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Electronic Supporting Information

for

Mechanism and origin of selectivities for NHC-catalyzed synthesis of axially chiral benzothiophene/benzofuran-fused biaryls

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Part 1: Computational methods

Using the Gaussian 09 suite of programs, the density functional theory (DFT) calculations were performed to locate all the reactants, intermediates, transition states, and products involved in the possible reaction pathways. After the optimization at the B3LYP-D3/6-31G(d, p)/$SMD_{dichloroethane}$ level, we performed frequency calculations to confirm if the numbers of imaginary frequencies associated with the local minima and transition state are correct.

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-D3/6-31G(d, p)/$SMD_{dichloroethane}$ level and the single-point energies (SPE) at a higher computational level of B3LYP-D3/6-311++G(2df, 2pd)/$SMD_{dichloroethane}$. To check whether the selected method is reliable, the additional calculations by employing different DFT methods (including M06-2X/6-311++G(2df, 2pd)/$SMD_{dichloroethane}$//M06-2X/6-31G(d, p)/$SMD_{dichloroethane}$ and ωB97X-D/6-311++G(2df, 2pd)/$SMD_{dichloroethane}$//ωB97X-D/6-31G(d, p)/$SMD_{dichloroethane}$) have been performed for the key transition states involved in the stereoselectivity-determining step, and the computed and test 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 **TS4RR/SR** Calculated by Using the Three DFT Methods.

Method	B3LYP-D3	M06-2X	ωB97XD
TS4RR	2.8	1.3	2.8
TS4SR	0.0	0.0	0.0

We further computed the single-point energies for the key transition states **TS4RR/RS/SR/SS** optimized at the B3LYP-D3/6-31G(d, p)/$SMD_{dichloroethane}$ level by using the higher basis set 6-311++G(2df, 2pd). As summarized in **Table S2**, the relative energies of transition states **TS4RR/RS/SR/SS** 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 **TS4RR/RS/SR/SS** Calculated by 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)
TS4RR	2.8	2.6
TS4RS	3.9	5.0
TS4SR	0.0	0.0
TS4SS	2.1	2.1

Atom-in-molecule (AIM) analyses were carried out by using Multiwfn (version 3.3.8). Most of the significant three-dimensional structures were refined and snapshotted with the software CYLview[1]. In addition, the extent of enantioselectivity, in terms of enantiomeric excess (*ee*), was calculated by using the Boltzmann distribution of diastereomeric transition states with the following equations:

$$\frac{[SR]}{[RS]} = \frac{exp(-\Delta G^{\ddagger}_{[SR]}/RT)}{exp(-\Delta G^{\ddagger}_{[RS]}/RT)} = exp(\Delta\Delta G^{\ddagger}_{[RS]-[SR]}/RT)$$

$$ee = \frac{[SR]-[RS]}{[SR]+[RS]} \times 100\% = \frac{\frac{[SR]}{[RS]}-1}{\frac{[SR]}{[RS]}+1} \times 100\%$$

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

References

1. Legault, C. Y. Cylview, version 1.0 b; Université de Sherbrooke, 2009; http://www.cylview.org/.

Part 2: Additionally computational results

2.1 Structural transformation between *pre*-NHC and NHC

The two-dimensional structures of organocatalytic species DDQ, DBU, DDQ are provided in **Figure S1.** The deprotonation process of *pre*-NHC for the formation of NHC has been considered and investigated (**Figure S2**). As shown in **Figure S2**, the energy barrier for DBU-assisted deprotonation process of *pre*-NHC via transition state **TS** is 5.1 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 it and NHC•H^+ exists in this reaction system.

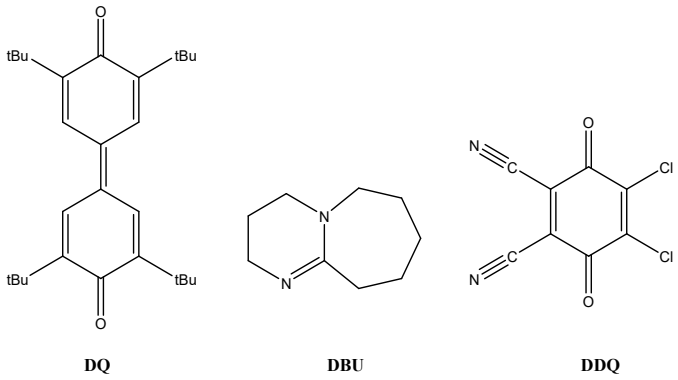


Figure S1. Two-dimensional structures of DQ, DBU, DDQ.

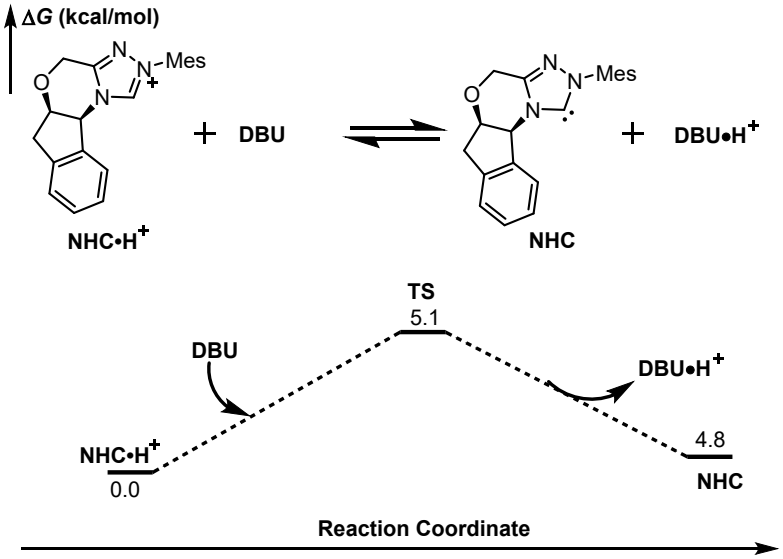


Figure S2. The Gibbs free energy profile for the structural transformation between NHC•H$^+$ and NHC.

2.2 Different deprotonation pathways of *pre*-R2

As shown in **Figure S3**, the C(sp^3)-H of the other reactant ***pre*-R2** can be deprotonated by base DBU or [DQH$^-$] species to generate the critical substrate **R2**, which happens through transition state $\mathbf{TS_{DBU}}$ or $\mathbf{TS_{[DQH-]}}$, respectively. Noteworthy, the energy barrier of the deprotonation pathway associated with DBU via $\mathbf{TS_{DBU}}$ ($\Delta G^{\neq}$=14.1 kcal/mol) is higher than that of the deprotonation pathway via $\mathbf{TS_{[DQH-]}}$ ($\Delta G^{\neq}$=10.6 kcal/mol), indicating that DQH$^-$ can abstract the proton more easily.

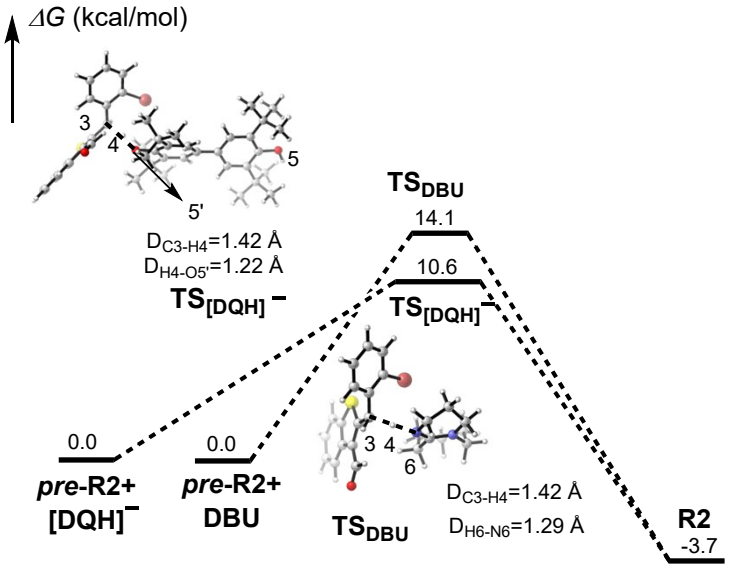


Figure S3. Relative Gibbs free energy profile of the possible deprotonation pathways of ***pre*-R2** (distance in angstrom).

2.3 Origin of stereoselectivity

Attracted by the puzzle of stereoselectivity, the topology and electron density distribution analyses on the key transition states **TS4RR/RS/SR/SS** were performed to characterize the stereoselectivity-determining factors, by using noncovalent interaction (NCI) and Bader's atoms-in-molecules (AIM) methods. As shown in **Figure S4**, the NCI analyses of the transition states **TS4RR/RS/SR/SS** indicate that hydrogen bond interactions would be significant for determining the stereoselectivity. As shown in **Figure S5**, the calculated energy barriers via **TS4RR**, **TS4RS, TS4SR**, and **TS4SS** are 3.6, 6.8, 2.4, and 3.9 kcal/mol, respectively. Subsequently, intramolecular [2+2] cycloaddition coupled with ring closure of the six-membered ring occurs to form the corresponding intermediate **M5RR/RS/SR/SS** through transition state **TS5RR/RS/SR/SS** with an energy barrier of 13.7/20.6/13.2/14.9 kcal/mol. As shown in **Figure S5**, it can be concluded that the central to axial chirality happens easily after the [2+2] cycloaddition transition state **TS5SR**. Correspondingly, Laplacian values at the bond critical points (BCPs) along the bond paths were summarized in **Table S3**. As shown in **Table S3**, three C-H…O (2.32, 2.42 and 2.32 Å), one C-H…Br (2.70 Å) interactions can be found in **TS4RR**. Three C-H…O (2.19, 2.34 and 2.29 Å) and one C-H…Br (2.67 Å) interactions can be found in **TS4RS**. Three C-H…O (2.11, 2.31 and 2.40 Å) interactions can be found in **TS4SS**, while two C-H…O (2.38, 2.33 Å), one C-H…π (2.47 Å), one C-H…S (3.48 Å), one C-H…Br (2.59 Å) interactions can be found in **TS4SR**. Moreover, we found that the **TS4SR** has the largest number of weak interactions based on the value of Laplacian of electron densities ($\nabla^2\rho$). That's why the **TS4SR** is more stable than **TS4RR/RS/SS**, and the corresponding pathway associated with **TS4SR** has a lower energy barrier. The calculated results are consistent with the experimental results, indicating that our model is reliable. Hence, the hydrogen-bond interactions are the main influencing factors for stabilizing **TS4SR**.

