588	669.4647	715.8175
722.9549	733.5434	762.9280
780.5298	793.3665	812.5881
825.5194	852.2907	865.1529
881.3969	936.9442	951.2867
952.5774	983.0897	983.7809
987.5080	991.2864	995.5212
1007.8488	1009.6104	1015.6571
1055.7968	1064.2439	1087.5377
1114.1314	1119.4923	1152.9004
1187.5978	1195.5796	1202.6489
1210.8925	1213.2693	1232.8609
1254.9199	1290.6873	1307.5448
1337.7042	1352.1694	1361.5482
1370.8726	1373.3614	1401.7166
1424.9401	1445.6168	1458.5386
1489.9023	1494.6310	1527.3640
1534.5172	1620.9652	1638.5603
1650.6961	1654.7182	1721.8125
3080.9476	3118.7738	3181.5557
3184.4474	3184.6774	3185.3930
3187.7836	3194.1672	3196.4962
3201.4252	3205.2541	3209.2543
3210.8712	3211.4774	3258.6625

TS5R(Φ=50°)

Zero-point correction= 0.671833

Thermal correction to Energy= 0.713984

Thermal correction to Enthalpy= 0.714928

Thermal correction to Gibbs Free Energy= 0.595186

Sum of electronic and zero-point Energies= -2462.463337

Sum of electronic and thermal Energies= -2462.421186

Sum of electronic and thermal Enthalpies= -2462.420242

Sum of electronic and thermal Free Energies= -2462.539984

Cartesian coordinates

C	-1.737690	-0.711123	-1.233108
C	-0.753272	0.128938	-0.672564
H	-1.378365	-1.461748	-1.928085
C	0.615466	-0.149189	-0.831594
O	1.151463	-1.096646	-1.448639
C	-3.105261	-0.211767	-1.489837
C	-3.868690	-0.807363	-2.509738
C	-3.676847	0.836871	-0.745890
C	-5.161265	-0.362773	-2.785441
H	-3.441985	-1.633982	-3.069393
C	-4.972215	1.275084	-1.018619
H	-3.114575	1.313080	0.049497
C	-5.718423	0.680105	-2.039783
H	-5.734075	-0.831197	-3.580721
H	-5.400131	2.081948	-0.430250
H	-6.725855	1.026053	-2.252573
C	1.581704	0.794888	-0.142940
C	3.400747	1.549274	0.828284
C	3.495743	-0.864398	0.279869

H	2.719928	-1.625313	0.237428
N	2.605037	2.584950	0.770977
N	1.473616	2.100496	0.154540
N	2.812742	0.439934	0.280094
C	4.714390	1.362456	1.510882
H	4.920916	2.201601	2.176649
H	5.529427	1.279902	0.779283
C	4.367466	-1.028399	1.584263
O	4.579909	0.189636	2.309977
C	5.724818	-1.425073	-0.393924
C	4.482199	-0.989618	-0.860664
C	4.257216	-0.741843	-2.213879
C	5.315851	-0.921570	-3.107011
C	6.567542	-1.351024	-2.646784
C	6.778660	-1.610790	-1.289866
C	5.698281	-1.655470	1.096421
H	3.274099	-0.433080	-2.552817
H	7.382136	-1.485673	-3.352887
H	7.749785	-1.947376	-0.937406
H	6.544392	-1.204074	1.624002
H	5.712282	-2.728134	1.323068
C	0.326908	2.954638	-0.011123
C	-0.470763	3.189976	1.118333
C	0.023236	3.443938	-1.287791
C	-1.636769	3.937451	0.928180
C	-1.151622	4.187650	-1.420424
C	-1.997890	4.431052	-0.331577
H	-2.282826	4.125394	1.781344
H	-1.419960	4.571990	-2.400854
C	0.896122	3.133921	-2.475528

H	0.749241	2.096891	-2.800496
H	1.958134	3.258688	-2.241223
H	0.649841	3.785148	-3.317397
C	-3.297763	5.169136	-0.528711
H	-4.062572	4.489068	-0.924846
H	-3.188819	5.987263	-1.247519
H	-3.675192	5.581778	0.411161
C	-0.100354	2.629236	2.467023
H	0.765432	3.154746	2.885192
H	0.168460	1.569679	2.405397
H	-0.932050	2.727333	3.167823
H	3.836112	-1.665920	2.289485
H	5.166505	-0.731924	-4.165975
H	-1.046380	0.987446	-0.090996
C	-2.388868	-1.581520	1.413878
C	-1.290143	-1.191187	2.225861
C	-1.509035	-0.519789	3.441114
C	-2.796259	-0.232794	3.872569
C	-3.886298	-0.602334	3.071044
C	-3.687892	-1.249518	1.855924
H	-0.643366	-0.242965	4.034635
H	-2.959194	0.276515	4.817582
H	-4.897711	-0.364561	3.389008
H	-4.537732	-1.473704	1.223845
C	0.088556	-1.501871	1.814300
H	0.177188	-2.203456	0.969728
O	1.089162	-1.040028	2.363442
N	-2.122636	-2.113738	0.150639
S	-2.679636	-3.562363	-0.352735
O	-2.252302	-3.696246	-1.761593

O	-2.280662	-4.615160	0.606073
C	-4.489015	-3.599521	-0.384350
H	-4.859832	-2.746937	-0.955000
H	-4.769282	-4.533409	-0.877230
H	-4.873087	-3.591285	0.635685

Vibrational frequencies

-233.5254	17.1847	20.3080
22.7776	30.0719	32.3165
39.1190	42.4783	54.6123
58.6782	61.4622	68.0784
72.4544	75.1849	85.3737
88.9248	92.1576	96.5569
105.8810	117.3036	128.9211
139.8039	147.8697	158.6188
171.3153	174.0033	179.9159
195.8468	203.6094	204.6493
220.5138	229.0404	234.4622
239.2346	250.2082	263.5648
274.9068	281.3339	286.9796
293.2558	299.9573	307.7879
323.8787	329.3114	333.5443
360.7431	372.6657	397.2495
401.0350	405.1842	409.6653
418.3095	439.3350	445.4917
463.3565	471.6114	481.4091
485.5970	493.7246	509.3110
511.7440	518.8501	527.6441
532.0256	534.1535	544.0175
548.1531	577.8776	582.0657
593.3717	599.9045	608.1665

614.4163	619.0187	632.0133
648.4338	650.6588	685.6527
693.2001	705.3109	708.0809
721.0979	733.3892	734.6356
749.8972	759.0974	763.8119
766.1690	780.6961	789.7236
795.0984	797.7508	814.1605
829.5067	842.8359	843.5410
861.2872	869.1009	870.9362
886.1428	895.2428	902.4088
903.4094	910.0908	933.0408
945.7068	947.3157	961.9701
974.1118	975.6371	978.2727
981.5708	984.4282	988.0182
989.5402	1002.3787	1002.4233
1004.1442	1013.3055	1032.5821
1040.9350	1041.9943	1043.5022
1046.8866	1051.6535	1053.6935
1057.1896	1060.7551	1064.3610
1065.4032	1070.6026	1072.5217
1078.9067	1094.4252	1102.1813
1111.1644	1116.2191	1117.1203
1124.9764	1154.2638	1184.9600
1185.0237	1186.9278	1189.5205
1191.4768	1201.1664	1211.3283
1213.4044	1224.1295	1226.6572
1234.4487	1244.9142	1259.8146
1267.8026	1275.7112	1285.6270
1288.0136	1291.2255	1301.2151
1308.8387	1312.0446	1325.5241

1331.8467	1334.2881	1342.7005
1345.9610	1348.0754	1359.2456
1368.3664	1369.3455	1379.2081
1380.0780	1412.3446	1418.6223
1421.8347	1423.0615	1429.7173
1440.8048	1449.8748	1466.5387
1467.7156	1470.0398	1470.9365
1479.2608	1486.0334	1486.9102
1488.5791	1489.4866	1492.9959
1496.4946	1498.9525	1503.2846
1506.8632	1509.2369	1512.3244
1520.7204	1531.1828	1533.4352
1566.9987	1606.7136	1628.2007
1632.0879	1641.1417	1641.7125
1642.0510	1651.3847	1653.2705
1654.7683	1660.1427	1725.1511
3027.2036	3037.0025	3043.6364
3044.2311	3048.2600	3054.2053
3073.9810	3100.7628	3100.8871
3106.9768	3109.8130	3129.5481
3139.3231	3142.8550	3146.0159
3151.1059	3168.7254	3173.6886
3181.3374	3182.0950	3183.9820
3185.4598	3186.2838	3189.6737
3192.0113	3192.1562	3198.4771
3200.6933	3203.9125	3208.5801
3210.8073	3212.0017	3215.2586
3217.3969	3238.8547	3277.5094

TS5R(Φ=90°)

Zero-point correction= 0.671551

Thermal correction to Energy= 0.713896

Thermal correction to Enthalpy= 0.714840

Thermal correction to Gibbs Free Energy= 0.594206

Sum of electronic and zero-point Energies= -2462.457850

Sum of electronic and thermal Energies= -2462.415505

Sum of electronic and thermal Enthalpies= -2462.414561

Sum of electronic and thermal Free Energies= -2462.535195

Cartesian coordinates

C	-1.698684	-0.496149	-1.357887
C	-0.782794	0.280732	-0.608383
H	-1.295387	-0.907268	-2.277894
C	0.584956	0.216471	-0.881667
O	1.186796	-0.401431	-1.797972
C	-3.127381	-0.118634	-1.457057
C	-3.901417	-0.662399	-2.495039
C	-3.745764	0.745676	-0.538431
C	-5.253230	-0.348282	-2.619403
H	-3.434404	-1.346737	-3.198053
C	-5.099141	1.057012	-0.659241
H	-3.175692	1.179248	0.275487
C	-5.857255	0.512132	-1.698610
H	-5.836026	-0.776834	-3.429593
H	-5.562372	1.724645	0.061499
H	-6.911806	0.756021	-1.790029
C	1.480177	0.973877	0.062685
C	3.185975	1.485973	1.340849
C	3.299372	-0.800450	0.360657
H	2.515590	-1.509038	0.086929
N	2.425159	2.548818	1.367133

N	1.361398	2.215143	0.553590
N	2.647152	0.506989	0.544897
C	4.393304	1.117141	2.137851
H	4.520104	1.803191	2.976502
H	5.299989	1.140711	1.519007
C	4.014840	-1.234074	1.701113
O	4.130182	-0.181588	2.668749
C	5.593982	-1.281763	-0.145464
C	4.415180	-0.737607	-0.661753
C	4.354730	-0.232444	-1.960108
C	5.512428	-0.265741	-2.740892
C	6.700150	-0.803713	-2.228569
C	6.747133	-1.319652	-0.930742
C	5.395354	-1.783446	1.262252
H	3.418989	0.158515	-2.344325
H	7.593402	-0.821351	-2.846684
H	7.668897	-1.738485	-0.536511
H	6.172404	-1.452073	1.958247
H	5.386607	-2.879443	1.287402
C	0.283963	3.136501	0.303719
C	-0.623337	3.394136	1.344339
C	0.149858	3.671224	-0.984862
C	-1.727254	4.193825	1.039482
C	-0.974887	4.463994	-1.233292
C	-1.930558	4.717539	-0.244064
H	-2.452726	4.401964	1.821576
H	-1.108874	4.883668	-2.226587
C	1.155063	3.386985	-2.072683
H	1.009017	2.389095	-2.501878
H	2.182105	3.433644	-1.696445

H	1.056230	4.112784	-2.883342
C	-3.173943	5.511712	-0.554728
H	-4.011719	4.836621	-0.770968
H	-3.034603	6.153910	-1.428894
H	-3.471831	6.138754	0.291445
C	-0.432905	2.813838	2.721573
H	0.506598	3.153919	3.168443
H	-0.409974	1.718845	2.705181
H	-1.252644	3.112624	3.379107
H	3.415186	-1.991348	2.206856
H	5.490559	0.125011	-3.754100
H	-1.121347	0.886934	0.219357
C	-2.918468	-2.345257	0.445971
C	-2.818280	-1.721501	1.716002
C	-3.936954	-1.697937	2.569228
C	-5.138931	-2.280859	2.195306
C	-5.240651	-2.899855	0.942123
C	-4.147407	-2.924347	0.083268
H	-3.829473	-1.203628	3.529876
H	-5.992964	-2.255708	2.865538
H	-6.176671	-3.357517	0.634574
H	-4.220888	-3.382257	-0.897020
C	-1.581465	-1.053471	2.176105
H	-0.681688	-1.229235	1.572508
O	-1.536032	-0.347987	3.181319
N	-1.916406	-2.297348	-0.553403
S	-0.588747	-3.259651	-0.377421
O	0.522689	-2.663209	0.415897
O	-1.026577	-4.604283	0.062251
C	0.001220	-3.362912	-2.068071