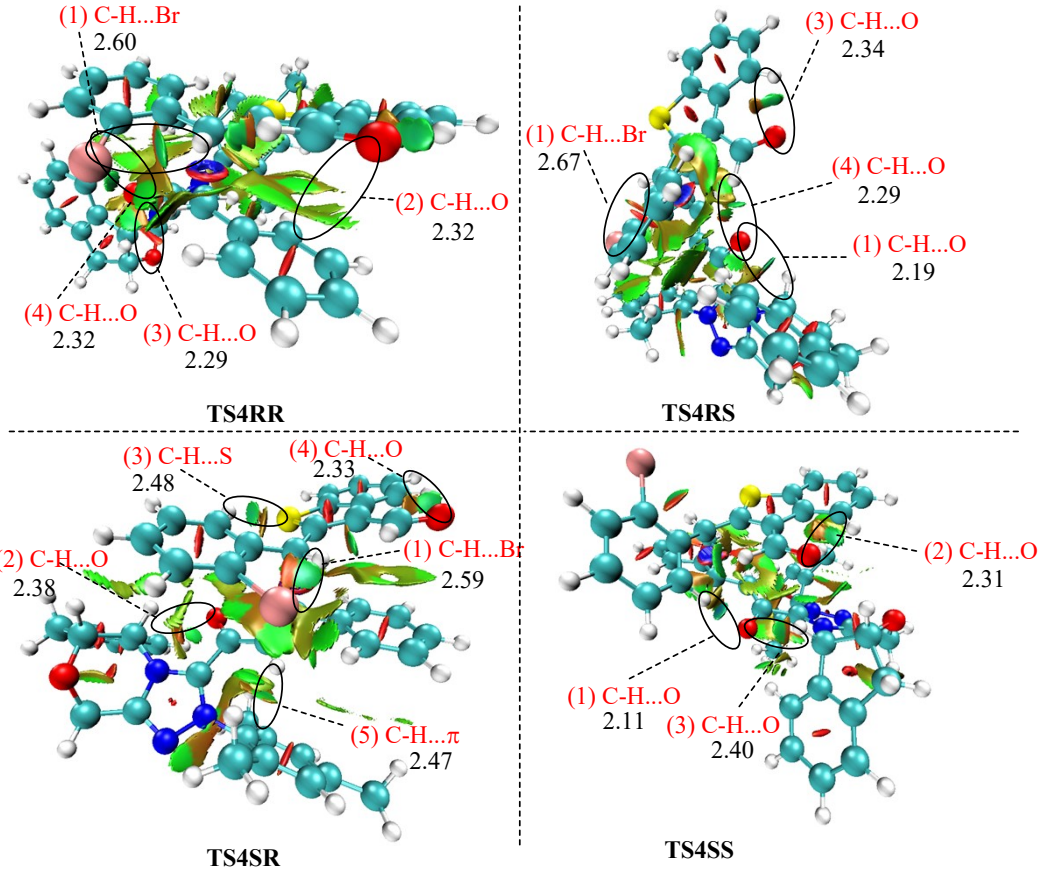


Figure S4. Non-covalent interactions (NCI) analyses of **TS4RR/RS/SR/SS** (Distances in Å).

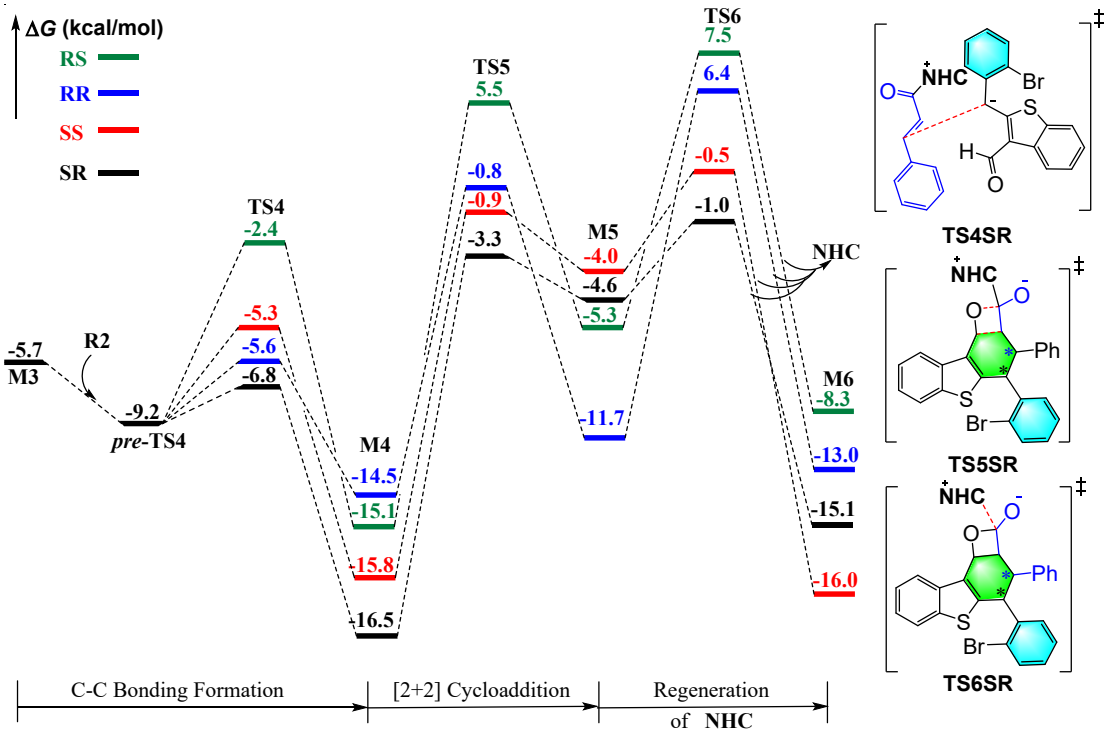


Figure S5. Relative Gibbs free energy profiles for transformation from intermediate **M3** to intermediate **M6** and the two-dimensional structures of the transition states.

Table S3. Summary of Type of Interaction, Electron Densities (ρ_{bcp}), Lagrangian Kinetic Energies (G_b), Potential Energy Densities (V_b), Energy Densities (H_b) at the Bond Critical Points (BCPs) along the Bond Paths in **TS4RR, TS4RS, TS4SR, TS4SS** (Units in a.u.)

BCP index of **TS4RR**	Type of interaction	$\rho_{bcp}*10^{-2}$	G_b*10^{-2}	V_b*10^{-2}	H_b*10^{-3}
1	C-H...Br	1.5811	1.1939	-0.9674	2.2648
2	C-H...O	1.5268	1.1841	-1.1055	0.7858
3	C-H...O	1.3326	1.0737	-0.9250	1.4871
4	C-H... O	1.4310	1.0759	-1.0267	0.4923
BCP index of **TS4RS**	Type of interaction	$\rho_{bcp}*10^{-2}$	G_b*10^{-2}	V_b*10^{-2}	H_b*10^{-3}
1	C-H...O	2.0144	1.6206	-1.5225	0.9807
2	C-H...Br	1.3962	1.0609	-0.8253	2.3564
3	C-H... O	1.5132	1.1711	-1.0931	0.7804
4	C-H...O	1.4780	1.0540	-1.0661	-0.1212
BCP index of **TS4SR**	Type of interaction	$\rho_{bcp}*10^{-2}$	G_b*10^{-2}	V_b*10^{-2}	H_b*10^{-3}
1	C-H...Br	1.5885	1.1951	-0.9732	2.2195
2	C-H...O	1.4392	1.1587	-1.0195	1.3925
3	C-H...S	1.5486	1.1354	-1.0142	1.2117
4	C-H...O	1.4913	1.1582	-1.0749	0.8334
5	C-H... π	1.2928	0.9227	-0.7358	1.8688
BCP index of **TS4SS**	Type of interaction	$\rho_{bcp}*10^{-2}$	G_b*10^{-2}	V_b*10^{-2}	H_b*10^{-3}
1	C-H...O	2.0940	1.4696	-1.5691	-0.9949
2	C-H...O	1.5778	1.2311	-1.1509	0.8016
3	C-H...O	1.3760	1.1061	-0.9666	1.3951

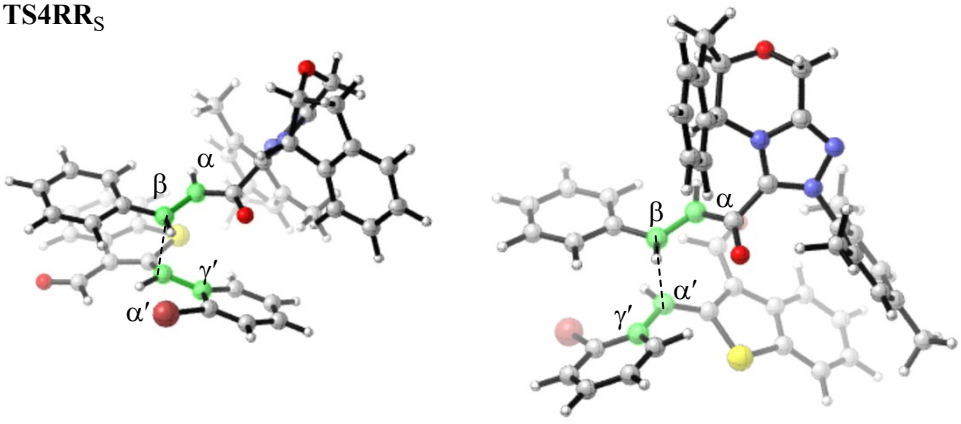
2.4 Different conformers and configurations

To ensure the selected configuration of the stereochemical transition state with the lowest energy, we have searched multiple possible conformations for the fourth step. By rotating the dihedral angle Φ(Cα−Cβ−Cα'−Cγ') with 90° per time in stereo-controlling transition states **TS4RR**, **TS4RS**, **TS4SR**, and **TS4SS**, we have totally constructed 4*4=16 conformations as the initial structures, which have subsequently been optimized at the B3LYP-D3/6-311++G(2df, 2pd)/$SMD_{dichloroethane}$//B3LYP-D3/6-31G(d,p)/$SMD_{dichloroethane}$ level. After the optimization, the corresponding dihedral Φ angles change to -156/147°/-69°/78°/, 21°/171°/-163°/-24°, -29°/-97°/63°/77° and -111°/-24°/59°/175° in the **TS4RR**s, **TS4RS**s, **TS4SR**s, and **TS4SS**s, respectively. As revealed by **Figures S6-9**, the most stable conformations with the lowest energies of the four diastereoselective transition states (denoted as **TS4RR**, **TS4RS**, **TS4SR**, and **TS4SS**) are associated

with the dihedral angles Φ(Cα−Cβ−Cα′−Cγ′) of -156°/21°/-29°/-111°, respectively.

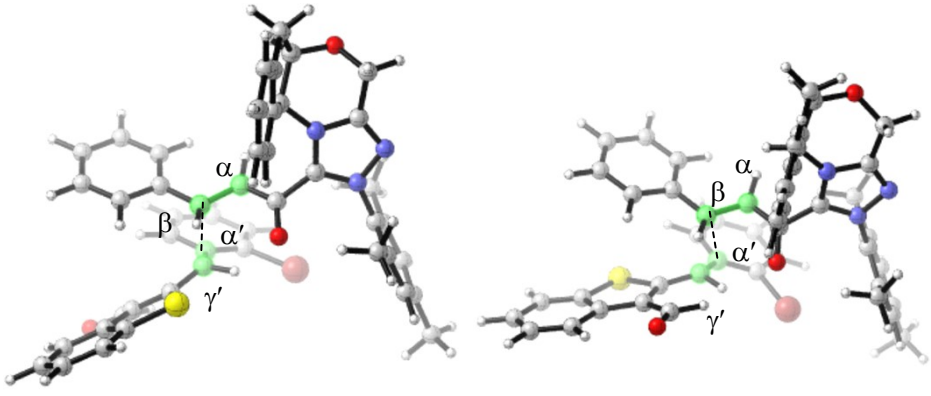
As shown in **Figure S10**, we have scanned the dihedral angles Φ(Cα−Cβ−Cα′−Cγ′) for 360° (24*15°) in the four stereoselective intermediates **M4RR**, **M4RS**, **M4SR**, and **M4SS**, and the most stable conformations with the lowest energies of the four intermediates are corresponding to the dihedral angles Φ(Cα−Cβ−Cα′−Cγ′) of -178°/62°/-63°/-88°, which belong to the same conformations of the four diastereoselective transition states **TS4RR**, **TS4RS**, **TS4SR**, and **TS4SS** with the dihedral angles Φ(Cα−Cβ−Cα′−Cγ′) -156°/21°/-29°/-111°, respectively. Noteworthy, we have always obtained the same transition states **TS4RR**, **TS4RS**, **TS4SR**, and **TS4SS** after the optimizations if we set the same dihedral angles Φ(Cα−Cβ−Cα′−Cγ′) -178°/62°/-63°/-88° in the initial structures.

TS4RR$_S$



Φ= -156°
TS4RR (0.0 kcal/mol)

Φ=147°
TS4RR' (2.4 kcal/mol)



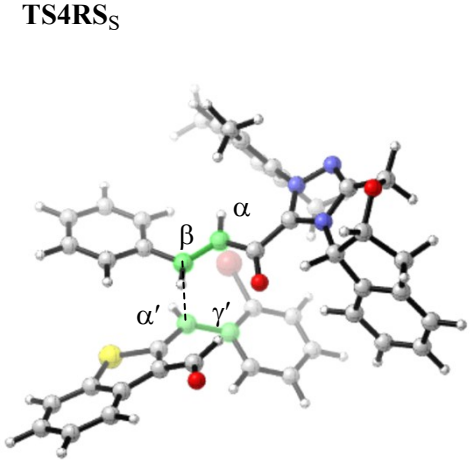
Φ= –69°
TS4RR'' (8.4 kcal/mol)

Φ=78°
TS4RR''' (2.4 kcal/mol)

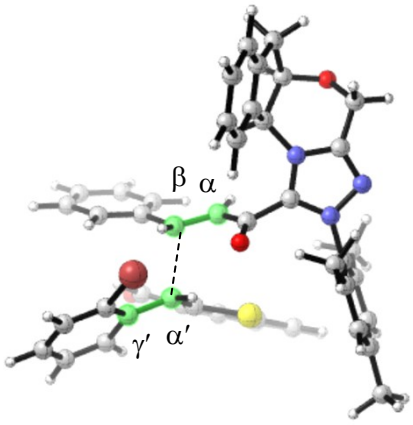
Figure S6. Different configurations of the transition states **TS4RR**s with different dihedral angles Φ(Cα−Cβ−Cα′−Cγ′) optimized at the B3LYP-D3/6-311++G (2df, 2pd)/ $SMD_{dichloroethane}$//B3LYP-

D3/6-31G(d, p)/ $SMD_{dichloroethane}$level of theory.

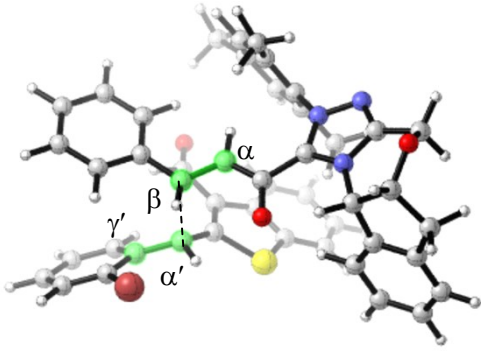
$TS4RS_S$



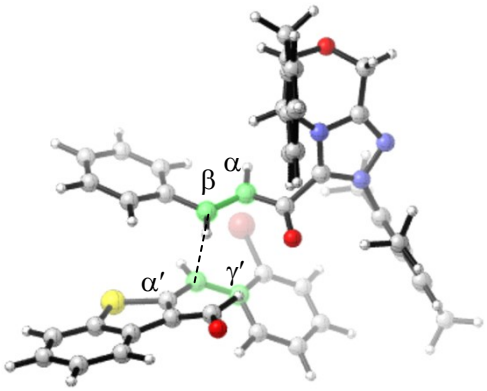
Φ=21°
TS4RS (0.0 kcal/mol)



Φ=171°
TS4RS' (3.4 kcal/mol)



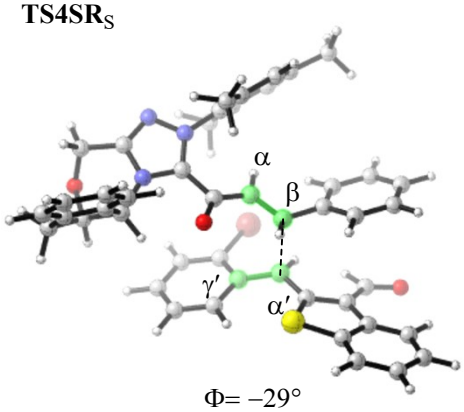
Φ= −163°
TS4RS'' (2.2 kcal/mol)



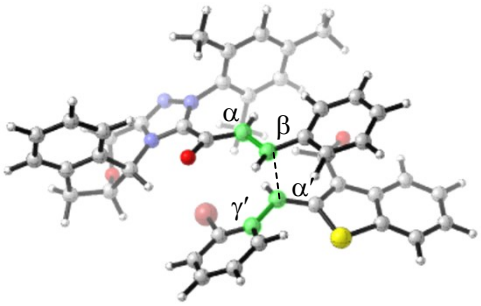
Φ=24°
TS4RS''' (3.6 kcal/mol)

Figure S7. Different configurations of the transition states **TS4RS**s with different dihedral angles Φ(Cα−Cβ−Cα'−Cγ') optimized at the B3LYP-D3/6-311++G (2df, 2pd)/$SMD_{dichloroethane}$//B3LYP-D3/6-31G(d, p)/ $SMD_{dichloroethane}$level of theory.

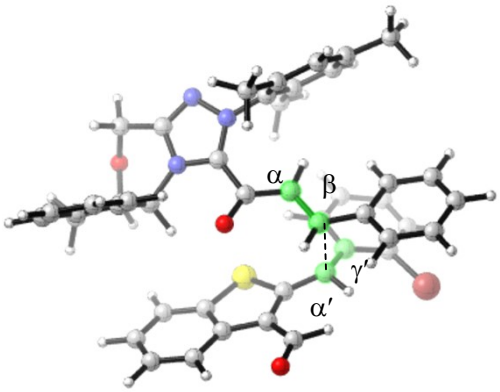
TS4SR$_S$



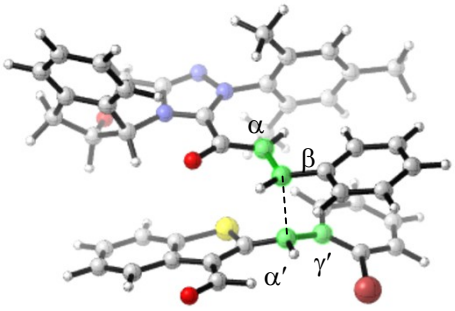
Φ= –29°
TS4SR (0.0 kcal/mol)



Φ= –97°
TS4SR' (3.7 kcal/mol)



Φ=63°
TS4SR'' (0.1 kcal/mol)



Φ=77°
TS4SR''' (0.7 kcal/mol)

Figure S8. Different configurations of the transition states **TS4SR**s with different dihedral angles Φ(Cα–Cβ–Cα'–Cγ') optimized at the B3LYP-D3/6-311++G (2df, 2pd)/SMD$_{dichloroethane}$//B3LYP-D3/6-31G(d, p)/ SMD$_{dichloroethane}$level of theory.