H	0.376849	-2.382854	-2.366384
H	0.818465	-4.087716	-2.060262
H	-0.809410	-3.711086	-2.708772

Vibrational frequencies

-285.2928	14.3316	18.1668
24.6910	27.8436	36.4014
41.0168	44.9596	49.5633
53.1516	59.7607	67.1459
69.5352	70.6459	78.0462
84.2329	90.1920	96.6753
109.8618	117.0197	125.9485
137.0732	140.0591	142.0476
153.7837	171.0926	183.5378
194.5138	203.9948	207.9330
218.4049	226.5896	234.6841
247.0091	258.9425	265.7783
268.0803	273.6041	285.3771
289.4541	293.1129	298.2748
305.6828	323.9139	330.8881
344.3688	372.0957	400.3277
403.4778	407.8373	413.9833
431.6901	441.7901	448.7717
457.6367	466.2905	480.2736
490.1585	493.4920	507.2284
511.1603	518.4962	525.7973
527.1615	532.2133	535.8994
559.9486	578.9645	584.9532
596.5668	603.0945	606.2177
608.2194	618.6985	632.4703
637.9811	641.5686	691.9790

695.8507 704.3026 705.0208
719.2118 730.6751 743.7897
753.5254 758.5577 762.6263
765.9177 782.5196 789.8485
794.3038 799.2545 806.8074
829.7215 836.2850 844.3691
857.9793 871.1466 873.2520
886.0507 894.3966 902.1732
907.3381 911.1048 933.5535
948.2966 950.3867 960.4244
975.3566 977.3406 978.3524
979.9178 989.1320 998.5066
998.7386 1004.0457 1006.8165
1007.7042 1015.1997 1033.4675
1033.9930 1042.8882 1044.5114
1047.3275 1053.1038 1054.8691
1058.3350 1062.4429 1067.5032
1068.2857 1070.8835 1072.7576
1076.4815 1089.9661 1098.0186
1108.8553 1114.0718 1117.0170
1125.7810 1157.7435 1183.1753
1185.3585 1187.0090 1190.0026
1194.4655 1205.4763 1213.3338
1220.7869 1221.2958 1225.4145
1232.2133 1234.4008 1249.1319
1249.7140 1265.0249 1271.7447
1292.0407 1294.8260 1296.8812
1305.3617 1311.8417 1327.3017
1332.0011 1340.9545 1345.3768
1345.5476 1358.1201 1368.4075

1370.0915	1370.2700	1377.7956
1381.5350	1411.2795	1422.6243
1427.4447	1440.3235	1446.5421
1449.8313	1455.5490	1467.1095
1468.8882	1470.7714	1478.1034
1483.1537	1483.6755	1483.9041
1485.0706	1490.2574	1491.5175
1493.2630	1498.6739	1499.6693
1505.5839	1507.4022	1517.7709
1521.7905	1532.5076	1536.1542
1565.3888	1607.8304	1622.7527
1635.1810	1639.4878	1641.0128
1642.6408	1644.2078	1653.6107
1657.3007	1658.9254	1739.0076
3039.2335	3043.6792	3047.0652
3053.2144	3055.8188	3067.2010
3078.1851	3102.1252	3102.7072
3108.0821	3119.2409	3121.1530
3130.5749	3135.2227	3138.8657
3139.2051	3153.5105	3170.9417
3181.4757	3181.8816	3181.9855
3185.7195	3186.2506	3186.9967
3188.5736	3190.3575	3193.9358
3197.3883	3197.8384	3204.1830
3207.6638	3208.8598	3217.3099
3219.0820	3222.1399	3244.1645

TS5R(Φ=177°)

Zero-point correction= 0.671510

Thermal correction to Energy= 0.713904

Thermal correction to Enthalpy= 0.714848

Thermal correction to Gibbs Free Energy= 0.593620

Sum of electronic and zero-point Energies= -2462.456537

Sum of electronic and thermal Energies= -2462.414144

Sum of electronic and thermal Enthalpies= -2462.413200

Sum of electronic and thermal Free Energies= -2462.534427

Cartesian coordinates

C	1.801830	0.210962	0.781788
C	0.612258	0.797360	0.292233
H	1.709044	-0.270247	1.750756
C	-0.625110	0.317026	0.721230
O	-0.877924	-0.541748	1.606685
C	3.106002	0.873929	0.539311
C	4.056896	0.938829	1.566724
C	3.431690	1.402190	-0.721236
C	5.301143	1.533254	1.348353
H	3.821619	0.513645	2.537971
C	4.676412	1.986337	-0.942462
H	2.716775	1.324087	-1.534320
C	5.615032	2.055542	0.093031
H	6.027684	1.575960	2.154690
H	4.921046	2.378837	-1.925291
H	6.587350	2.506618	-0.083053
C	-1.821111	0.833885	-0.032941
C	-3.727805	0.884145	-1.117565
C	-3.005921	-1.396712	-0.440508
H	-2.009791	-1.822514	-0.337809
N	-3.346606	2.132752	-1.065219
N	-2.152481	2.085836	-0.372283
N	-2.827343	0.062323	-0.489017

C	-4.830079	0.221242	-1.875977
H	-5.262597	0.910056	-2.602694
H	-5.623013	-0.128940	-1.202163
C	-3.685553	-1.900828	-1.774594
O	-4.216207	-0.850135	-2.592519
C	-4.949701	-2.665801	0.158012
C	-3.952679	-1.825582	0.659587
C	-3.897221	-1.484949	2.010864
C	-4.878377	-1.994282	2.864506
C	-5.884858	-2.833796	2.369246
C	-5.924307	-3.178690	1.015630
C	-4.777510	-2.903399	-1.320832
H	-3.094890	-0.851240	2.373753
H	-6.641988	-3.221745	3.044932
H	-6.705166	-3.831766	0.635689
H	-5.695596	-2.745790	-1.895955
H	-4.450238	-3.931030	-1.517021
C	-1.431110	3.300119	-0.094169
C	-0.733586	3.906676	-1.149600
C	-1.466139	3.820998	1.205826
C	-0.039784	5.084025	-0.862472
C	-0.753224	5.001032	1.438123
C	-0.035047	5.642122	0.422685
H	0.513586	5.573258	-1.659777
H	-0.762636	5.427975	2.437365
C	-2.222932	3.132376	2.312852
H	-1.701737	2.225783	2.641758
H	-3.225990	2.833102	1.990926
H	-2.324088	3.790714	3.178732
C	0.756075	6.893342	0.711179

H	1.806187	6.647862	0.913376
H	0.367398	7.420275	1.587348
H	0.742370	7.581647	-0.139635
C	-0.724933	3.300040	-2.529246
H	-1.729151	3.291106	-2.965965
H	-0.378522	2.260457	-2.505081
H	-0.066449	3.862030	-3.195171
H	-2.931348	-2.371201	-2.405732
H	-4.859066	-1.740971	3.920553
H	0.653086	1.506118	-0.524152
C	3.348285	-2.089231	0.351785
C	4.525973	-2.157309	-0.429282
C	5.702322	-2.683806	0.124864
C	5.730525	-3.138347	1.438295
C	4.567931	-3.070129	2.215597
C	3.391708	-2.550142	1.678893
H	6.588836	-2.721384	-0.501008
H	6.646462	-3.542158	1.859142
H	4.580409	-3.420501	3.243926
H	2.492875	-2.486867	2.284219
C	4.541328	-1.672665	-1.827243
H	3.589835	-1.250945	-2.189282
O	5.526841	-1.721267	-2.551253
N	2.185476	-1.465508	-0.161085
S	1.051951	-2.427939	-0.837475
O	0.012586	-1.562297	-1.438235
O	1.709469	-3.415995	-1.721147
C	0.253397	-3.378393	0.474743
H	-0.201682	-2.677262	1.175582
H	-0.502631	-4.016377	0.011015

H	1.008435	-3.996108	0.963551

Vibrational frequencies

-294.0774	13.9377	21.8239
22.6988	26.6613	34.0563
38.4393	43.5599	48.3633
51.2431	53.7310	60.8912
64.6546	69.0361	72.3853
82.4810	87.7981	103.5605
108.8689	121.3418	129.9805
134.5483	139.1497	141.5142
160.5891	176.3011	182.1326
194.5953	203.6342	207.6608
215.1578	217.4407	237.2641
241.2898	251.1204	265.3479
270.0035	280.1627	281.0950
287.4518	295.6160	298.5888
314.3423	318.5534	328.7406
354.6430	369.6094	389.0677
394.2728	401.5137	406.4781
417.0446	443.6695	447.0933
465.4775	478.6154	482.4222
487.7523	492.6045	509.3115
513.9425	524.1376	529.6356
530.7132	535.9410	542.0306
560.8164	580.6827	587.4125
597.7749	602.5348	606.4959
618.2039	624.3568	633.6214
637.1583	645.6234	693.5491
700.3710	705.6659	707.3918
718.3250	731.6319	737.9009

750.5686	761.0964	766.4738
768.1791	782.1590	789.0042
793.8009	800.6048	813.3131
829.0346	838.7437	844.7820
857.9335	871.6432	877.6121
886.1105	906.5331	906.8484
907.2710	912.0385	928.4873
933.6943	948.5915	960.5502
976.0710	978.1250	979.5094
981.7672	987.8051	989.0823
1000.7016	1003.9178	1006.9114
1007.4260	1015.0545	1032.4454
1033.6137	1041.7831	1044.2517
1046.0649	1053.1012	1054.6592
1057.3102	1064.5548	1067.5307
1069.3592	1070.9289	1071.2592
1079.2754	1088.7832	1097.5171
1109.3844	1117.1542	1118.7292
1141.1870	1164.2232	1184.4707
1186.8251	1187.0111	1188.0419
1194.0079	1203.0060	1210.1087
1216.8364	1219.7359	1227.1150
1236.0243	1245.3737	1252.7141
1256.7375	1268.9129	1280.0665
1292.7767	1296.1957	1297.6206
1305.0392	1311.1982	1323.9159
1331.9876	1338.6193	1342.9177
1344.0304	1354.3830	1359.4541
1364.1471	1369.7853	1377.4448
1381.8791	1411.0163	1423.1029

1425.6945	1428.5450	1431.4888
1445.1354	1448.7110	1458.4188
1470.9381	1472.6070	1479.1769
1480.9516	1481.9563	1485.2373
1485.6390	1489.0309	1490.4074
1492.1520	1494.9954	1499.1516
1507.5032	1511.3105	1518.1713
1522.5833	1533.4960	1538.3240
1565.9124	1615.9643	1623.2817
1635.4810	1639.1968	1641.1709
1642.6659	1643.9514	1654.2980
1656.8323	1658.6530	1764.0847
3024.7106	3040.0760	3045.7224
3046.5809	3048.3453	3057.4435
3066.8416	3101.1886	3102.5376
3106.9751	3107.0855	3129.5044
3133.1880	3139.8795	3144.0008
3154.4084	3167.5403	3170.1514
3182.0921	3182.7109	3183.5319
3184.7592	3184.9038	3186.3709
3188.0125	3189.5663	3192.7971
3196.8140	3197.0226	3204.3188
3204.4938	3206.3021	3211.1878
3212.8721	3214.3309	3247.2070

TS5R(Φ=-54°)

Zero-point correction= 0.672148

Thermal correction to Energy= 0.713908

Thermal correction to Enthalpy= 0.714852

Thermal correction to Gibbs Free Energy= 0.597547

Sum of electronic and zero-point Energies= -2462.451871

Sum of electronic and thermal Energies= -2462.410110

Sum of electronic and thermal Enthalpies= -2462.409166

Sum of electronic and thermal Free Energies= -2462.526471

Cartesian coordinates

C	1.902185	-0.853214	0.971076
C	1.009386	0.106012	0.423397
H	1.429252	-1.552910	1.655283
C	-0.371167	0.018632	0.633597
O	-1.015497	-0.787168	1.349143
C	3.281750	-0.475221	1.375205
C	4.083832	-1.411475	2.046708
C	3.793847	0.813755	1.156860
C	5.363845	-1.075541	2.476832
H	3.697396	-2.411659	2.216033
C	5.080802	1.149263	1.578599
H	3.180344	1.571795	0.683464
C	5.871008	0.205785	2.237496
H	5.970769	-1.813308	2.993784
H	5.457962	2.152812	1.401807
H	6.871427	0.467540	2.570290
C	-1.215259	1.035424	-0.108819
C	-2.928212	1.943952	-1.144714
C	-3.384296	-0.337317	-0.267311
H	-2.740635	-1.207097	-0.149983
N	-1.996189	2.857764	-1.189823
N	-0.932675	2.281118	-0.528347
N	-2.495664	0.822333	-0.484387
C	-4.264121	1.878966	-1.808354
H	-4.331945	2.628503	-2.598332