TS4SS$_S$

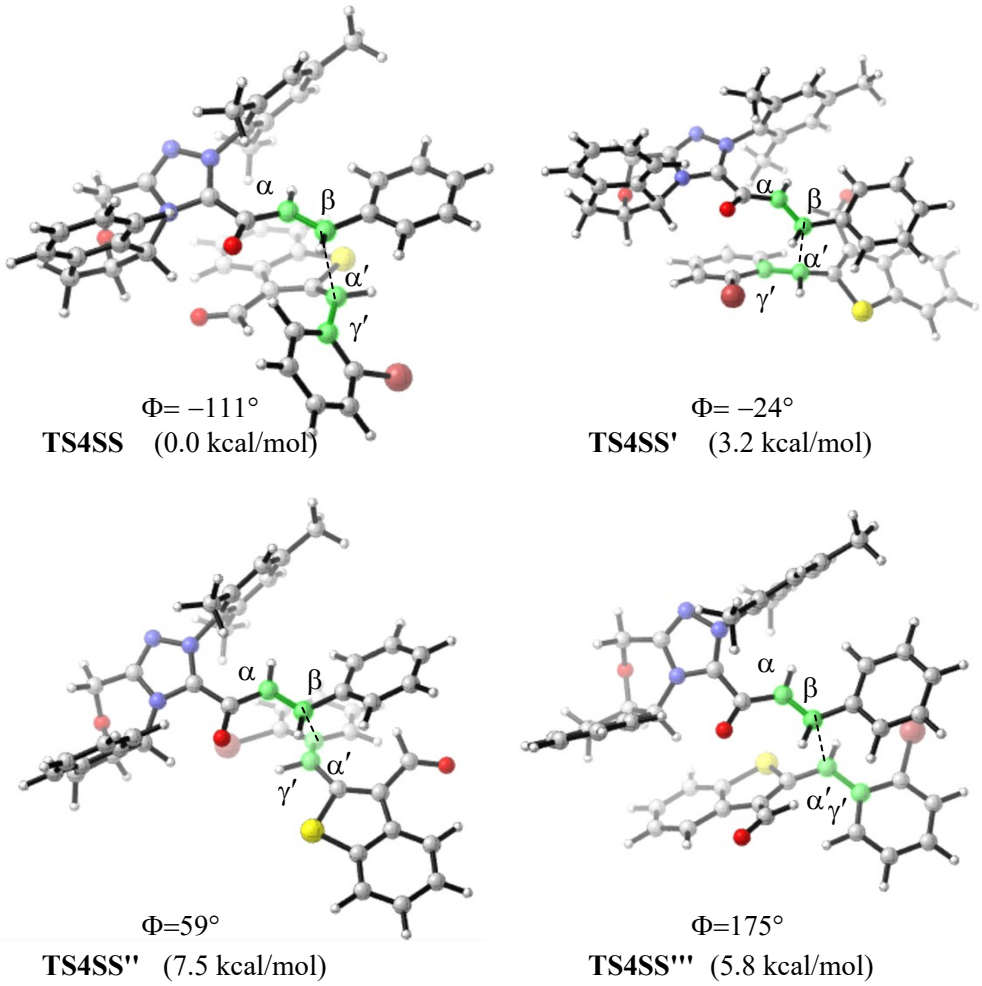


Figure S9. Different configurations of the transition states **TS4SS**s with different dihedral angles Φ(C*α*–C*β*–C*α*′–C*γ*′) optimized at the B3LYP-D3/6-311++G (2df, 2pd)/SMD$_{dichloroethane}$//B3LYP-D3/6-31G(d, p)/SMD$_{dichloroethane}$level of theory.

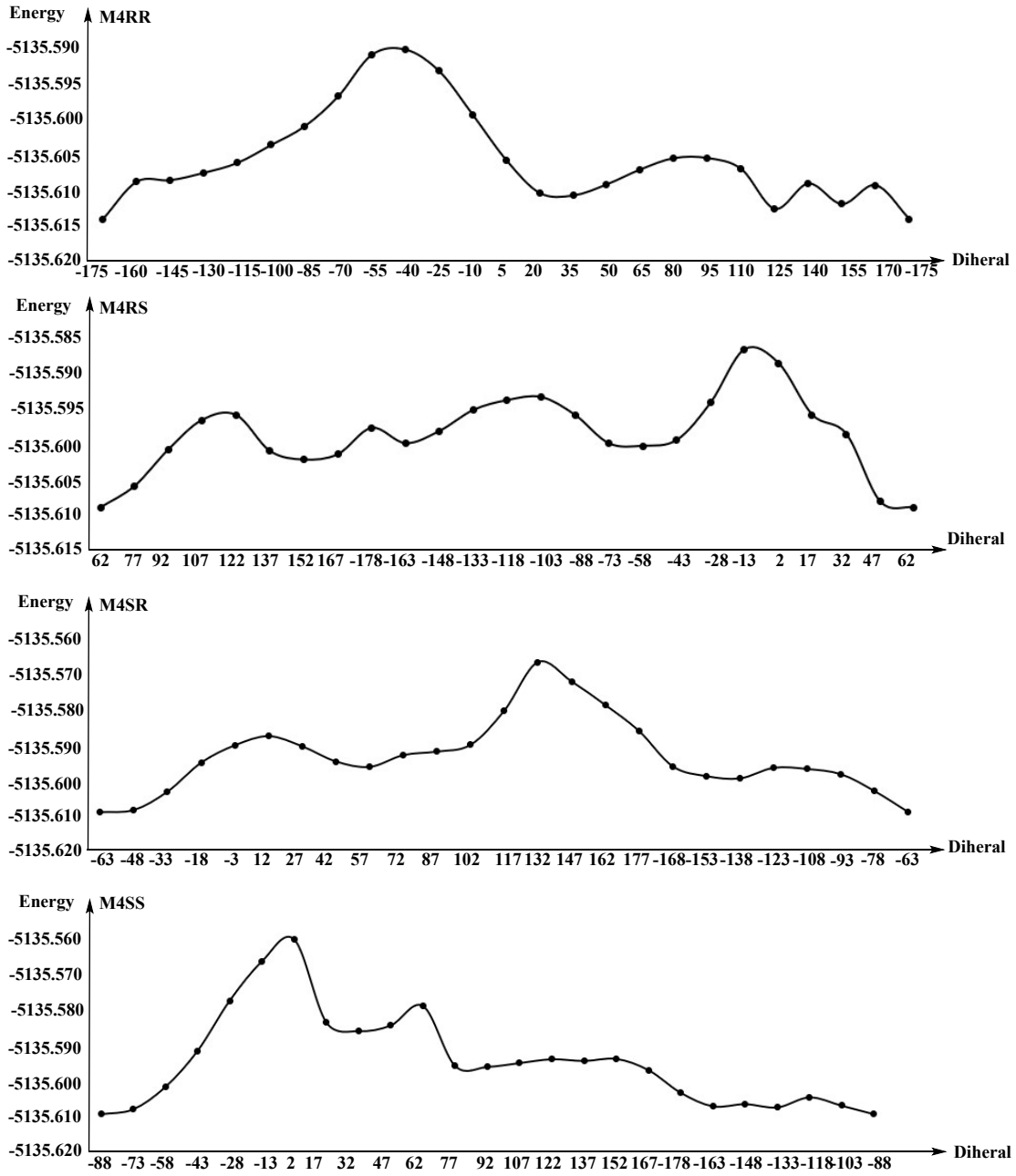


Figure S10 Potential energy surface scan of the intermediates **M4RR**, **M4RS**, **M4SR**, and **M4SS.**

2.5 Molecular orbital overlap mode analysis of TS5SR' and TS5SR

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. We have tracked and compared the FMO changes with the intrinsic reaction coordinate (IRC) results of the key transition states **TS5SR'** without the presence of NHC and **TS5SR** with the presence of NHC. As shown in **Figure S11**, the orbital interaction between the center atoms involved in HOMO of **TS5SR'** along the IRC is gradually changed from a shoulder-to-head overlap mode to a head-to-

head overlap mode, which results in the formation of $\sigma_{C2-C\alpha}$ bond/orbital. In contrast, only the head-to-head overlap mode formation of $\sigma_{C2-C\alpha}$ bond/orbital can be observed in the HOMO of **TS5SR** along the IRC **(Figure S12)**. Therefore, the intramolecular [2+2] cycloaddition reaction with the presence of NHC can avoid the unfavorable shoulder-to-head overlap mode, thus the energy barrier can be reduced significantly.

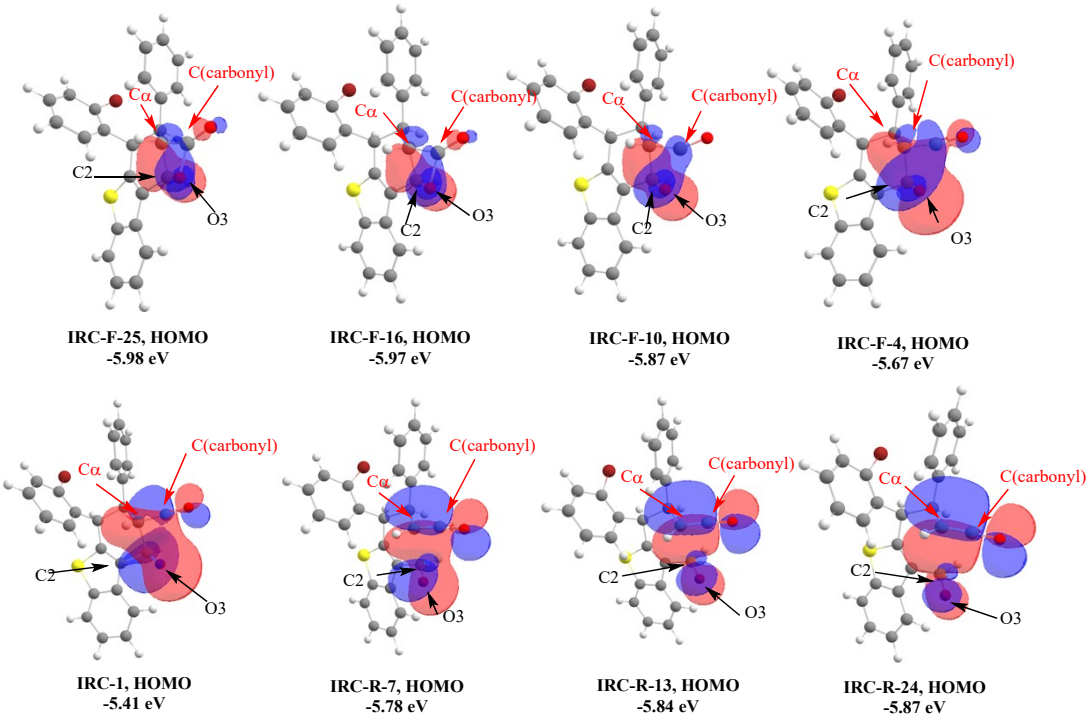


Figure S11. The HOMO changes along the several representative IRC points of **TS5SR′**.("F" and "R" represent forward and reverse directions, respectively; IRC-1 is the structure of **TS5SR′**, only the orbitals of the key C(carbonyl), C2, O3, and Cα atoms of **TS5SR′** and **TS5SR** are shown for clarity).