H	-5.075628	2.049295	-1.088658
C	-4.371801	-0.502501	-1.488899
O	-4.339537	0.589642	-2.414733
C	-5.624872	-0.329542	0.590543
C	-4.284859	-0.132194	0.931174
C	-3.903943	0.196704	2.231923
C	-4.900995	0.346546	3.197846
C	-6.248608	0.158855	2.862745
C	-6.618661	-0.185785	1.560325
C	-5.774631	-0.709397	-0.860380
H	-2.852970	0.309886	2.475413
H	-7.013561	0.278635	3.624820
H	-7.664138	-0.335702	1.305381
H	-6.518838	-0.107918	-1.392700
H	-6.080940	-1.756803	-0.961543
C	0.293451	3.020561	-0.374431
C	1.145594	3.119484	-1.485306
C	0.603756	3.552216	0.882889
C	2.364989	3.773585	-1.298286
C	1.836139	4.200654	1.014376
C	2.728034	4.315511	-0.057595
H	3.052635	3.851254	-2.136150
H	2.107898	4.613965	1.981811
C	-0.325767	3.389830	2.056999
H	-0.276609	2.367843	2.451005
H	-1.366591	3.586947	1.780854
H	-0.050581	4.070974	2.865406
C	4.051656	5.018430	0.109966
H	4.366108	5.037159	1.157238
H	3.986573	6.058334	-0.233774

H	4.836163	4.532447	-0.478386
C	0.771319	2.512443	-2.812191
H	-0.058282	3.057677	-3.275505
H	0.445523	1.473127	-2.698687
H	1.619170	2.529192	-3.500684
H	-4.065922	-1.362103	-2.086362
H	-4.629772	0.604365	4.217459
H	1.393976	0.885010	-0.214027
C	0.860682	-2.769388	-0.694457
C	0.262341	-3.708086	0.186386
C	-1.061683	-4.123281	-0.016887
C	-1.799593	-3.656323	-1.097205
C	-1.204677	-2.753768	-1.988353
C	0.097963	-2.306895	-1.784806
H	-1.485044	-4.833734	0.686481
H	-2.820567	-3.991366	-1.253885
H	-1.765859	-2.382823	-2.842060
H	0.529543	-1.602615	-2.483833
C	1.024721	-4.291118	1.308028
H	2.100727	-4.040075	1.323135
O	0.539869	-5.024070	2.160985
N	2.135217	-2.277415	-0.353833
S	3.257990	-2.045186	-1.560114
O	4.589821	-2.130593	-0.940255
O	2.950873	-2.942902	-2.693441
C	3.113031	-0.356592	-2.189429
H	3.353472	0.347472	-1.394240
H	3.840966	-0.265884	-2.998853
H	2.107981	-0.186959	-2.572327

Vibrational frequencies

-318.8218	16.9877	27.1419
28.0403	32.4423	46.4259
48.4610	53.4710	55.3387
59.4146	63.0992	66.7978
73.2622	79.8438	88.8451
94.1405	105.8914	124.8450
127.0413	131.2828	133.4130
145.3993	151.5450	163.0189
168.8702	181.3404	186.4553
201.3348	204.9914	215.1866
219.6595	225.7375	235.9460
237.9865	248.2153	263.2487
283.5822	284.7371	289.3188
293.0381	301.0217	316.8220
326.5456	328.0558	341.4283
357.2110	373.0831	383.7863
402.4424	403.7606	419.6730
437.2060	442.6188	448.4292
458.4568	471.2356	476.0664
487.9240	492.9053	507.0187
509.0678	514.1157	527.6084
529.2768	537.3397	548.5914
560.4626	578.8572	587.7675
598.7810	604.1528	609.1910
615.2377	623.7706	632.8141
645.3897	657.8842	676.9131
681.5223	704.8639	706.0340
718.0239	732.7864	735.3231
752.0947	753.6497	761.5988
765.1558	775.6880	785.3611

791.8319	799.1262	804.7392
828.9062	838.3550	846.4284
858.9804	871.0848	874.3012
877.1478	882.1348	896.0316
904.9600	905.8547	927.3574
944.2187	948.9770	960.1864
964.5989	973.0043	974.1171
976.3723	981.2050	989.1409
992.0292	998.5495	1003.6288
1003.9974	1015.4582	1034.1603
1039.4774	1041.7140	1045.0610
1045.5436	1053.8432	1054.9745
1057.6475	1060.8958	1065.4819
1069.1862	1070.5041	1071.8267
1093.9670	1099.0848	1100.8294
1113.8343	1118.6176	1120.5888
1138.8737	1169.4423	1184.6847
1186.6463	1188.0904	1190.0275
1194.5036	1201.7938	1213.2795
1214.9499	1217.0997	1224.7507
1232.2597	1245.3860	1249.4367
1269.2445	1272.6326	1280.6156
1289.8072	1290.4446	1304.7281
1304.8533	1310.4072	1324.7832
1330.5222	1336.9733	1341.9546
1342.5838	1349.7970	1361.8757
1364.7945	1369.8699	1373.9039
1377.4438	1406.9717	1418.4383
1420.1998	1424.3608	1426.3462
1438.6989	1447.9408	1457.2512

1466.2745	1472.1178	1472.5348
1483.6308	1483.7235	1485.8162
1486.5252	1488.9736	1491.6798
1494.8732	1496.8753	1499.5697
1503.8798	1508.4681	1512.2674
1522.4340	1528.7271	1532.8347
1558.0546	1611.6219	1629.3429
1635.0419	1640.5405	1641.5920
1642.2010	1649.3868	1653.0512
1656.0175	1659.6404	1758.7227
2991.2177	3041.6496	3047.4299
3049.0561	3050.3823	3057.1893
3088.2868	3098.7652	3103.4743
3109.7316	3110.0867	3126.8641
3130.5494	3140.4579	3141.5513
3151.7067	3153.3846	3171.6685
3179.9816	3180.7668	3183.8169
3184.4059	3185.0008	3187.1963
3189.4627	3194.3973	3195.7182
3200.0344	3205.9079	3209.4059
3209.5249	3219.1181	3219.2188
3220.4415	3232.2708	3272.7401

TS5R(Φ=-128°)

Zero-point correction= 0.671790

Thermal correction to Energy= 0.714042

Thermal correction to Enthalpy= 0.714986

Thermal correction to Gibbs Free Energy= 0.594113

Sum of electronic and zero-point Energies= -2462.455711

Sum of electronic and thermal Energies= -2462.413459

Sum of electronic and thermal Enthalpies= -2462.412515

Sum of electronic and thermal Free Energies= -2462.533388

Cartesian coordinates

C	-1.722572	0.127998	-1.044246
C	-0.578693	0.700691	-0.494141
H	-1.579636	-0.729694	-1.692629
C	0.644745	0.003785	-0.494231
O	0.864610	-1.142828	-0.953522
C	-2.960785	0.889879	-1.248511
C	-3.818600	0.527213	-2.299907
C	-3.315629	1.973774	-0.423662
C	-4.988484	1.246197	-2.543938
H	-3.561077	-0.321799	-2.927477
C	-4.485460	2.686993	-0.666834
H	-2.694412	2.223089	0.428759
C	-5.322882	2.330964	-1.730834
H	-5.639142	0.957508	-3.364351
H	-4.753474	3.517253	-0.019471
H	-6.235481	2.890240	-1.916238
C	1.829036	0.676124	0.164975
C	3.797152	0.966169	1.100057
C	3.358986	-1.387551	0.443509
H	2.444014	-1.975673	0.452760
N	3.267952	2.160413	1.065012
N	2.042146	1.967511	0.474874
N	2.953732	0.031045	0.558996
C	5.065903	0.486889	1.722355
H	5.445231	1.226421	2.428824
H	5.832703	0.304909	0.957030
C	4.316249	-1.792004	1.636096

O	4.732999	-0.692355	2.450123
C	5.379418	-2.270135	-0.503024
C	4.175077	-1.632310	-0.807860
C	3.836569	-1.305381	-2.120972
C	4.737789	-1.621939	-3.139055
C	5.948376	-2.261697	-2.841532
C	6.274644	-2.593314	-1.524357
C	5.510189	-2.530932	0.975071
H	2.886241	-0.830410	-2.337971
H	6.639723	-2.503040	-3.643914
H	7.213644	-3.090470	-1.297315
H	6.454506	-2.167569	1.394048
H	5.457759	-3.603538	1.192918
C	1.180454	3.102105	0.253046
C	0.379929	3.547351	1.314410
C	1.153076	3.666722	-1.029001
C	-0.501514	4.597727	1.042368
C	0.253219	4.712641	-1.245100
C	-0.589746	5.178924	-0.228416
H	-1.145531	4.957683	1.840139
H	0.201474	5.164718	-2.231851
C	2.023969	3.128604	-2.133997
H	1.684391	2.133261	-2.444771
H	3.067421	3.034490	-1.815503
H	1.989987	3.781162	-3.009168
C	-1.609399	6.253012	-0.508879
H	-2.555416	5.800070	-0.831765
H	-1.279292	6.924829	-1.306668
H	-1.820559	6.850276	0.382964
C	0.397636	2.867952	2.658535

H	1.415950	2.649867	2.993294
H	-0.158616	1.923102	2.612222
H	-0.082375	3.496567	3.412525
H	3.775107	-2.439322	2.326660
H	4.496430	-1.375438	-4.168794
H	-0.652923	1.647452	0.011145
C	-2.858634	-2.540729	-0.080526
C	-4.148900	-3.120174	0.033972
C	-4.389692	-4.402188	-0.486166
C	-3.387020	-5.108356	-1.139339
C	-2.116899	-4.530125	-1.275507
C	-1.853402	-3.266871	-0.752749
H	-5.385967	-4.819196	-0.370862
H	-3.585569	-6.096308	-1.544290
H	-1.326822	-5.072895	-1.788033
H	-0.869969	-2.814001	-0.847580
C	-5.259204	-2.378893	0.668355
H	-5.049204	-1.319316	0.888094
O	-6.354383	-2.870306	0.911544
N	-2.590655	-1.250577	0.399211
S	-2.232190	-1.041471	1.956625
O	-1.974933	0.401478	2.170450
O	-3.222135	-1.696486	2.846892
C	-0.669209	-1.898558	2.262792
H	0.085705	-1.500375	1.585215
H	-0.381835	-1.734186	3.303440
H	-0.813584	-2.964257	2.075520

Vibrational frequencies

-90.9815	15.3859	16.7621
22.6449	25.8656	32.6285

36.3537	40.8277	49.8067
51.5592	58.3211	65.7084
66.2059	74.9746	81.1803
83.1446	91.4089	93.1511
105.9537	118.3188	129.7890
134.3233	143.4073	156.0905
184.6284	187.2189	194.2344
201.7795	205.9656	213.7685
220.4364	224.8865	230.6608
241.9319	244.8362	255.4650
266.7326	271.4963	287.3283
290.4072	293.8629	301.8123
320.5043	330.0976	331.9509
367.4747	370.8440	386.9112
392.5932	397.4610	408.9335
416.8893	441.1855	448.3422
463.2585	476.5830	478.7560
487.8081	492.5401	509.2413
513.6990	519.3531	530.7852
533.4490	537.6197	550.1237
557.6265	575.2210	581.7158
593.9184	599.2609	608.8126
618.9715	621.6220	632.7517
642.2955	645.9952	675.8742
701.4736	702.5539	707.2890
715.1528	731.5854	743.3390
752.5870	757.5458	765.3282
767.9814	780.6482	793.8523
796.0604	801.7951	817.2268
828.6336	840.5206	848.5726