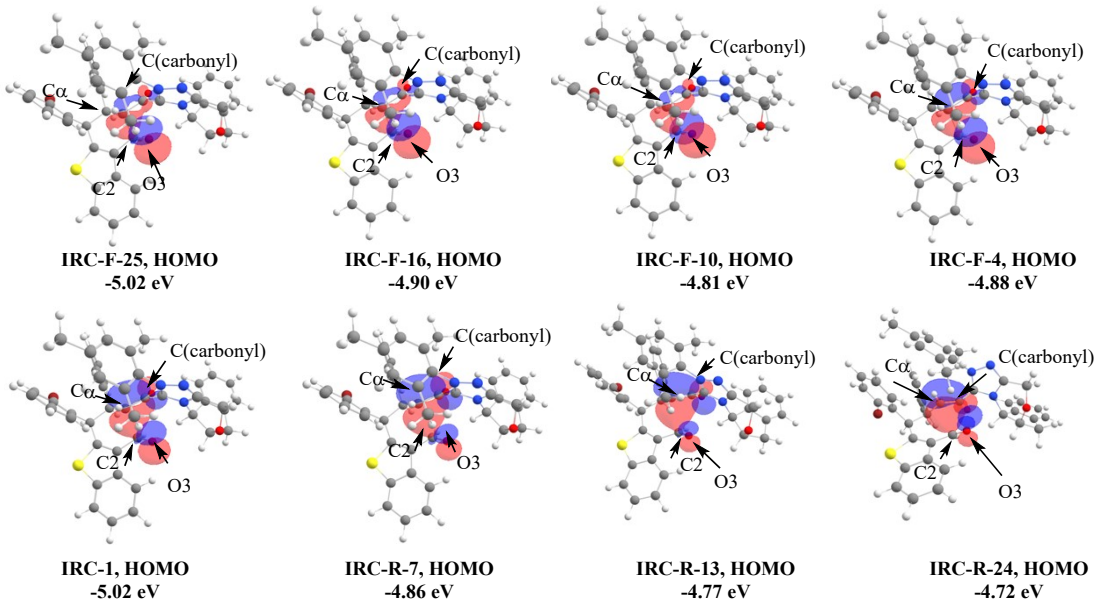


Figure S12. The HOMO changes along several representative IRC points of **TS5SR** ("F" and "R" represent forward and reverse directions, respectively; IRC-1 is the structure of **TS5SR**, only the orbitals of the key C(carbonyl), C2, O3, and C*α* atoms of **TS5SR′** and **TS5SR** are shown for clarity)

2.6 Possible CO_2 Release Pathways

As shown in **Figure S13**, the energy barrier for DBU•H^+-assisted decarboxylation process via transition state **TS7SR** is 5.0 kcal/mol, indicating that this process occurs more easily than the direct decarboxylation and NHC•H^+-assisted decarboxylation process, which the energy barriers via transition state **TS7SR′ and TS7SR″** are 15.4 and 17.3 kcal/mol. Therefore, DBU•H^+ can indeed work as a good hydrogen bond donor to stabilize the transition state structures.

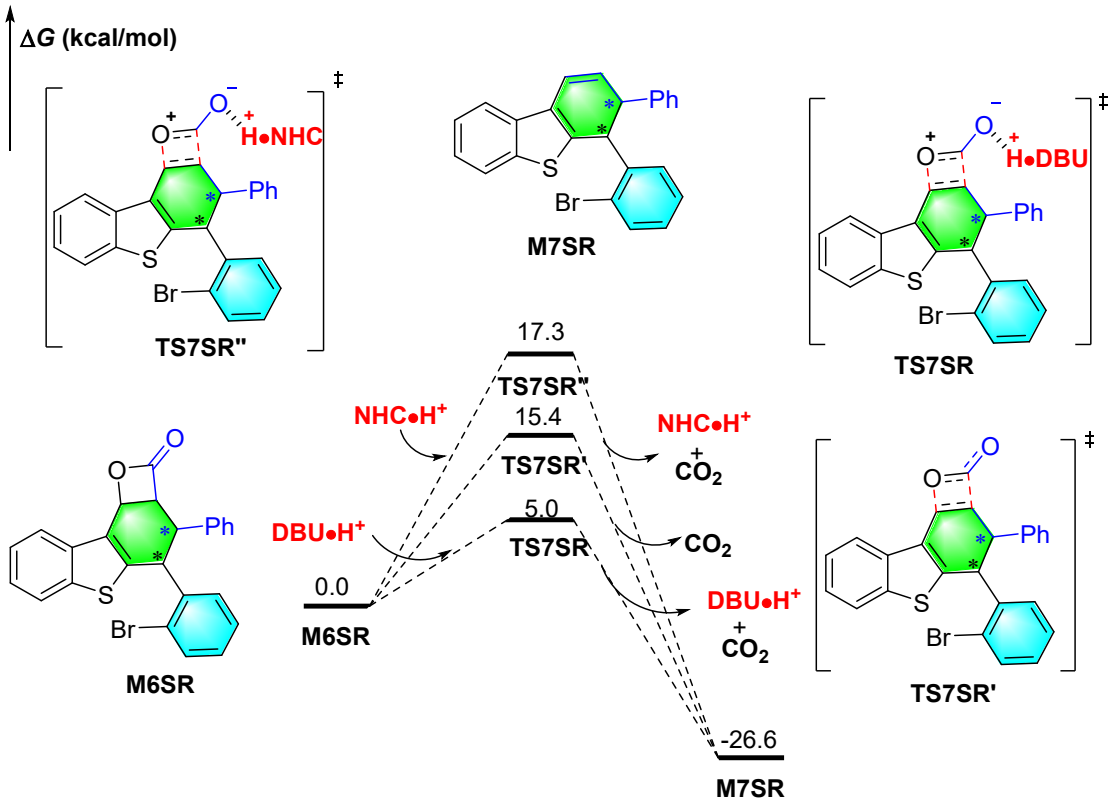


Figure S13. Relative Gibbs free energy profiles of the possible release pathways of CO_2.

2.7 The volume of R

To obtain the relationship of substituent groups and the energy barriers of corresponding racemization processes, the typical functional groups, *i.e.* bromophenyl, chlorophenyl, fluorophenyl, and phenyl groups, were employed for molecular simulations. The molecular volume of organic compounds has good additivity, that is, the molecular volume of organic compounds is equal to the sum of the topological volumes of the functional groups of its components, and the molecular volume of organic compounds can be calculated by the following formula, in which V_m is the molecular volume, d is molecular radius.

$$V_M = \frac{M(molecular\ weight)}{d \times 6.023 \times 10^{23}} = \frac{1.6603M}{d}$$

Table S4. Summary of the volumes of the groups.

Groups	Volume (cm^3/mol)
PhBr	93.457
PhCl	90.518
PhF	77.051
Ph	64.444

Part 3: Cartesian coordinates and energy values of optimized structures

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

Table S5. Absolute SPE and GFE of the Optimized Structures by using B3LYP-D3 method

	SPE (a.u.)	GFEC (a.u.)	GFE (a.u.)
NHC	-1052.722651	0.330062	-1052.392589
R1	-423.149197	0.109413	-423.039784
NHC+R1	-1475.887096	0.459669	-1475.427427
pre-R2	-3664.196978	0.178050	-3664.018928
R2	-3663.696213	0.165066	-3663.531147
$DBU.H^+$	-462.773956	0.226838	-462.547118
DQ	-1242.013953	0.555343	-1241.458610
DQH^-	-1242.757414	0.567119	-1242.190295
DQH_2	-1243.63555	0.652655	-1242.982895
$DDQH^-$	-1486.180361	0.033599	-1486.146762
DDQ	-1485.378001	0.023306	-1485.354695
CO_2	-188.656013	-0.009263	-188.665276
DBU	-462.289420	0.211341	-462.078079
TS	-1515.514533	0.575211	-1514.939322
pre-R2+DBU	-4123.706967	0.412168	-4123.294799
TS_{DBU}	-4123.680570	0.408281	-4123.272288
pre-R2+DQH^-	-4903.959678	0.767233	-4903.192445
TS_{DQH^-}	-4903.940686	0.765199	-4903.175487
TS1	-1475.870108	0.463895	-1475.406213
M1	-1475.881187	0.466889	-1475.414298
TS2	-1938.655044	0.707965	-1937.947079
M2	-1475.889996	0.462417	-1475.427579

pre-TS3	-2717.940651	1.047390	-2716.893261
TS3	-2717.934709	1.042764	-2716.891945
M3	-1475.161046	0.457006	-1474.704040
pre-TS4	-5138.889104	0.647436	-5138.241668
$TS4_{chemo}$	-5138.864223	0.652498	-5138.211725
$M4_{chemo}$	-5138.867315	0.653582	-5138.213733
TS4RR	-5138.883510	0.647751	-5138.235779
TS4RS	-5138.879616	0.648864	-5138.230752
TS4SR	-5138.884272	0.646500	-5138.237772
TS4SS	-5138.873156	0.647854	-5138.235302
TS4RR'	-4812.819093	0.653516	-4812.165577
TS4SR'	-4812.816741	0.652655	-4812.164086
M4RR	-5138.906615	0.656679	-5138.249936
M4RS	-5138.899452	0.648459	-5138.250993
M4SR	-5138.904039	0.650885	-5138.253154
M4SS	-5138.904717	0.652630	-5138.252087
M4SR'	-5138.879024	0.650852	-5138.228172
TS5SR'	-5138.872717	0.654589	-5138.218128
TS5RR	-5138.895147	0.653550	-5138.241597
TS5RS	-5138.883523	0.651972	-5138.231551
TS5SR	-5138.900980	0.655396	-5138.245584
TS5SS	-5138.889114	0.653729	-5138.241757
M5RR	-5138.898068	0.657227	-5138.240841
M5RS	-5138.87512	0.657377	-5138.217743
M5SR	-5138.875097	0.658470	-5138.216627
M5SS	-5138.868911	0.654932	-5138.213979
TS6RR	-5138.88472	0.654530	-5138.23019
TS6RS	-5138.881103	0.652668	-5138.228435
TS6SR	-5138.89436	0.652370	-5138.241990
TS6SS	-5138.890988	0.649795	-5138.241193
M6RR	-4086.155079	0.299071	-4085.856008
M6RS	-4086.148422	0.299909	-4085.848513
M6SR	-4086.156642	0.297285	-4085.859357
M6SS	-4086.156167	0.298245	-4085.857922
TS7SR	-4548.944018	0.545525	-4548.398493
TS7SR'	-4086.128197	0.293097	-4085.835100
TS7SR"	-5139.363203	0.662097	-5138.701106
NHC-H^+	-4359.042066	0.504170	-4358.537896

M7SR	-3897.521098	0.284699	-3897.236399
TS8R	-5382.901405	0.327767	-5382.573638
TS8R'	-5382.885140	0.324066	-5382.561074
TS8R"	-5139.518440	0.863210	-5138.655230
TS8R"'	-5139.502509	0.860178	-5138.642331
M8R	-3896.737580	0.274277	-3896.463303
M8R-1	-3896.724404	0.273484	-3896.450920
TS9R	-4359.042066	0.504170	-4358.537896
TS10	-3893.555177	0.263461	-3893.291716
TS11	-6464.663052	0.250371	-6464.412681
TS12	-4353.153002	0.252174	-4352.900828
TS13	-3992.786582	0.254214	-3992.532368
P-Ph	-3893.618759	0.262442	-3893.356317
P-PhBr	-6464.727072	0.249471	-6464.477601
P-PhCl	-4353.216995	0.251166	-4352.965829
P-PhF	-3992.850630	0.252921	-3992.597709
PR	-3896.345932	0.262432	-3896.083500
PS	-3896.345943	0.262435	-3896.083508

Table S6. Relative Gibbs Free Energies of the Stationary Points (SPs) Involved in Energy Profiles Calculated at the B3LYP-D3/6-311++G(2df, 2pd)/ $SMD_{dichloroethane}$//B3LYP-D3/6-31G(d, p)/$SMD_{dichloroethane}$ level. The Energy of NHC+R1 was Set as 0.0 kcal/mol, and the Superscripts a, b, c, and d Represent Addition of the Energies of NHC+R1, *pre*-TS3, *pre*-TS4, M7SR, respectively.

SP	Δ*G* (kcal/mol)
TS1[a]	13.3
M1[a]	8.2
TS2[a]	6.1
M2[a]	0.5
pre-TS3[a]	-5.0
TS3[b]	2.7
M3[b]	-0.7
pre-TS4[b]	-4.2
TS4RR[c]	3.6
TS4RS[c]	6.8
TS4SR[c]	2.4
TS4SS[c]	3.9
M4SR[c]	-7.3
TS5SR[c]	5.9
M5SR[c]	4.6
TS6SR[c]	8.2

M6SR[c]	-5.9
TS7SR[c]	-2.3
TS7SR'[c]	9.5
TS7SR''[c]	11.4
M7SR[c]	-32.9
TS8R[d]	11.0
TS8R'[d]	18.8
TS8R''[d]	25.0
TS8R'''[d]	33.1
M8R[d]	-11.9
M8R-1[d]	-4.1
TS9R[d]	-9.7
PR[d]	-15.9

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

Table S7. Absolute SPE and GFE of the Optimized Structures at the M06-2X/6-311++G(2df, 2pd)/$SMD_{dichloroethane}$ //M06-2X /6-31G(d, p)/$SMD_{dichloroethane}$ Level

	SPE (a.u.)	GFEC (a.u.)	CFE(a.u.)	$\Delta\Delta G^{\neq}$
$TS4RR_{M06-2X}$	-5134.814826	0.655156	-5134.159670	1.3
$TS4SR_{M06-2X}$	-5134.817810	0.646500	-5134.171310	0.0

Table S8. Absolute SPE and GFE of the Optimized Structures at the ωB97X-D/6-311++G(2df, 2pd)/$SMD_{dichloroethane}$//ωB97X-D /6-31G(d, p)/$SMD_{dichloroethane}$Level

	SPE(a.u.)	GFEC(a.u.)	CFE(a.u.)	$\Delta\Delta G^{\neq}$
$TS4RR_{\omega B97X-D}$	-5134.989987	0.657989	-5134.331998	2.8
$TS4SR_{\omega B97X-D}$	-5134.994494	0.656056	-5134.338438	0.0

Table S9. Absolute SPE and GFE of the different conformers of **TS4RR/RS/SR/SS** .

	SPE(a.u.)	GFEC(a.u.)	CFE(a.u.)
TS4RR (Φ= -156°)	-5138.883530	0.647751	-5138.235779
TS4RR′ (Φ=147°)	-5138.882574	0.650607	-5138.231967
TS4RR″ (Φ= -69°)	-5138.869741	0.647314	-5138.222427
TS4RR‴ (Φ=78°)	-5138.88006	0.648129	-5138.231931
TS4RS (Φ=21°)	-5138.879616	0.648864	-5138.230752
TS4RS′ (Φ=171°)	-5138.873305	0.648046	-5138.225259
TS4RS″ (Φ= -163°)	-5138.879208	0.651940	-5138.227268
TS4RS‴ (Φ=24°)	-5138.874885	0.649832	-5138.225053

TS4SR (Φ= -29°)	-5138.884272	0.646500	-5138.237772
TS4SR′ (Φ= -97°)	-5138.881012	0.649160	-5138.231852
TS4SR″ (Φ=63°)	-5138.886715	0.649035	-5138.237680
TS4SR‴ (Φ=77°)	-5138.885717	0.649055	-5138.236662
TS4SS (Φ= -111°)	-5138.883156	0.647854	-5138.235302
TS4SS′ (Φ= -24°)	-5138.879162	0.648931	-5138.230231
TS4SS″ (Φ=59°)	-5138.872333	0.648955	-5138.223378
TS4SS‴ (Φ=175°)	-5138.875355	0.649244	-5138.226111

3.3 The Cartesian coordinates of all the stationary points

NHC

Zero-point correction= 0.380341

Thermal correction to Energy= 0.401265

Thermal correction to Enthalpy= 0.402209

Thermal correction to Gibbs Free Energy= 0.330062

Sum of electronic and zero-point Energies= -1052.042674

Sum of electronic and thermal Energies= -1052.021750

Sum of electronic and thermal Enthalpies= -1052.020806

Sum of electronic and thermal Free Energies= -1052.092954

Cartesian coordinates

C	0.126978	0.014276	0.810248
C	-0.528154	-1.681115	-0.539646
C	-2.295396	-0.714539	0.964206
H	-2.224101	-0.977312	2.021980
N	0.737532	-1.536039	-0.813590
N	1.107307	-0.483112	0.028384
N	-0.928858	-0.770681	0.409993
C	-1.484420	-2.666135	-1.135176
H	-0.991949	-3.631157	-1.275461
H	-1.819976	-2.317171	-2.121827
C	-3.228591	-1.696186	0.187779
O	-2.583016	-2.884289	-0.254447
C	-3.890904	0.542028	-0.314727
C	-2.966308	0.621069	0.735233
C	-2.759186	1.814864	1.424276
C	-3.493747	2.943272	1.049221
C	-4.420857	2.868328	0.002431
C	-4.627781	1.667491	-0.683496

C	-3.926110	-0.845175	-0.905368
H	-2.036737	1.865101	2.232643
H	-4.989708	3.751152	-0.275821
H	-5.352625	1.612820	-1.491194
H	-3.372112	-0.872976	-1.851113
H	-4.936949	-1.206179	-1.114517
C	2.470211	-0.037752	-0.008132
C	2.791668	1.095616	-0.766281
C	3.439165	-0.767565	0.699472
C	4.130733	1.504107	-0.794414
C	4.762423	-0.324488	0.638820
C	5.126414	0.809367	-0.100323
H	4.399398	2.381798	-1.376874
H	5.527292	-0.875166	1.181482
C	3.050274	-1.981988	1.503442
H	2.583667	-2.743843	0.869935
H	2.318627	-1.721955	2.276664
H	3.921688	-2.425483	1.991560
C	6.564632	1.266019	-0.131523
H	7.232867	0.450935	-0.431429
H	6.892624	1.598959	0.860609
H	6.708845	2.097092	-0.827579
C	1.725425	1.845820	-1.523367
H	0.979501	2.266126	-0.840437
H	1.187521	1.181415	-2.208902
H	2.159483	2.662759	-2.105062
H	-3.986171	-2.039936	0.896242
H	-3.347733	3.882270	1.575120

Vibrational frequencies

28.8727	35.7067	50.5629

54.5658	72.4383	82.9132
122.5262	131.5069	139.6615
166.0430	171.2556	197.9030
208.7604	235.9302	241.0969
263.3128	284.7624	295.3659
319.0352	331.8876	351.1504
386.0806	412.9476	455.2183
469.8351	497.6101	513.5562
520.3690	526.8415	530.8798
563.8376	580.9697	599.5863
604.6560	617.5762	628.4888
647.0712	676.9672	694.7421
728.8901	758.3892	768.0756
785.4928	819.0470	841.6731
877.5641	879.7084	885.8266
901.7329	903.4603	954.2580
958.3917	958.6285	973.2557
979.1493	1001.9921	1010.7689
1035.0860	1036.8375	1044.6267
1049.2564	1051.4489	1065.1222
1066.5543	1069.1553	1069.3689
1072.4109	1123.8774	1132.7668
1159.5789	1183.1079	1185.6835
1192.8449	1216.5996	1233.4047
1247.8712	1253.2967	1269.3709
1286.2923	1290.1491	1300.9138
1322.3515	1328.0110	1338.1331
1344.2209	1354.5895	1367.8507
1379.7203	1411.8360	1415.7084
1417.8453	1423.3751	1425.6650

1440.7097	1447.6018	1478.6169
1479.7125	1481.1659	1482.1727
1485.1873	1490.0948	1498.3481
1501.5640	1506.2184	1520.4183
1534.9670	1627.7473	1638.2191
1639.0051	1657.1935	1662.7151
3028.8015	3039.5714	3045.5220
3046.2103	3056.5624	3097.2294
3098.5317	3104.8971	3105.1966
3105.3930	3116.2110	3124.9722
3126.4652	3134.7775	3135.8089
3174.8991	3180.1528	3182.1213
3193.2390	3203.0253	3215.5021

R1

Zero-point correction= 0.143672

Thermal correction to Energy= 0.152220

Thermal correction to Enthalpy= 0.153164

Thermal correction to Gibbs Free Energy= 0.109413

Sum of electronic and zero-point Energies= -422.870879

Sum of electronic and thermal Energies= -422.862332

Sum of electronic and thermal Enthalpies= -422.861388

Sum of electronic and thermal Free Energies= -422.905139

Cartesian coordinates

C	0.932966	-0.596040	0.000049
C	1.995039	0.240501	0.000059
H	1.141007	-1.666854	0.000052
C	3.353005	-0.291678	0.000019
O	4.365620	0.398416	-0.000008
C	-0.484646	-0.242259	0.000022

C	-1.438846	-1.278206	0.000039
C	-0.941653	1.091866	-0.000037
C	-2.803373	-0.994664	0.000000
H	-1.100412	-2.310974	0.000085
C	-2.303858	1.372835	-0.000077
H	-0.228482	1.909753	-0.000059
C	-3.239834	0.331760	-0.000059
H	-3.524831	-1.806375	0.000016
H	-2.640161	2.405451	-0.000126
H	-4.302496	0.556086	-0.000092
H	3.423124	-1.401666	0.000049
H	1.894489	1.322566	0.000054