855.2896 870.7549 875.1515

881.6721 903.2026 906.4783

910.1006 913.3176 935.4142

937.8051 950.6250 962.4155

973.6446 974.7441 976.6824

979.9281 981.1530 982.0197

991.5531 1003.0121 1004.3067

1011.4650 1014.3743 1033.9390

1035.1533 1041.2427 1044.1195

1046.2558 1052.4923 1055.3063

1056.9827 1059.1392 1062.1865

1066.0415 1069.6782 1070.7188

1076.5674 1100.5028 1105.2202

1106.9621 1114.6254 1118.4972

1120.4582 1160.3429 1185.1530

1185.8850 1187.1132 1190.3375

1194.5553 1204.3509 1213.2761

1216.0487 1221.8753 1228.6546

1241.7823 1244.7434 1246.5196

1265.5843 1269.8509 1291.0164

1291.2873 1294.0964 1302.7420

1308.4608 1313.6612 1332.4703

1335.2565 1340.0078 1343.2044

1343.7408 1346.5604 1353.7230

1369.2481 1369.7964 1375.0179

1388.4606 1408.4551 1416.4920

1420.0759 1430.2286 1436.6063

1439.5712 1448.2687 1457.4320

1462.4630 1465.4999 1470.3299

1473.1064 1483.8761 1487.4554

1487.7705	1492.3319	1492.6510
1492.9284	1497.1634	1498.7739
1506.7199	1509.2136	1510.4622
1522.4287	1528.2180	1536.4735
1582.5236	1607.1038	1623.8939
1634.3418	1640.4684	1641.3454
1641.5928	1643.4329	1652.5310
1655.9186	1658.4025	1760.5647
3022.0662	3040.0114	3041.3238
3041.8356	3045.3684	3060.4906
3076.6494	3099.2935	3104.2774
3106.6573	3112.8773	3133.0521
3134.3293	3138.8411	3140.3447
3152.9496	3165.5662	3172.5817
3177.9921	3182.5802	3184.9574
3186.1249	3187.8181	3188.5635
3189.0053	3195.1659	3195.5028
3197.8220	3198.1747	3205.6399
3206.8220	3207.3704	3209.2945
3225.1697	3225.4415	3302.8515

TS5R(Φ=-175°)

Zero-point correction= 0.671632

Thermal correction to Energy= 0.713949

Thermal correction to Enthalpy= 0.714893

Thermal correction to Gibbs Free Energy= 0.594528

Sum of electronic and zero-point Energies= -2462.456488

Sum of electronic and thermal Energies= -2462.414171

Sum of electronic and thermal Enthalpies= -2462.413227

Sum of electronic and thermal Free Energies= -2462.533592

Cartesian coordinates

C	1.813638	0.292065	0.654734
C	0.607317	0.824751	0.145737
H	1.738288	-0.126112	1.653995
C	-0.610221	0.361524	0.641426
O	-0.827048	-0.448674	1.581376
C	3.107649	0.948222	0.353532
C	4.076518	1.069601	1.359435
C	3.410345	1.407768	-0.939039
C	5.315179	1.653310	1.087995
H	3.859305	0.695719	2.355704
C	4.649442	1.981687	-1.212676
H	2.682735	1.282262	-1.734831
C	5.605658	2.108270	-0.198837
H	6.055475	1.739913	1.878102
H	4.876394	2.320416	-2.219428
H	6.573685	2.550499	-0.416141
C	-1.845528	0.848022	-0.069347
C	-3.812419	0.870612	-1.040060
C	-2.964206	-1.407600	-0.520146
H	-1.947839	-1.799534	-0.489255
N	-3.475527	2.130147	-0.951385
N	-2.241097	2.098518	-0.330886
N	-2.846194	0.057705	-0.504000
C	-4.941535	0.194843	-1.744774
H	-5.455161	0.894429	-2.405377
H	-5.664905	-0.213937	-1.027189
C	-3.685183	-1.874619	-1.844765
O	-4.346466	-0.818384	-2.555954
C	-4.803647	-2.813389	0.097199

C	-3.841192	-1.931917	0.596567
C	-3.758135	-1.637317	1.957092
C	-4.676025	-2.236896	2.822814
C	-5.647254	-3.118039	2.330120
C	-5.714136	-3.415941	0.966245
C	-4.667547	-2.984791	-1.394819
H	-2.984545	-0.967678	2.317581
H	-6.355628	-3.575166	3.015336
H	-6.467927	-4.100788	0.587663
H	-5.615083	-2.891962	-1.934599
H	-4.254786	-3.971048	-1.637639
C	-1.543617	3.319990	-0.025226
C	-0.886881	3.984759	-1.072034
C	-1.549559	3.779348	1.297042
C	-0.201654	5.156882	-0.750415
C	-0.847385	4.959671	1.564186
C	-0.169053	5.656516	0.559124
H	0.325148	5.689538	-1.537984
H	-0.831002	5.338276	2.582445
C	-2.266157	3.024196	2.387499
H	-1.756534	2.082235	2.621279
H	-3.291024	2.773418	2.092929
H	-2.309923	3.617073	3.303970
C	0.584084	6.926965	0.864698
H	0.593946	7.142139	1.936530
H	0.131859	7.784102	0.351964
H	1.622302	6.860050	0.520949
C	-0.913086	3.442002	-2.477572
H	-1.931321	3.436622	-2.880959
H	-0.550120	2.408657	-2.514529

H	-0.286509	4.045630	-3.137840
H	-2.941772	-2.244577	-2.551668
H	-4.634949	-2.019988	3.886320
H	0.615661	1.484708	-0.712052
C	3.372202	-2.030462	0.402569
C	4.570199	-2.118893	-0.344543
C	5.739349	-2.600339	0.263198
C	5.740759	-2.988077	1.598223
C	4.558417	-2.896962	2.342960
C	3.388995	-2.421626	1.752637
H	6.641500	-2.656014	-0.338619
H	6.650975	-3.357533	2.060969
H	4.550275	-3.194288	3.387950
H	2.474880	-2.340096	2.332414
C	4.613131	-1.704145	-1.764185
H	3.664571	-1.315688	-2.168894
O	5.616971	-1.772959	-2.460906
N	2.216364	-1.450116	-0.170895
S	1.097727	-2.454924	-0.803649
O	0.068705	-1.626951	-1.472577
O	1.769163	-3.495168	-1.614258
C	0.272724	-3.324342	0.547568
H	-0.188907	-2.581946	1.199821
H	-0.480664	-3.983582	0.109910
H	1.015440	-3.917558	1.083313

Vibrational frequencies

-283.8410	14.8147	22.9248
24.3553	30.6635	36.8863
40.2810	44.2037	49.7977
53.8843	57.1372	63.0197

69.5535	74.0995	81.2765
86.9999	99.2739	103.6946
109.8880	118.6884	133.6545
134.9075	142.4373	143.1265
150.0953	158.3245	174.9995
192.4344	203.9650	208.0060
211.1185	217.4742	239.0802
244.7092	248.8742	263.4356
267.3510	282.1809	285.7477
287.1719	297.5840	298.6893
314.2680	317.5856	329.1233
355.2482	366.7780	391.1108
398.3869	403.1020	406.5449
416.0484	443.2257	446.2576
463.1316	478.4766	482.8602
488.5046	492.0426	506.5133
511.9192	523.3269	529.1220
533.2139	535.4554	540.6478
560.5345	580.9457	592.1155
596.8878	602.3487	606.7293
615.7755	623.8066	633.3948
635.8254	645.6423	697.3489
703.5580	707.6442	707.6617
721.2876	732.6106	738.7670
753.1703	760.7117	766.4065
767.2519	783.7644	789.3389
794.2010	799.5114	812.9291
830.6216	838.6669	843.3980
859.4196	871.8938	879.7904
887.3229	906.2137	908.4253

909.3842	912.7702	929.6352
934.3190	946.7293	961.3366
975.0649	979.1587	979.8041
981.5425	983.5947	988.0114
999.5615	1001.6673	1005.7902
1008.7712	1014.8513	1031.0042
1036.1197	1041.0923	1042.8673
1049.1100	1053.4153	1055.4805
1059.7580	1067.0861	1068.8664
1069.0220	1071.8950	1073.8607
1077.8356	1086.8681	1096.4841
1109.6425	1117.0833	1118.8347
1137.6428	1163.1306	1185.3379
1187.3514	1187.6356	1188.8272
1193.5449	1204.1188	1210.7978
1219.1405	1221.0667	1229.2805
1233.4798	1246.6477	1254.1631
1256.2808	1266.4012	1278.8346
1291.6026	1296.0663	1299.1544
1304.8758	1311.1514	1324.1135
1331.0597	1340.2614	1343.4887
1347.1142	1352.8911	1357.0825
1365.1529	1370.4164	1377.2990
1380.5649	1410.1647	1420.1362
1427.9917	1429.2702	1433.9043
1446.4970	1450.0132	1459.8130
1468.1437	1470.2987	1479.1880
1482.2454	1484.4357	1485.5270
1485.8623	1489.6423	1491.3466
1492.5570	1498.9558	1500.5606

1507.6500	1512.7022	1517.2622
1522.5104	1533.3312	1540.0833
1565.2193	1615.8453	1622.2518
1635.6685	1639.4284	1641.0696
1643.4144	1644.2954	1654.8905
1656.8069	1659.1029	1763.6910
3024.5576	3042.8196	3045.8241
3047.8393	3048.8924	3055.0987
3066.4505	3101.6241	3102.7171
3105.7398	3107.4993	3131.1007
3131.8701	3138.7126	3142.2351
3147.3596	3157.4805	3169.7911
3182.0943	3183.0036	3183.2130
3184.8792	3185.0580	3186.1914
3190.0964	3190.2737	3193.3755
3196.9992	3197.4547	3204.8819
3205.1222	3206.5756	3211.6473
3212.8137	3219.1591	3240.2100

TS5S(Φ=168°)

Zero-point correction= 0.671871

Thermal correction to Energy= 0.714018

Thermal correction to Enthalpy= 0.714962

Thermal correction to Gibbs Free Energy= 0.595674

Sum of electronic and zero-point Energies= -2462.456931

Sum of electronic and thermal Energies= -2462.414784

Sum of electronic and thermal Enthalpies= -2462.413839

Sum of electronic and thermal Free Energies= -2462.533127

Cartesian coordinates

C 1.604941 0.125883 -0.801067

C	0.316936	0.597894	-0.456039
H	1.617047	-0.586945	-1.621646
C	-0.836831	0.142322	-1.100485
O	-0.957039	-0.660851	-2.058828
C	2.795118	1.001973	-0.747994
C	3.907980	0.680060	-1.544605
C	2.845991	2.166492	0.040262
C	5.041352	1.494254	-1.554491
H	3.879254	-0.213417	-2.161131
C	3.977542	2.976452	0.030420
H	2.006111	2.431005	0.668910
C	5.080264	2.644546	-0.765557
H	5.890468	1.228399	-2.177483
H	3.999876	3.871538	0.645969
H	5.960493	3.281262	-0.771025
C	-2.137150	0.751509	-0.615706
C	-4.285315	1.105243	-0.332517
C	-3.714429	-1.230669	-1.137137
H	-3.433310	-1.288442	-2.186980
N	-3.715048	2.235731	-0.008786
N	-2.373041	1.998999	-0.182305
N	-3.355754	0.159314	-0.694367
C	-5.755684	0.825337	-0.343145
H	-6.280409	1.685375	-0.766016
H	-6.116682	0.687676	0.685221
C	-5.240157	-1.433674	-0.881504
O	-6.038216	-0.293774	-1.166334
C	-4.046098	-2.768075	0.673117
C	-3.118141	-2.333631	-0.286242
C	-1.888154	-2.975331	-0.431100

C	-1.572330	-4.026583	0.433108
C	-2.475664	-4.429524	1.422704
C	-3.724264	-3.810742	1.540167
C	-5.346581	-2.017942	0.550439
H	-1.203526	-2.657702	-1.206637
H	-2.215667	-5.247178	2.089006
H	-4.440661	-4.151418	2.282454
H	-5.418254	-1.232201	1.311356
H	-6.227778	-2.655162	0.660729
C	-1.436271	3.072108	0.049389
C	-1.001664	3.821334	-1.054613
C	-0.987618	3.296803	1.356262
C	-0.059032	4.821347	-0.814920
C	-0.044987	4.315666	1.540398
C	0.435879	5.077083	0.471346
H	0.305567	5.409414	-1.653037
H	0.330628	4.502710	2.542644
C	-1.418193	2.427161	2.509177
H	-0.793904	1.525482	2.553000
H	-2.463566	2.117920	2.427239
H	-1.291882	2.956632	3.456925
C	1.479093	6.145863	0.679968
H	1.802876	6.195569	1.722984
H	1.096857	7.132948	0.394972
H	2.360776	5.952185	0.058742
C	-1.497901	3.526565	-2.445952
H	-2.588163	3.430245	-2.473110
H	-1.075096	2.586065	-2.818597
H	-1.206833	4.320567	-3.137306
H	-5.568286	-2.193996	-1.593901