Vibrational frequencies

56.5310	114.3573	121.1480
184.9379	306.8313	337.5724
354.0179	411.1270	511.3692
594.2398	619.6988	632.0868
699.3054	768.2216	856.6668
859.3327	877.4694	943.3104
984.8909	1006.4108	1012.1350
1014.9937	1050.1369	1054.7124
1113.5788	1151.6649	1191.4416
1212.2600	1234.5907	1274.2423
1338.8922	1366.9852	1376.0126
1442.9595	1490.5006	1535.9975
1625.2540	1651.5844	1683.1353
1750.4314	2908.8192	3147.3868
3185.3898	3191.2264	3195.0332
3200.5928	3209.4459	3215.9759

pre-TS1

Zero-point correction= 0.525224

Thermal correction to Energy= 0.556490

Thermal correction to Enthalpy= 0.557434

Thermal correction to Gibbs Free Energy= 0.459669

Sum of electronic and zero-point Energies= -1474.929074

Sum of electronic and thermal Energies= -1474.897809

Sum of electronic and thermal Enthalpies= -1474.896864

Sum of electronic and thermal Free Energies= -1474.994629

Cartesian coordinates

C	5.383472	-0.460634	-0.458178
C	4.014624	-0.738545	-0.479615
C	3.489211	-1.853341	0.173018
C	4.367070	-2.702492	0.851861
C	5.741834	-2.433604	0.873923
C	6.258582	-1.311603	0.219591
C	5.696460	0.798752	-1.227434
C	4.318996	1.442442	-1.540530
C	3.253996	0.309909	-1.268937
H	2.422403	-2.058251	0.168932
H	3.977468	-3.575289	1.368135
H	6.412197	-3.100511	1.409008
H	7.324303	-1.100564	0.245830
H	6.322629	1.502651	-0.669495
H	4.258447	1.769498	-2.579632
H	6.226463	0.568760	-2.159468
H	2.883010	-0.095824	-2.212867
N	2.101501	0.827878	-0.540519
O	4.089401	2.641100	-0.789526
C	0.802001	0.389497	-0.595281

C	2.256470	1.797905	0.420456
N	0.253772	1.149992	0.378864
N	1.125890	2.043748	1.016409
C	3.596190	2.446993	0.538980
H	4.280625	1.832185	1.140038
H	3.514690	3.430471	1.005055
C	-1.109988	1.115799	0.822995
C	-1.418410	0.398732	1.989847
C	-2.083476	1.810754	0.092642
C	-2.748464	0.395852	2.420106
C	-3.400972	1.779533	0.562661
C	-3.750425	1.084636	1.724641
H	-3.007967	-0.158875	3.318703
H	-4.171131	2.303182	0.002651
C	-2.402430	-1.771090	-1.263584
C	-1.761833	-2.357613	-0.228567
H	-1.821341	-1.573380	-2.164630
C	-3.789043	-1.315852	-1.306018
C	-4.194510	-0.485024	-2.367869
C	-4.733092	-1.652102	-0.315171
C	-5.494620	0.013115	-2.429341
H	-3.475200	-0.220553	-3.138131
C	-6.033888	-1.163938	-0.384787
H	-4.446875	-2.299204	0.507574
C	-6.418367	-0.325177	-1.437581
H	-5.787390	0.660999	-3.250217
H	-6.751732	-1.433510	0.383894
H	-7.433943	0.056739	-1.485009
C	-0.349701	-2.697362	-0.341845
H	0.099723	-2.532179	-1.339913

O	0.327737	-3.140747	0.583259
C	-0.356354	-0.373506	2.730400
H	-0.003973	-1.222366	2.133978
H	0.514198	0.252160	2.950408
H	-0.747040	-0.763249	3.674120
C	-1.722118	2.548338	-1.171081
H	-0.908565	3.261093	-0.996460
H	-1.373957	1.853554	-1.942801
H	-2.582613	3.094787	-1.564993
C	-5.171611	1.087176	2.231358
H	-5.456221	0.106383	2.625288
H	-5.294530	1.811017	3.047043
H	-5.877356	1.354616	1.440653
H	-2.239203	-2.543773	0.729199

Vibrational frequencies

13.1432	18.5239	25.5217
29.2272	34.4529	40.4362
52.2548	58.6250	74.6488
78.9005	86.6140	92.7481
103.0507	123.6255	133.7091
151.3534	159.7191	164.5944
173.8830	194.4537	203.2343
205.5362	217.6424	219.9936
242.2745	274.2863	280.6775
289.2163	309.8608	328.4262
334.1094	349.5788	361.2670
368.8592	400.6373	413.9506
424.5806	445.0121	479.9351
487.5317	496.3065	513.8250
517.2690	527.4824	530.1033

568.5344	581.8538	597.2360
599.5709	604.8415	613.2194
618.8494	622.3784	631.9935
681.7186	700.9361	702.2364
718.1900	731.6268	758.1892
760.6876	766.0954	789.4448
818.2910	840.2474	854.9928
858.2847	870.9175	872.4219
872.7217	878.1644	900.5418
907.7878	940.9651	945.9036
947.0889	960.1411	975.4133
976.3387	983.3328	988.7901
995.3585	1005.3188	1008.0459
1012.5067	1029.6479	1033.3785
1036.7029	1038.4127	1046.5969
1050.7635	1051.5607	1055.6325
1062.8841	1066.8642	1067.8608
1073.1476	1096.4801	1112.3674
1116.5494	1156.4459	1172.8097
1183.7378	1187.4446	1188.2626
1196.3481	1212.8546	1214.4018
1226.6550	1239.7224	1248.0525
1248.4132	1268.1336	1277.4534
1289.0473	1296.5897	1299.6950
1309.6702	1327.0340	1338.1363
1338.6244	1341.5151	1367.5180
1368.5540	1370.0237	1372.6629
1376.2067	1406.4256	1415.0764
1419.0587	1421.7440	1431.5289
1443.9502	1444.6321	1448.0216

1468.4277	1478.6303	1484.0725
1486.8970	1488.0997	1488.3049
1491.8305	1496.6217	1498.2268
1507.2786	1521.3485	1536.1231
1536.5422	1625.4109	1638.0051
1640.1275	1643.9374	1652.2707
1656.7339	1657.7911	1685.0445
1729.6487	2965.3255	3031.2419
3037.2207	3046.4596	3050.3357
3052.3972	3095.9593	3098.7863
3104.8923	3105.7163	3116.8383
3122.2516	3132.4681	3133.1854
3135.2742	3141.9254	3151.9482
3174.8757	3180.3343	3182.7978
3184.8087	3190.1058	3190.9229
3197.9032	3200.1581	3201.5081
3207.4306	3208.9825	3215.9185

preR2

Zero-point correction= 0.223791

Thermal correction to Energy= 0.239644

Thermal correction to Enthalpy= 0.240588

Thermal correction to Gibbs Free Energy= 0.178050

Sum of electronic and zero-point Energies= -3661.300646

Sum of electronic and thermal Energies= -3661.284793

Sum of electronic and thermal Enthalpies= -3661.283849

Sum of electronic and thermal Free Energies= -3661.346387

Cartesian coordinates

C	2.837102	0.150629	-0.065589
C	2.387705	-1.131863	0.322884

C	3.224938	-2.058886	0.949311
C	4.544533	-1.689231	1.192383
C	5.012821	-0.418922	0.815120
C	4.175992	0.499643	0.191169
C	1.779252	0.926047	-0.698628
C	0.584053	0.238586	-0.783041
H	2.857068	-3.038670	1.237468
H	5.216276	-2.390829	1.677682
H	6.046075	-0.149948	1.013848
H	4.534037	1.478426	-0.100286
S	0.692252	-1.367002	-0.088614
C	1.946063	2.294573	-1.189884
O	2.985092	2.941279	-1.115893
H	1.052313	2.750197	-1.654926
C	-0.740938	0.707789	-1.331465
H	-0.586373	1.601100	-1.938327
H	-1.150340	-0.055317	-1.998180
C	-1.734770	1.027601	-0.226265
C	-2.715107	0.132253	0.219287
C	-1.664669	2.272136	0.416773
C	-3.597530	0.451084	1.252000
C	-2.534615	2.610964	1.450278
H	-0.905851	2.978677	0.092144
C	-3.504336	1.697573	1.869204
H	-4.345854	-0.266924	1.568321
H	-2.455737	3.583057	1.926879
H	-4.188335	1.948478	2.673986
Br	-2.886657	-1.610180	-0.584425

Vibrational frequencies

16.6712	38.5357	55.6216

84.9609	117.0847	127.4522
140.7624	177.1957	210.6269
226.0935	248.9807	295.2197
307.2203	356.4239	379.6519
420.2415	440.3520	450.6743
454.1771	488.0745	503.2530
520.8951	534.4737	591.5535
613.8878	663.4542	673.8535
708.0116	749.3093	753.6496
756.3256	775.9365	778.7949
792.7606	835.7675	885.6744
890.3747	965.3654	967.7346
972.0565	1004.3962	1006.7118
1015.3595	1028.1727	1046.3810
1057.5670	1071.4332	1079.5455
1142.8679	1151.4084	1175.8062
1189.5119	1193.5904	1220.9029
1229.6076	1294.6434	1309.9739
1335.2822	1348.4682	1363.2342
1381.1941	1448.3267	1471.8210
1474.4158	1498.2303	1507.3625
1512.1586	1565.5962	1610.9039
1619.6061	1643.4293	1644.2126
1741.3267	2968.8792	3088.4104
3142.1285	3190.6794	3190.9950
3201.4348	3201.5341	3212.7667
3213.5075	3222.9925	3247.0192