H	-0.619658	-4.536900	0.326627
H	0.228559	1.325246	0.331079
C	3.237674	-2.028556	0.115868
C	3.066640	-3.011447	-0.897368
C	4.183466	-3.665124	-1.444294
C	5.463729	-3.388648	-0.984905
C	5.635107	-2.439180	0.033935
C	4.546689	-1.758909	0.568472
H	4.010804	-4.401924	-2.223312
H	6.323510	-3.899550	-1.407594
H	6.633576	-2.211122	0.397112
H	4.693824	-1.005603	1.332169
C	1.714417	-3.384705	-1.348916
H	0.897113	-2.885270	-0.803668
O	1.475889	-4.194390	-2.237796
N	2.111418	-1.303411	0.512321
S	1.833565	-0.943085	2.100816
O	2.800979	-1.618465	2.992338
O	1.627224	0.510439	2.290141
C	0.229918	-1.711688	2.360957
H	0.327092	-2.787954	2.219413
H	-0.092543	-1.486194	3.380382
H	-0.466617	-1.296805	1.632635

Vibrational frequencies

-266.3713	14.1374	17.0387
29.0939	33.8290	38.9714
43.0278	49.7425	52.1536
55.2036	58.6515	62.9920
67.7432	80.8904	82.8941
91.9022	95.4685	111.3816

126.0013 127.9639 138.3487
139.4724 153.3090 156.4450
160.1041 181.5203 187.7068
197.9069 205.2940 206.9321
218.8208 224.1404 237.9299
244.5994 247.6185 259.6932
263.3087 269.0563 282.2987
286.1449 297.7979 305.8279
316.1065 324.2234 339.2340
348.4619 360.3361 371.6812
394.1141 400.1390 412.8531
419.9770 429.3232 452.6600
460.8547 470.7648 475.7385
485.9610 493.8265 509.7073
513.3165 525.2284 528.8261
535.9425 538.1398 545.6132
547.0182 579.6506 581.9156
589.6011 595.0841 604.6707
618.3408 627.3525 632.5603
637.7988 649.3084 654.9114
682.7074 695.5128 702.6531
712.0936 726.9352 746.2712
750.5605 752.9436 760.5061
770.2162 778.7168 784.0251
790.1944 795.3697 797.9217
839.2123 842.5445 845.0517
858.6946 873.2769 883.2173
884.8227 886.3412 902.6180
904.9349 907.2448 932.2442
935.4569 962.9287 971.7002

972.0625	974.6141	981.3129
983.0279	988.2940	990.9665
996.3990	1002.1303	1007.5600
1014.2211	1015.6246	1038.0135
1043.1397	1047.9768	1048.9118
1050.4227	1054.8009	1056.0273
1060.8270	1066.6501	1067.7031
1070.0110	1073.8708	1076.6701
1082.0884	1104.9572	1112.4775
1119.2507	1124.0716	1130.2551
1138.4174	1141.5910	1165.4131
1182.8478	1188.4647	1188.7529
1191.2169	1200.6959	1212.0080
1215.6444	1223.8464	1230.8911
1233.7149	1244.6222	1256.1710
1265.9417	1276.7321	1282.3509
1286.9916	1291.7443	1299.8176
1313.1399	1318.1299	1322.0917
1330.5144	1342.4269	1345.4838
1345.9009	1349.3313	1362.3011
1369.4135	1372.7943	1379.6928
1383.3545	1415.8953	1417.6240
1420.3670	1421.7191	1430.7050
1436.1802	1449.5763	1456.1410
1457.5917	1460.7041	1466.3796
1481.0649	1485.4741	1486.2404
1487.2755	1489.4493	1492.9452
1496.2740	1500.9716	1502.4536
1504.3622	1506.1592	1507.4360
1516.8330	1528.1474	1535.0253

1563.9526	1606.0910	1619.5371
1630.5975	1636.4428	1641.7256
1642.2034	1648.0640	1653.3790
1654.8535	1661.9110	1755.5420
3026.6289	3036.0368	3039.7213
3042.7622	3047.4888	3062.7029
3073.7355	3102.1352	3109.1962
3110.6469	3112.7446	3123.2642
3129.7612	3131.4882	3141.3829
3142.1113	3162.3183	3176.8728
3177.4757	3179.2981	3183.9706
3185.0631	3185.3929	3186.5776
3188.2086	3195.6425	3196.0263
3196.2916	3196.5329	3206.6098
3207.7431	3208.8345	3235.1312
3240.0515	3243.1837	3308.5162

TS5S(Φ=-61°)

Zero-point correction= 0.671405

Thermal correction to Energy= 0.713719

Thermal correction to Enthalpy= 0.714663

Thermal correction to Gibbs Free Energy= 0.593195

Sum of electronic and zero-point Energies= -2462.452146

Sum of electronic and thermal Energies= -2462.409833

Sum of electronic and thermal Enthalpies= -2462.408888

Sum of electronic and thermal Free Energies= -2462.530356

Cartesian coordinates

C	0.966773	1.612864	-0.331424
C	0.076893	0.700961	0.292885
H	0.655469	1.927314	-1.321054

C	-0.920177	0.078127	-0.459228
O	-1.188178	0.168628	-1.679778
C	1.632046	2.691118	0.431942
C	1.998213	3.871229	-0.238018
C	1.920639	2.580790	1.802588
C	2.614879	4.918795	0.442390
H	1.794486	3.960289	-1.301699
C	2.543840	3.625910	2.482842
H	1.674263	1.669598	2.337007
C	2.889950	4.798474	1.807156
H	2.886045	5.824939	-0.091436
H	2.766922	3.521385	3.540616
H	3.376681	5.610798	2.338951
C	-1.918501	-0.757627	0.323434
C	-3.733398	-1.443764	1.344395
C	-3.557992	1.074758	1.051529
H	-2.832208	1.523753	1.731595
N	-3.021767	-2.523564	1.159556
N	-1.888216	-2.075605	0.515317
N	-3.094488	-0.333549	0.837823
C	-5.058929	-1.331555	2.029591
H	-5.104104	-2.042794	2.856994
H	-5.865919	-1.579863	1.327391
C	-4.997784	1.025366	1.650357
O	-5.211569	-0.029384	2.577473
C	-5.131627	1.877615	-0.561393
C	-3.772569	1.869716	-0.215190
C	-2.837624	2.598752	-0.948160
C	-3.275089	3.314001	-2.064664
C	-4.626297	3.303186	-2.429933

C	-5.565408	2.593349	-1.675734
C	-5.949444	1.089057	0.429476
H	-1.795066	2.615543	-0.652093
H	-4.951359	3.865947	-3.300413
H	-6.617314	2.609608	-1.946332
H	-6.175533	0.089818	0.039027
H	-6.901634	1.561132	0.684638
C	-0.815659	-2.993278	0.217299
C	0.056751	-3.337285	1.260511
C	-0.710704	-3.511318	-1.078439
C	1.076838	-4.243662	0.964725
C	0.334223	-4.406438	-1.320866
C	1.236995	-4.777254	-0.320474
H	1.768791	-4.529466	1.752340
H	0.452180	-4.811040	-2.322168
C	-1.666838	-3.097844	-2.164296
H	-1.548520	-2.031627	-2.383384
H	-2.707828	-3.261580	-1.861763
H	-1.483778	-3.666559	-3.078967
C	2.394338	-5.692246	-0.630076
H	2.161820	-6.369816	-1.456945
H	2.679522	-6.291975	0.239815
H	3.272651	-5.104481	-0.925225
C	-0.073706	-2.720842	2.629363
H	-1.079713	-2.852648	3.040508
H	0.127072	-1.643634	2.590168
H	0.640098	-3.167012	3.325427
H	-5.116653	1.940835	2.234489
H	-2.561581	3.885901	-2.650278
H	0.144009	0.481888	1.351714

C	3.275846	0.102584	0.069360
C	4.360156	0.803162	0.657314
C	4.962810	0.313541	1.827145
C	4.522001	-0.863958	2.416915
C	3.459863	-1.566611	1.831678
C	2.838023	-1.091639	0.680554
H	5.784345	0.883233	2.250988
H	4.995855	-1.238013	3.319744
H	3.105344	-2.489714	2.281454
H	2.009826	-1.630723	0.241572
C	4.889945	2.041311	0.048623
H	4.442080	2.313399	-0.922064
O	5.772482	2.725210	0.551035
N	2.603942	0.691837	-1.023636
S	2.364654	-0.330142	-2.325382
O	3.692808	-0.636269	-2.907933
O	1.489569	-1.495031	-2.057006
C	1.487529	0.743408	-3.465306
H	2.014310	1.694280	-3.553122
H	1.496033	0.218462	-4.423159
H	0.460928	0.859501	-3.115190

Vibrational frequencies

-261.3796	7.8359	17.6973
22.1036	22.8541	30.7139
34.6601	43.8552	48.4229
50.4350	57.0314	61.4937
63.3734	72.9279	85.4510
91.5902	93.1839	105.8823
113.0341	118.8605	138.8697
146.5362	155.6937	160.9036

173.3710	181.1460	187.8849
192.4599	198.7423	207.4836
218.1218	229.6925	240.8021
244.7318	249.5748	255.1191
259.8833	280.3584	284.2355
289.4788	291.1952	294.9504
309.6464	317.0194	324.8115
331.2319	354.1654	371.0282
395.2235	411.0760	413.9192
437.6462	450.3273	456.5785
462.7719	468.6226	470.7497
481.7032	501.1919	506.4142
517.1900	520.7407	527.3203
528.7787	535.8341	537.0345
576.3630	581.9323	586.9834
593.0055	597.7642	606.6416
617.5803	620.4686	630.3786
632.3608	652.9532	656.0953
691.9733	701.3745	705.0877
716.5411	731.8096	735.8947
748.5906	757.7984	762.1934
766.1371	771.9183	787.2638
793.9530	801.6716	805.6650
838.5541	839.6357	844.0983
859.0151	869.4746	884.7562
886.3804	895.2359	899.8640
901.9701	905.6913	925.3115
939.7964	962.4689	967.0160
975.8708	977.1163	979.0130
979.7731	986.4674	1001.0892

1001.3800	1004.0598	1005.1527
1008.2746	1014.5812	1036.6536
1040.4655	1044.1784	1047.9820
1051.9135	1054.3830	1054.7379
1062.5692	1067.4004	1070.6786
1071.1596	1076.7597	1080.0582
1088.3782	1092.3411	1106.2618
1110.6215	1120.6840	1127.0451
1132.9603	1156.0380	1172.4584
1183.8694	1187.7983	1189.7689
1190.0434	1202.0753	1209.4240
1216.5496	1223.2166	1226.5214
1232.0249	1242.8219	1251.7295
1255.8264	1261.9892	1274.6307
1290.7938	1292.7008	1296.5292
1305.5284	1320.5930	1323.1513
1336.5117	1340.1534	1343.4265
1346.1464	1348.9609	1355.5900
1364.2370	1371.8018	1374.9728
1381.4925	1414.1668	1416.1405
1420.1023	1421.3331	1423.7665
1427.0339	1450.1794	1455.0437
1461.2236	1471.3965	1482.4089
1483.8910	1484.6070	1486.5079
1488.8662	1489.0198	1490.1033
1495.1276	1502.0688	1503.9596
1510.0178	1511.4170	1519.5670
1522.0100	1530.6222	1539.2190
1559.7924	1609.7455	1620.8844
1633.0483	1638.6547	1640.4807

1644.0548	1650.6367	1655.8763
1657.2154	1662.9319	1760.5163
3011.2668	3038.6122	3039.0079
3040.0167	3046.0523	3067.4655
3069.6341	3101.5274	3107.0560
3107.2153	3110.4383	3121.9812
3128.1184	3128.1535	3137.2846
3138.8446	3139.8235	3172.8640
3181.2064	3182.8827	3185.7484
3186.4911	3187.0382	3187.8810
3191.2587	3196.9289	3196.9579
3198.8731	3203.3264	3207.0999
3207.2920	3208.8935	3213.8969
3217.1495	3223.3198	3254.7991

TS5S(Φ=-75°)

Zero-point correction= 0.671760

Thermal correction to Energy= 0.713793

Thermal correction to Enthalpy= 0.714738

Thermal correction to Gibbs Free Energy= 0.595935

Sum of electronic and zero-point Energies= -2462.451702

Sum of electronic and thermal Energies= -2462.409668

Sum of electronic and thermal Enthalpies= -2462.408724

Sum of electronic and thermal Free Energies= -2462.527527

Cartesian coordinates

C	1.489011	0.659279	-0.850819
C	0.322968	0.479325	-0.062659
H	1.350904	0.414818	-1.899272
C	-0.825727	-0.097860	-0.617633
O	-1.017841	-0.565214	-1.764869

C	2.384354	1.821090	-0.643999
C	3.163826	2.274377	-1.721017
C	2.498729	2.480447	0.591370
C	4.029311	3.357099	-1.573086
H	3.091515	1.763966	-2.677400
C	3.370057	3.557303	0.742712
H	1.924926	2.138599	1.445638
C	4.137457	4.000244	-0.338048
H	4.625265	3.691687	-2.416990
H	3.455383	4.048285	1.707741
H	4.817481	4.838339	-0.217035
C	-2.028797	-0.112052	0.301542
C	-3.650183	0.387639	1.691122
C	-2.273717	2.376798	0.917242
H	-1.270639	2.474360	1.330972
N	-3.756066	-0.900193	1.496004
N	-2.743523	-1.193631	0.613385
N	-2.612147	0.918399	0.959404
C	-4.485024	1.235527	2.599342
H	-4.640231	0.707581	3.543090
H	-5.470439	1.412662	2.149470
C	-3.345143	3.149519	1.752645
O	-3.803301	2.444428	2.898250
C	-3.649909	3.683933	-0.546982
C	-2.430183	2.997210	-0.455794
C	-1.526948	3.001015	-1.519493
C	-1.873695	3.675094	-2.692612
C	-3.099009	4.343217	-2.793509
C	-3.990055	4.360546	-1.717079
C	-4.428210	3.596262	0.739301

H	-0.569524	2.502900	-1.432712
H	-3.352897	4.867224	-3.710528
H	-4.930343	4.900068	-1.786967
H	-5.234892	2.858998	0.654449
H	-4.887367	4.542916	1.035484
C	-2.520040	-2.555482	0.196514
C	-1.716584	-3.365030	1.006900
C	-3.127906	-2.999513	-0.983785
C	-1.520244	-4.683828	0.592181
C	-2.900243	-4.327400	-1.352659
C	-2.098016	-5.178905	-0.582139
H	-0.890191	-5.332733	1.194104
H	-3.355543	-4.702329	-2.265604
C	-3.960394	-2.070557	-1.826476
H	-3.322903	-1.279182	-2.234881
H	-4.751978	-1.593120	-1.237978
H	-4.429259	-2.607541	-2.654488
C	-1.831001	-6.595128	-1.028201
H	-2.639874	-6.978646	-1.657283
H	-1.709980	-7.268212	-0.173830
H	-0.905162	-6.647199	-1.614861
C	-1.075848	-2.816749	2.253232
H	-1.824504	-2.422509	2.949504
H	-0.390061	-2.005472	1.992539
H	-0.500064	-3.589322	2.766929
H	-2.843931	4.036005	2.147612
H	-1.180206	3.686959	-3.528085
H	0.286630	0.826110	0.963225
C	3.501123	-0.582195	0.655437
C	4.780850	0.027410	0.647699

C	5.400277	0.375812	1.858150
C	4.786665	0.113139	3.075979
C	3.533299	-0.512964	3.089487
C	2.894666	-0.851784	1.899619
H	6.375297	0.850986	1.810580
H	5.274379	0.384887	4.007357
H	3.045244	-0.728304	4.036449
H	1.920723	-1.324615	1.913064
C	5.501846	0.284633	-0.616996
H	4.994361	-0.077713	-1.527400
O	6.595609	0.831439	-0.678862
N	2.839570	-0.785402	-0.578050
S	2.265867	-2.335343	-0.802893
O	3.422162	-3.261523	-0.794757
O	1.132651	-2.701456	0.080209
C	1.633609	-2.242441	-2.477926
H	2.407672	-1.842791	-3.134277
H	1.395100	-3.271463	-2.756853
H	0.725144	-1.636487	-2.487838

Vibrational frequencies

-268.5024	16.8781	23.4782
27.2499	29.1944	38.6930
41.4490	43.9145	47.0961
64.5900	69.6297	71.6245
76.9647	77.4121	81.6499
88.7600	89.8123	107.5185
113.2922	118.9759	135.0550
139.2742	150.0516	168.3673
176.4850	185.0547	193.7852
199.9366	208.2814	212.9477

218.8428	236.2442	240.1905
244.1600	254.9147	260.5735
264.2544	283.6989	287.3280
291.0107	296.1834	303.1236
307.5425	313.7159	325.2030
332.9567	351.3459	377.5467
400.2536	412.0181	415.8501
434.7633	449.3724	453.7074
460.9197	467.3462	474.9262
483.6041	495.2780	513.7362
517.5471	522.7096	527.5639
530.8000	535.6371	538.6112
572.1842	582.4002	586.6542
588.6018	598.9697	606.4311
618.1779	624.8206	629.4592
632.6130	650.4373	653.0424
688.7795	698.4172	701.9062
713.2422	725.3840	733.6971
745.6453	756.2679	762.1331
773.6570	775.8829	786.5399
798.3870	802.6511	804.5102
837.8256	839.7681	843.0012
856.8860	871.6354	881.4079
886.4883	890.4947	899.7142
902.5669	905.8089	926.0176
938.1150	962.6249	969.6591
972.2679	976.8114	978.0761
980.9106	991.9149	997.9260
1004.8147	1007.9319	1010.3067
1014.6508	1015.7207	1038.4808

1039.4681	1043.5390	1045.9345
1049.7007	1054.8392	1055.6739
1063.7062	1067.9268	1069.6816
1071.2570	1075.8032	1078.6634
1089.0351	1096.7195	1110.3739
1111.9989	1120.9769	1126.9543
1134.6246	1155.6903	1171.4352
1185.1189	1188.6335	1188.8818
1189.6120	1200.8033	1211.3355
1215.6019	1221.2252	1231.1941
1234.8328	1242.2401	1249.4586
1253.2090	1266.9837	1269.9984
1289.9773	1293.5557	1300.1905
1301.3527	1319.1894	1326.2369
1338.4524	1339.1776	1342.4481
1346.9781	1347.9370	1366.7312
1369.6971	1370.6374	1376.2127
1379.9092	1411.5855	1415.7141
1416.3593	1418.8481	1420.3889
1423.8453	1450.9196	1458.9905
1460.6367	1474.6745	1483.5564
1484.3051	1485.2315	1486.4572
1487.6811	1489.2512	1489.7700
1494.7865	1497.2325	1502.8082
1510.2371	1511.4896	1518.3035
1522.3713	1531.4799	1538.6097
1560.2719	1612.7390	1619.1749
1632.5076	1638.9303	1640.0899
1645.3231	1646.5927	1655.6304
1656.5680	1660.6810	1759.8798

3003.6546	3039.3522	3043.5853
3050.5124	3053.0998	3058.2082
3063.7793	3101.3725	3107.1697
3109.2102	3118.7428	3120.5197
3128.0184	3131.7651	3137.8398
3142.8629	3146.0491	3163.8253
3182.5100	3182.9028	3183.1042
3183.6533	3186.1874	3187.1855
3187.7914	3189.9635	3197.0022
3197.2182	3198.0810	3207.0413
3208.4753	3209.8942	3211.5028
3218.0538	3237.3274	3241.5248

TS5S(Φ=129°)

Zero-point correction= 0.622393

Thermal correction to Energy= 0.665746

Thermal correction to Enthalpy= 0.666690

Thermal correction to Gibbs Free Energy= 0.544184

Sum of electronic and zero-point Energies= 0.611633

Sum of electronic and thermal Energies= 0.654986

Sum of electronic and thermal Enthalpies= 0.655931

Sum of electronic and thermal Free Energies= 0.533424

Cartesian coordinates

C	1.239832	-1.676253	-0.279343
C	0.186758	-0.895135	-0.718964
H	1.319825	-1.910987	0.797373
C	-0.822126	-0.475360	0.183138
O	-1.049768	-0.788015	1.328312
C	2.038442	-2.512355	-1.188880
C	3.204407	-3.142806	-0.716995

C	1.623506	-2.751358	-2.515503
C	3.950445	-3.972855	-1.559621
H	3.549454	-2.963071	0.307135
C	2.363570	-3.588533	-3.348499
H	0.712883	-2.287281	-2.891737
C	3.533919	-4.195470	-2.873596
H	4.870373	-4.427161	-1.190221
H	2.037157	-3.768377	-4.370798
H	4.120280	-4.836347	-3.531330
C	-1.904085	0.449725	-0.463115
C	-3.822692	1.215143	-1.358148
C	-3.907674	-1.205960	-0.571914
H	-3.175958	-2.050999	-0.669704
N	-2.958967	2.253067	-1.350852
N	-1.795684	1.781654	-0.796983
N	-3.195057	0.072035	-0.794154
C	-5.196746	1.060686	-1.920406
H	-5.388185	1.728727	-2.787965
H	-5.978687	1.190167	-1.145560
C	-5.089800	-1.365819	-1.614460
O	-5.254800	-0.253167	-2.505169
C	-5.977567	-1.461352	0.642750
C	-4.587929	-1.231035	0.778706
C	-4.011589	-1.081043	2.032823
C	-4.841131	-1.154775	3.163934
C	-6.212504	-1.377670	3.030034
C	-6.796311	-1.535846	1.761101
C	-6.373246	-1.616096	-0.794730
H	-2.932757	-0.910424	2.152801
H	-6.842414	-1.433083	3.918986

H	-7.864568	-1.714947	1.665774
H	-7.178025	-0.914563	-1.090804
H	-6.782368	-2.627132	-0.991831
C	-0.635352	2.608871	-0.600719
C	0.180784	2.929586	-1.717906
C	-0.306240	3.052889	0.705589
C	1.385573	3.584643	-1.492785
C	0.925842	3.688600	0.890478
C	1.800838	3.916453	-0.183066
H	2.044735	3.823194	-2.327088
H	1.225570	3.982561	1.898537
C	-1.204700	2.847294	1.869310
H	-0.774882	2.088565	2.577868
H	-2.218276	2.520863	1.628974
H	-1.297890	3.763471	2.473357
C	3.160361	4.453670	0.042461
H	3.297849	4.939760	1.014169
H	3.502127	5.142408	-0.737734
H	3.889420	3.590273	0.020927
C	-0.231682	2.553409	-3.102322
H	-1.190999	3.024583	-3.372316
H	-0.347619	1.468132	-3.219672
H	0.498272	2.877687	-3.859111
H	-4.874467	-2.176176	-2.346604
H	-4.399739	-1.037884	4.155310
H	0.141044	-0.563679	-1.751489
C	3.370281	-0.522391	1.554903
C	2.519764	-0.278683	2.674880
C	2.888599	-0.742450	3.955289
C	4.087152	-1.403299	4.162282

C	4.967797	-1.582731	3.072735
C	4.630568	-1.158095	1.804876
H	2.201800	-0.551515	4.785117
H	4.364004	-1.761856	5.146429
H	5.928600	-2.069777	3.244915
H	5.330332	-1.300951	0.975199
C	1.333383	0.555475	2.523107
H	1.106726	0.903719	1.498898
O	0.611761	0.905867	3.452036
N	2.932808	-0.203846	0.284259
S	4.009184	0.371857	-0.854075
O	4.455607	1.725634	-0.496064
O	5.069147	-0.594923	-1.141182
C	3.028574	0.549571	-2.307548
H	2.197648	1.243603	-2.135168
H	3.617590	0.953401	-3.139146
H	2.612776	-0.400028	-2.656923

Vibrational frequencies

-194.5709	-6.6489	11.0854
20.0486	26.0118	30.1171
36.8650	41.4108	42.5267
49.8679	52.6412	59.3066
65.5875	69.4571	76.7153
89.7466	97.3295	103.5217
108.1951	112.0633	113.4476
119.6919	122.1744	129.9685
139.9240	143.6301	171.1905
176.3262	182.9015	191.5284
195.8001	197.2320	204.2725
212.3968	222.7357	230.9563

244.1864	245.0143	251.8917
265.9716	283.2311	289.4208
290.7212	305.0130	320.3734
328.0194	328.5433	354.6942
360.6606	373.4350	398.4752
405.0260	412.5562	425.1870
431.4574	440.9582	450.4406
456.6854	465.0955	469.9892
478.4563	480.4872	482.3281
500.2471	501.2718	509.6560
525.1718	552.4822	554.6743
556.4954	567.7968	570.1343
584.8367	596.9654	610.5589
624.6259	633.3327	637.1439
639.2443	651.5489	664.6545
682.7518	702.3064	714.7894
716.1916	749.2495	778.3924
792.5019	799.8045	810.5944
817.3005	819.8841	820.0946
839.5379	851.3305	869.3142
870.8089	876.1510	880.6670
885.0564	899.5670	905.9318
912.1667	923.1764	931.2600
939.3597	943.0732	950.9328
961.6222	969.1512	972.5232
976.1971	987.0412	987.7164
988.1110	989.6910	990.8511
994.4724	996.2509	1006.7760
1010.1286	1013.0610	1017.6741
1026.9629	1027.7363	1033.1273

1043.3910	1045.1125	1070.8620
1079.6878	1086.9224	1093.2249
1096.4863	1107.4057	1107.8209
1111.2482	1115.9080	1120.4001
1131.8469	1140.3553	1142.4700
1149.6515	1157.3706	1158.8825
1172.6136	1173.6291	1182.7712
1186.2133	1189.5919	1193.5335
1201.4616	1205.0636	1211.8200
1215.0909	1217.8216	1218.6147
1220.3467	1222.3412	1226.0195
1226.7844	1230.2853	1232.4724
1234.6897	1236.6621	1240.2393
1241.0264	1248.1193	1249.1075
1251.0621	1259.3990	1272.9781
1278.9797	1288.9190	1296.7240
1298.3861	1301.6786	1309.7552
1310.7189	1316.1904	1334.0389
1336.1607	1340.0848	1348.1674
1361.4906	1362.2683	1366.3878
1400.5849	1445.2016	1476.3586
1477.1021	1485.1554	1491.5592
1499.9870	1502.6579	1502.9715
1513.0138	1515.1722	1535.6620
1562.3674	1594.2811	1604.0825
1607.0223	1625.1173	1637.8188
1642.1725	1652.0634	1662.0376
1665.1444	1723.8263	1809.8375
2559.2696	2564.4320	2645.3461
2645.4567	2660.8846	2663.4001

2676.8549	2681.6934	2687.9930
2689.1076	2691.3267	2694.9476
2695.6718	2700.9287	2702.2865
2705.3641	2714.0952	2721.1895
2736.7461	2741.8853	2744.6333
2744.8285	2748.7654	2748.9279
2751.4176	2751.7566	2755.1948
2758.4118	2764.0574	2765.6867
2771.8191	2776.9804	2777.5556
2779.7260	2785.1277	2798.2308

TS5S(Φ=137°)

Zero-point correction= 0.671845

Thermal correction to Energy= 0.713988

Thermal correction to Enthalpy= 0.714932

Thermal correction to Gibbs Free Energy= 0.595946

Sum of electronic and zero-point Energies= -2462.449940

Sum of electronic and thermal Energies= -2462.407797

Sum of electronic and thermal Enthalpies= -2462.406852

Sum of electronic and thermal Free Energies= -2462.525839

Cartesian coordinates

C	1.114490	-1.430821	-0.326626
C	-0.035922	-0.713258	-0.762810
H	1.127317	-1.571706	0.750326
C	-0.804229	-0.042672	0.190168
O	-0.660125	0.017157	1.433846
C	1.645017	-2.594574	-1.071229
C	2.318694	-3.600998	-0.358249
C	1.485133	-2.749189	-2.458433
C	2.829161	-4.721449	-1.012170

H	2.440220	-3.498060	0.715429
C	1.990906	-3.869749	-3.111844
H	0.962406	-1.992213	-3.033856
C	2.668901	-4.858467	-2.392497
H	3.346997	-5.488796	-0.443825
H	1.859368	-3.972386	-4.185295
H	3.064406	-5.731052	-2.904441
C	-2.011584	0.722315	-0.325064
C	-4.005742	1.376988	-0.957252
C	-3.713246	-1.142205	-0.756365
H	-3.132835	-1.590855	-1.563784
N	-3.312587	2.478971	-0.836358
N	-2.069569	2.050134	-0.432245
N	-3.244078	0.272512	-0.641184
C	-5.430051	1.236083	-1.395735
H	-5.634663	1.946735	-2.199388
H	-6.104876	1.469306	-0.561555
C	-5.243890	-1.123058	-1.054932
O	-5.652796	-0.067752	-1.915472
C	-4.910137	-1.942239	1.153768
C	-3.647683	-1.909425	0.543700
C	-2.555993	-2.568963	1.106963
C	-2.736612	-3.245977	2.315035
C	-3.990216	-3.266654	2.937106
C	-5.087207	-2.622679	2.356916
C	-5.935022	-1.205265	0.329080
H	-1.590211	-2.560946	0.614548
H	-4.115163	-3.799516	3.875461
H	-6.063151	-2.658584	2.832452
H	-6.122746	-0.209084	0.745947

H	-6.898417	-1.718069	0.268366
C	-0.963057	2.960599	-0.275537
C	-0.229022	3.292836	-1.425259
C	-0.645118	3.425812	1.004864
C	0.895551	4.099630	-1.251562
C	0.499464	4.223195	1.123470
C	1.287787	4.551312	0.017342
H	1.491812	4.364576	-2.120863
H	0.791953	4.565977	2.110766
C	-1.467844	3.045631	2.205548
H	-1.281191	1.998048	2.457915
H	-2.538832	3.161623	2.005757
H	-1.207068	3.664862	3.066058
C	2.563732	5.337798	0.175448
H	2.637957	5.794230	1.166119
H	2.643197	6.129885	-0.576789
H	3.430890	4.678789	0.044613
C	-0.629283	2.771168	-2.781292
H	-1.648189	3.077153	-3.041644
H	-0.603650	1.675717	-2.802672
H	0.047737	3.139257	-3.555185
H	-5.459579	-2.038343	-1.611027
H	-1.897917	-3.762735	2.771611
H	-0.322047	-0.662015	-1.806519
C	3.316546	-0.465674	1.063086
C	2.883670	0.161082	2.258275
C	3.478707	-0.184211	3.481843
C	4.505293	-1.118969	3.540047
C	4.955145	-1.717205	2.355702
C	4.365670	-1.403318	1.133855

H	3.122755	0.315988	4.377616
H	4.960811	-1.376774	4.491511
H	5.762971	-2.443453	2.387026
H	4.698306	-1.885144	0.221592
C	1.872775	1.244628	2.230681
H	1.503649	1.521677	1.233496
O	1.497264	1.839125	3.232951
N	2.619673	-0.180288	-0.135086
S	3.579897	0.172814	-1.445228
O	4.528318	1.245122	-1.063919
O	4.162999	-1.010799	-2.120204
C	2.371019	0.891174	-2.556399
H	1.932267	1.759319	-2.068984
H	2.913090	1.186663	-3.457271
H	1.609889	0.153393	-2.801220

Vibrational frequencies

-301.9863	16.5829	23.4317
28.2051	33.4241	33.9988
40.8489	47.1104	53.8571
56.1430	66.2356	68.9911
73.4329	75.0720	82.9237
94.6293	96.2888	108.2829
117.2860	120.3963	135.4957
139.7534	148.0700	156.2604
164.8983	171.1307	190.0642
205.1345	207.4556	208.6701
227.4881	231.5452	240.4129
245.3698	250.5555	254.4879
261.8850	273.7221	282.3324
285.1274	293.3590	295.9215

308.3765	316.4579	326.9003
343.4255	349.9405	370.3994
390.5009	413.6151	418.3816
435.4997	447.9126	454.9467
459.1407	468.4145	471.6340
482.9718	501.7603	508.4535
511.9135	516.0199	527.4984
530.0003	532.9181	547.6608
566.0075	580.9029	588.2944
590.5914	599.7471	607.0586
617.5717	623.9868	627.8939
633.9251	649.7627	652.7919
679.2037	701.5050	702.9013
718.5835	729.7991	736.1024
745.3992	755.8190	766.2271
767.8535	775.2966	784.9768
795.1461	796.9016	800.6892
838.5638	839.8375	841.5222
856.7350	866.8786	883.0122
887.5607	898.7812	902.9473
903.5287	906.4377	922.4453
933.5884	960.1252	969.5006
976.3634	977.0949	978.1510
981.1820	996.1475	999.7296
1002.6200	1003.4220	1007.4763
1011.1122	1013.8991	1032.3835
1037.8257	1041.0242	1045.3077
1050.7639	1053.8084	1056.4480
1061.9700	1065.8148	1070.4690
1071.1738	1072.9951	1080.0160

1087.4087	1098.8045	1111.0629
1118.4318	1127.6706	1133.6584
1152.8202	1169.6452	1183.9096
1188.1374	1188.8946	1189.2788
1194.7265	1201.1962	1208.5525
1218.1973	1221.2427	1230.2419
1235.7043	1242.3991	1246.6251
1250.8477	1266.6648	1281.3821
1290.5382	1291.6039	1300.8708
1303.6958	1321.3356	1325.9039
1332.2738	1339.5975	1340.4064
1349.7974	1353.8437	1370.3938
1371.4356	1372.1035	1373.6248
1384.3102	1414.1595	1416.9777
1417.7389	1419.5078	1421.4984
1423.9049	1449.6535	1456.9363
1464.2758	1466.7451	1468.1563
1479.7918	1483.4966	1485.2297
1486.9689	1487.4849	1488.8052
1492.8230	1498.7768	1502.9281
1506.9272	1510.2969	1516.0648
1519.1520	1527.7982	1537.2837
1557.9295	1612.1658	1616.8536
1632.9619	1639.1124	1641.2083
1642.0922	1647.3388	1654.2793
1657.8172	1662.0941	1757.0693
3040.4914	3044.8220	3045.8669
3049.5079	3058.4505	3063.0585
3092.5311	3101.5357	3104.1673
3108.6441	3120.7536	3120.9318

3129.5639	3131.1366	3133.6733
3142.2711	3148.5618	3167.7075
3181.1002	3183.7706	3184.6294
3187.0059	3188.4240	3193.4649
3196.8683	3197.7071	3198.2455
3202.2901	3203.8679	3208.3881
3208.7832	3210.4324	3216.9397
3223.3194	3223.9085	3224.6957

TS6'

Zero-point correction= 0.671406

Thermal correction to Energy= 0.713800

Thermal correction to Enthalpy= 0.714744

Thermal correction to Gibbs Free Energy= 0.594118

Sum of electronic and zero-point Energies= -2462.425868

Sum of electronic and thermal Energies= -2462.383473

Sum of electronic and thermal Enthalpies= -2462.382529

Sum of electronic and thermal Free Energies= -2462.503155

Cartesian coordinates

C	2.059045	0.286786	0.475217
C	0.596557	0.361598	0.099708
H	2.135981	-0.092632	1.496947
C	-0.308521	-0.103266	0.949451
O	-0.854137	-0.563853	1.887588
C	2.801892	1.622188	0.443224
C	4.118714	1.661797	0.924606
C	2.216510	2.801963	-0.017796
C	4.840347	2.854493	0.929377
H	4.579588	0.750390	1.295418
C	2.938663	3.998311	-0.017841
H	1.194722	2.800072	-0.375177

C	4.252076	4.029858	0.452116
H	5.859456	2.866913	1.305581
H	2.468962	4.904060	-0.389518
H	4.812508	4.960474	0.450548
C	-2.415735	0.419424	-0.445076
C	-4.663128	0.564851	-0.509324
C	-3.691121	-1.671242	-1.127804
H	-3.288730	-1.704726	-2.142673
N	-4.278564	1.769056	-0.192447
N	-2.889483	1.645520	-0.155430
N	-3.579477	-0.272632	-0.658823
C	-6.068888	0.078295	-0.677793
H	-6.666045	0.833280	-1.194476
H	-6.526205	-0.090364	0.307571
C	-5.186004	-2.108351	-1.077720
O	-6.101241	-1.098437	-1.477818
C	-4.009170	-3.264813	0.630804
C	-3.045295	-2.672324	-0.197737
C	-1.708731	-3.056955	-0.131044
C	-1.335983	-4.040949	0.788237
C	-2.292010	-4.623369	1.627909
C	-3.635404	-4.242088	1.551965
C	-5.383508	-2.717584	0.334742
H	-0.970890	-2.606832	-0.785148
H	-1.989601	-5.389026	2.336826
H	-4.377494	-4.709477	2.193337
H	-5.659050	-1.950948	1.068779
H	-6.170189	-3.476815	0.345272
C	-2.108597	2.810108	0.153929
C	-1.515116	3.527030	-0.893558

C	-1.983690	3.199775	1.496953
C	-0.768655	4.665159	-0.563630
C	-1.224961	4.338710	1.775965
C	-0.607957	5.081523	0.761422
H	-0.301418	5.234728	-1.362846
H	-1.111584	4.653472	2.810436
C	-2.645332	2.408566	2.596351
H	-2.260662	1.384071	2.629215
H	-3.726937	2.342019	2.438316
H	-2.468363	2.871539	3.570352
C	0.232803	6.286395	1.103930
H	-0.255459	6.912140	1.858539
H	0.428907	6.903967	0.222702
H	1.200815	5.977162	1.515848
C	-1.653492	3.078768	-2.326262
H	-2.691854	2.835018	-2.572697
H	-1.056910	2.179024	-2.516215
H	-1.309649	3.857005	-3.012231
H	-5.307392	-2.904276	-1.817137
H	-0.300901	-4.362726	0.841607
H	0.283603	0.783152	-0.839561
C	3.185997	-1.977743	0.317705
C	4.524518	-2.421513	0.322949
C	4.837657	-3.644942	0.934941
C	3.854622	-4.404236	1.559249
C	2.532927	-3.946243	1.572842
C	2.197105	-2.748528	0.943772
H	5.873061	-3.970131	0.921419
H	4.112033	-5.343328	2.039176
H	1.757884	-4.527183	2.063930

H	1.167385	-2.409971	0.936572
C	5.628528	-1.607242	-0.250517
H	5.364653	-0.580038	-0.545694
O	6.772734	-2.019917	-0.357902
N	2.843811	-0.738034	-0.314790
S	2.707705	-0.750898	-2.003600
O	2.388439	0.622757	-2.409390
O	3.903724	-1.422399	-2.531123
C	1.300816	-1.804619	-2.388451
H	0.400623	-1.329494	-2.001687
H	1.257589	-1.892014	-3.476330
H	1.463217	-2.784263	-1.936682

Vibrational frequencies

-74.8401	8.5564	17.9443
23.2153	31.1644	35.3582
39.8084	45.6522	54.1952
56.7459	59.5433	67.2562
74.0049	77.4183	86.9250
93.2073	97.9171	112.1454
121.7657	124.2971	135.0214
139.4565	149.3448	152.7950
155.1972	167.2947	180.4642
196.9644	200.7090	205.7566
214.3824	225.4363	233.5488
241.3791	250.3054	257.4306
268.8637	274.7510	277.8227
287.1974	300.9191	307.5108
323.8353	325.8657	329.6220
333.1865	355.1168	372.3983
379.8820	393.5789	408.7545

419.9684	423.0288	449.6382
464.1988	468.5292	477.3074
487.2162	498.8676	502.3463
513.4434	525.5174	529.2302
531.3674	536.4715	546.3813
557.3806	570.8326	574.1356
581.2478	593.5339	602.7693
605.7298	617.4791	630.3346
633.3973	641.2087	649.1425
666.7786	682.4245	688.3580
695.2558	709.1269	716.3820
725.9018	742.4338	748.8248
756.4749	770.7020	778.0597
788.1824	798.6519	820.7585
831.8152	839.0240	855.7048
866.9545	876.0503	882.5588
888.7788	900.5196	902.6496
904.9444	921.0019	949.6754
955.7166	959.0719	963.3654
972.7148	974.6060	983.0903
988.4299	990.6103	1003.5398
1004.3454	1007.4833	1013.5897
1014.2140	1016.6805	1019.1534
1037.4863	1039.5592	1040.5976
1046.1830	1048.7056	1052.2365
1056.6419	1062.3122	1063.2674
1067.1947	1070.9939	1072.2868
1075.2180	1077.0773	1112.1555
1115.1225	1124.5919	1126.8565
1136.9685	1139.7753	1161.6388

1183.8261	1187.3412	1192.2649
1194.8718	1196.4114	1213.1526
1216.0260	1219.4752	1224.3495
1234.7512	1245.5656	1254.8691
1257.8229	1266.4359	1277.2798
1289.2224	1292.4203	1305.7999
1307.9562	1310.9734	1323.3419
1329.0075	1340.3412	1344.4919
1347.8225	1350.9195	1355.7067
1363.3985	1364.6188	1366.3186
1372.0250	1384.7729	1415.6102
1417.4533	1420.3783	1422.8129
1425.5455	1430.6094	1436.1292
1445.4821	1448.3836	1450.0006
1473.9807	1477.6323	1483.6135
1486.3325	1486.7016	1487.5580
1488.6448	1489.6700	1493.4124
1505.5947	1506.7167	1507.3928
1519.8396	1522.6601	1533.8666
1536.8431	1624.4770	1626.4492
1639.5106	1639.7463	1640.1017
1645.4640	1656.3961	1657.7439
1664.8590	1773.6349	2142.2677
3024.5545	3036.9685	3040.1935
3047.0114	3050.8133	3059.5595
3082.5016	3093.5333	3099.5630
3101.1068	3107.5914	3107.8663
3115.8677	3117.9717	3125.8375
3125.9919	3135.5579	3136.0139
3178.3082	3180.1701	3181.0394

3183.0473	3184.1175	3188.7242
3195.6258	3197.8922	3199.0621
3207.4195	3207.4535	3208.0345
3217.1094	3219.7208	3232.2015
3233.1491	3248.7567	3301.6564

M6'

Zero-point correction= 0.287508

Thermal correction to Energy= 0.308728

Thermal correction to Enthalpy= 0.309672

Thermal correction to Gibbs Free Energy= 0.235378

Sum of electronic and zero-point Energies= -1410.315421

Sum of electronic and thermal Energies= -1410.294201

Sum of electronic and thermal Enthalpies= -1410.293257

Sum of electronic and thermal Free Energies= -1410.367551

Cartesian coordinates

C	0.663523	-0.222665	-1.057948
C	0.205404	-1.612055	-1.441490
H	0.716087	0.372245	-1.975140
C	0.806069	-2.728711	-1.081139
O	1.310075	-3.750558	-0.807732
C	2.047234	-0.246738	-0.422137
C	2.262730	-0.868320	0.817485
C	3.133278	0.328789	-1.091744
C	3.542736	-0.917545	1.370647
H	1.426277	-1.304735	1.355838
C	4.414187	0.280763	-0.537297
H	2.974709	0.820748	-2.047066
C	4.621793	-0.342269	0.694697
H	3.695944	-1.402119	2.330616

H	5.247392	0.733240	-1.067119
H	5.617400	-0.377609	1.127333
H	-0.640710	-1.748268	-2.108332
C	-1.740407	0.061103	-0.305115
C	-2.421395	-0.590234	0.742059
C	-3.761636	-0.968723	0.560222
C	-4.419647	-0.707304	-0.635010
C	-3.739752	-0.056705	-1.670202
C	-2.409719	0.326459	-1.504841
H	-4.266477	-1.470009	1.379723
H	-5.456135	-1.003255	-0.764246
H	-4.247389	0.157108	-2.606051
H	-1.885873	0.834602	-2.308748
C	-1.765361	-0.893080	2.035528
H	-0.710860	-0.578746	2.120498
O	-2.327156	-1.452199	2.964886
N	-0.350449	0.434937	-0.129712
S	-0.147910	2.148168	0.055261
O	0.516669	2.699852	-1.138665
O	-1.451196	2.684315	0.469130
C	0.967766	2.320324	1.449274
H	1.946547	1.918018	1.195904
H	1.036140	3.394225	1.640097
H	0.538698	1.809507	2.311619

Vibrational frequencies

16.7017	31.9321	34.5311
48.2324	53.5978	82.1561
87.0336	98.5243	129.2795
134.1594	172.5765	191.0944
197.9862	215.2901	228.3815

242.6404	263.6786	275.6318
295.0472	304.2672	343.6796
375.4149	408.9135	424.5507
461.9465	480.9928	486.5476
504.4534	520.7237	533.9997
537.1861	555.9864	569.2170
630.8820	634.8564	651.4005
686.3936	716.8662	732.6634
755.9002	768.1072	781.9106
798.3119	833.5711	835.7083
871.2058	877.3559	912.3174
945.5108	968.5591	988.0221
991.4916	993.0479	999.1805
1004.3877	1011.7569	1015.0659
1016.9361	1035.8660	1054.6319
1066.9936	1107.6107	1111.3666
1115.0440	1139.0711	1180.5241
1181.6819	1201.7669	1204.6420
1220.9547	1232.2443	1294.0224
1300.4795	1308.1529	1330.5058
1347.1975	1360.1149	1365.5026
1388.7525	1417.7020	1426.4115
1445.5170	1456.5618	1485.8593
1493.2480	1519.4032	1535.4482
1625.9158	1638.2515	1643.9062
1656.3407	1771.4301	2208.3050
3009.7185	3070.7789	3084.8876
3183.8459	3187.2798	3193.1852
3196.2168	3199.8018	3202.9776
3205.1347	3206.2907	3213.1750

3213.5318 3215.3675 3220.1432

Zero-point correction= 0.288956

Thermal correction to Energy= 0.308451

Thermal correction to Enthalpy= 0.309395

Thermal correction to Gibbs Free Energy= 0.240133

Sum of electronic and zero-point Energies= -1410.312740

Sum of electronic and thermal Energies= -1410.293246

Sum of electronic and thermal Enthalpies= -1410.292301

Sum of electronic and thermal Free Energies= -1410.361564

Cartesian coordinates

C	-0.607185	0.705807	-0.536381
C	0.350899	1.845288	-0.159878
H	-0.950720	0.845978	-1.562175
C	0.380813	3.008154	-0.938004
O	0.295008	3.758265	-1.805728
C	-1.805681	0.596322	0.386013
C	-3.091390	0.822542	-0.116995
C	-1.645710	0.246818	1.734577
C	-4.206426	0.707237	0.717407
H	-3.219310	1.081131	-1.164883
C	-2.758631	0.130047	2.565542
H	-0.652062	0.056773	2.129886
C	-4.041860	0.360694	2.059294
H	-5.200408	0.882452	0.316412
H	-2.626004	-0.142782	3.608442
H	-4.907572	0.267631	2.708351
H	0.423388	2.067534	0.901300
C	1.363193	-0.683658	0.332013
C	2.285260	0.378919	0.393218

C	3.350875	0.328921	1.288405
C	3.550635	-0.805478	2.077007
C	2.652955	-1.872885	1.994517
C	1.547625	-1.806884	1.143958
H	4.016611	1.184698	1.340083
H	4.395971	-0.855247	2.756987
H	2.798195	-2.756230	2.609191
H	0.842216	-2.628508	1.110690
C	2.043996	1.590457	-0.480645
H	2.030507	1.256538	-1.543536
O	2.557253	2.759558	-0.198866
N	0.233549	-0.534468	-0.538295
S	-0.228157	-1.770428	-1.598134
O	-0.804078	-1.121871	-2.784872
O	0.916047	-2.675753	-1.729533
C	-1.565552	-2.639617	-0.769727
H	-2.386813	-1.940419	-0.607535
H	-1.878633	-3.448842	-1.433402
H	-1.206436	-3.040276	0.178455

Vibrational frequencies

-561.4925	22.4141	32.6975
49.1113	67.6243	73.8778
88.7877	129.3070	153.1707
165.5944	185.4464	216.6069
222.1746	238.6618	241.6382
270.4925	287.3768	302.8153
321.5266	359.3850	373.1077
378.3469	414.1309	463.1006
469.7665	480.9107	515.3826
518.9316	525.6477	542.2787

569.8743	620.2191	629.4465
633.3634	644.0171	661.0513
712.0886	726.0293	744.0749
760.9358	772.4913	807.4879
844.3621	849.2708	860.7822
887.7422	915.3638	935.6054
957.4577	982.0299	986.7404
991.6298	993.3287	1007.8840
1014.2532	1025.9559	1031.1338
1055.3951	1069.1119	1100.6073
1107.7812	1112.3033	1120.2418
1124.6307	1185.0445	1187.8062
1200.1623	1210.3428	1216.0229
1228.6100	1247.6135	1274.9194
1298.5303	1313.2208	1322.4997
1334.9894	1349.8477	1362.9300
1375.3400	1399.1628	1414.9076
1435.5243	1446.6667	1456.4476
1490.0838	1495.4076	1513.0477
1535.3671	1627.5065	1639.6980
1650.2049	1656.6172	2182.7557
2836.7172	3080.6026	3130.1385
3181.0044	3182.4600	3184.8642
3186.9164	3189.4120	3194.3260
3197.0097	3202.2590	3202.3928
3211.3272	3211.4019	3230.0654