R2

Zero-point correction= 0.209808

Thermal correction to Energy= 0.225529

Thermal correction to Enthalpy= 0.226474

Thermal correction to Gibbs Free Energy= 0.165066

Sum of electronic and zero-point Energies= -3660.800015

Sum of electronic and thermal Energies= -3660.784294

Sum of electronic and thermal Enthalpies= -3660.783350

Sum of electronic and thermal Free Energies= -3660.844757

Cartesian coordinates

C	3.012523	0.324169	-0.107587
C	3.241092	-1.008230	0.320539
C	4.519729	-1.531248	0.490066
C	5.623837	-0.707226	0.239621
C	5.426178	0.612337	-0.183663
C	4.140785	1.128952	-0.361157
C	1.604837	0.642906	-0.280134
C	0.725555	-0.418809	0.138232
H	4.659714	-2.559644	0.811811
H	6.628994	-1.096063	0.375580
H	6.286107	1.248138	-0.379277
H	3.984513	2.144799	-0.701520
S	1.717053	-1.868612	0.585071
C	1.150885	1.763435	-1.039156
O	1.842299	2.716225	-1.449589
H	0.074260	1.736254	-1.302019
C	-0.642958	-0.559784	0.261553
H	-1.006440	-1.577242	0.376508
C	-1.673011	0.454022	0.380276
C	-3.040824	0.182150	0.123694
C	-1.418273	1.763062	0.873702
C	-4.059232	1.114877	0.312102

C	-2.418797	2.704517	1.063046
H	-0.393887	2.020054	1.121982
C	-3.754839	2.392578	0.778186
H	-5.084469	0.840315	0.087405
H	-2.158023	3.687544	1.446159
H	-4.544404	3.124678	0.916124
Br	-3.579501	-1.558488	-0.530660

Vibrational frequencies

36.0110	40.7748	64.3233
90.5490	121.3958	138.3911
164.5245	197.9334	204.6955
213.1521	278.5167	284.5335
314.5392	353.7178	358.5934
390.1912	426.4725	450.8050
461.2062	491.9606	524.7374
540.6192	558.8245	596.3419
620.7119	661.5690	667.6136
704.6773	716.4783	743.0482
755.3424	761.2336	766.0236
770.9273	829.2960	874.2702
878.4048	901.2669	929.0308
955.8537	981.1970	998.4558
1012.2999	1023.1107	1046.1176
1057.8865	1071.6123	1094.2996
1138.9874	1142.1202	1180.7331
1187.8460	1208.0003	1254.3438
1293.3270	1316.8846	1326.9576
1351.9601	1384.6371	1424.4050
1457.4470	1465.8939	1481.9348
1495.8849	1501.5880	1556.7762

1588.0940	1601.9658	1624.5234
1634.8024	1671.9428	2929.6690
3162.9464	3173.2506	3180.6451
3183.0774	3197.7828	3198.5593
3204.8738	3214.3661	3235.4641

DBU

Zero-point correction= 0.261443

Thermal correction to Energy= 0.271172

Thermal correction to Enthalpy= 0.272116

Thermal correction to Gibbs Free Energy= 0.226838

Sum of electronic and zero-point Energies= -462.387477

Sum of electronic and thermal Energies= -462.377748

Sum of electronic and thermal Enthalpies= -462.376803

Sum of electronic and thermal Free Energies= -462.422081

Cartesian coordinates

C	1.973301	1.282149	0.558611
C	2.816459	0.014949	0.371289
C	2.024263	-1.297860	0.363649
C	0.917350	1.513665	-0.546302
C	0.952167	-1.369165	-0.729178
C	-0.330813	0.692396	-0.361976
H	1.477203	1.270712	1.536649
H	3.364840	0.097837	-0.576898
H	1.546152	-1.468723	1.336298
H	1.338691	-0.996357	-1.683096
H	1.346560	1.288393	-1.529313
H	2.639205	2.151145	0.555898
H	3.570736	-0.027393	1.165181
H	2.718837	-2.129488	0.200427

H	0.622902	2.565624	-0.567506
H	0.646526	-2.403095	-0.893545
C	-1.484434	-1.451815	-0.097751
H	-1.147192	-2.339604	0.441670
H	-1.918283	-1.777197	-1.049927
C	-2.496473	-0.676005	0.736418
H	-3.425330	-1.247010	0.802112
H	-2.109246	-0.537095	1.750991
C	-2.758333	0.683921	0.100752
H	-3.346708	1.329596	0.755170
H	-3.292467	0.578854	-0.850157
N	-1.469264	1.339387	-0.136858
N	-0.286131	-0.633429	-0.388340
H	-1.425591	2.348679	-0.090637

Vibrational frequencies

81.1865	103.8594	177.3297
217.4791	273.8399	313.4554
343.3962	371.2817	410.8996
436.2144	480.4744	516.7052
530.3213	533.5410	646.6477
701.2616	709.4934	804.7438
842.7326	865.0208	876.0118
905.5196	912.6442	928.8418
981.8098	1001.7873	1011.8146
1023.7094	1090.0215	1102.1420
1114.9728	1124.7363	1135.3090
1180.5633	1214.2049	1233.0435
1247.9941	1250.8295	1270.3053
1296.5511	1309.5576	1321.1522
1352.9178	1356.5833	1372.2184

1387.0862	1392.6732	1401.7008
1403.0673	1418.7477	1426.6290
1477.1729	1480.4804	1489.8370
1493.5637	1499.3160	1501.0371
1508.5209	1533.6280	1619.1139
1683.6507	3032.8344	3044.7573
3049.7398	3062.0596	3065.4357
3069.4304	3077.1339	3077.9984
3085.2878	3094.4349	3099.7783
3125.3873	3128.6637	3136.0538
3141.5628	3145.5038	3632.6226

DQ

Zero-point correction= 0.618514

Thermal correction to Energy= 0.650796

Thermal correction to Enthalpy= 0.651740

Thermal correction to Gibbs Free Energy= 0.555343

Sum of electronic and zero-point Energies= -1241.060866

Sum of electronic and thermal Energies= -1241.028584

Sum of electronic and thermal Enthalpies= -1241.027640

Sum of electronic and thermal Free Energies= -1241.124037

Cartesian coordinates

C	2.820085	-1.280539	0.004125
C	1.462449	-1.231589	0.020798
C	0.702864	0.000002	0.009864
C	1.462451	1.231594	0.020358
C	2.820086	1.280536	0.003600
C	3.583003	-0.000008	-0.023434
H	0.916336	-2.161270	0.046469
H	0.916342	2.161291	0.045542

C	-0.702853	0.000002	-0.009568
C	-1.462441	1.231592	-0.020205
C	-1.462438	-1.231589	-0.020646
C	-2.820076	1.280529	-0.003455
H	-0.916335	2.161288	-0.045551
C	-2.820074	-1.280534	-0.003973
H	-0.916328	-2.161268	-0.046477
C	-3.582976	-0.000009	0.024170
O	-4.822100	-0.000019	0.064461
O	4.822093	-0.000019	-0.064798
C	-3.589286	2.610657	-0.007785
C	-4.503090	2.685150	-1.255514
C	-4.443067	2.726722	1.278615
C	-2.639922	3.823787	-0.049268
H	-3.910877	2.613869	-2.174887
H	-5.242685	1.884170	-1.256425
H	-5.031499	3.645098	-1.269742
H	-3.808870	2.688194	2.171528
H	-4.973426	3.685720	1.284275
H	-5.178964	1.924914	1.341797
H	-3.232806	4.743946	-0.051169
H	-1.980175	3.861665	0.824499
H	-2.019359	3.832198	-0.952063
C	-3.589286	-2.610656	-0.009000
C	-4.443130	-2.727397	1.277298
C	-4.503029	-2.684482	-1.256813
C	-2.639925	-3.823767	-0.051053
H	-3.808984	-2.689311	2.170268
H	-5.179049	-1.925643	1.340856
H	-4.973457	-3.686415	1.282436

H	-3.910763	-2.612763	-2.176118
H	-5.031486	-3.644397	-1.271558
H	-5.242592	-1.883468	-1.257355
H	-3.232811	-4.743923	-0.053422
H	-2.019333	-3.831750	-0.953830
H	-1.980206	-3.862059	0.822718
C	3.589286	-2.610671	0.008948
C	4.503742	-2.684260	1.256250
C	2.639939	-3.823765	0.051783
C	4.442387	-2.727694	-1.277819
H	5.243268	-1.883209	1.256240
H	3.911999	-2.612416	2.175882
H	5.032253	-3.644147	1.270849
H	1.979619	-3.862137	-0.821529
H	3.232813	-4.743929	0.053844
H	2.019968	-3.831646	0.954988
H	4.972606	-3.686772	-1.283113
H	3.807736	-2.689679	-2.170432
H	5.178359	-1.926034	-1.341920
C	3.589283	2.610674	0.007734
C	4.503940	2.684831	1.254856
C	4.442176	2.727128	-1.279223
C	2.639934	3.823781	0.050198
H	3.912352	2.613360	2.174617
H	5.243491	1.883806	1.255068
H	5.032414	3.644745	1.268950
H	3.807376	2.688720	-2.171713
H	4.972403	3.686198	-1.285031
H	5.178136	1.925436	-1.343086
H	3.232805	4.743949	0.051783

H	1.979483	3.861797	-0.823031
H	2.020099	3.832027	0.953494

Vibrational frequencies

7.2564	10.0204	20.4340
40.9879	62.5048	62.9359
64.4477	71.7742	109.0853
127.1539	153.4367	159.7998
161.5360	163.4123	170.5052
209.3764	222.2071	230.6480
236.4165	242.5062	268.7047
269.0546	273.2006	275.0010
283.0860	284.6107	285.1617
299.6905	300.6296	308.4739
316.5499	320.6912	328.2328
342.2443	360.0740	361.1645
365.6960	366.5013	366.7034
373.7830	389.9993	392.8024
394.0077	407.0100	408.2084
411.7417	416.1595	448.0026
449.8900	456.2216	459.3999
476.4655	527.8516	535.9969
537.9294	558.2339	580.2059
585.9086	592.3091	637.2081
670.7434	687.5037	688.0514
753.2994	755.8046	795.4109
812.7164	818.7277	820.1486
827.0065	852.7369	881.4327
896.2363	897.9021	901.2184
904.2042	924.4372	935.0886
941.7275	941.8094	942.4903

942.8112	946.2603	947.8848
947.9689	948.8484	977.3210
977.3908	977.3954	977.4498
1030.5889	1049.3152	1059.2133
1059.5723	1060.1761	1060.4534
1061.8232	1062.7849	1073.7026
1111.9916	1117.0692	1210.5837
1213.5383	1224.9689	1225.0737
1225.1210	1225.6130	1238.5435
1239.1697	1240.2534	1240.8096
1280.6770	1284.3174	1287.0567
1294.0512	1328.2444	1382.6992
1391.1114	1392.4910	1398.1087
1398.1879	1398.4727	1398.7629
1408.9403	1409.6224	1411.0327
1412.7919	1434.6538	1435.3462
1435.6675	1436.3823	1447.9970
1456.0486	1483.0931	1483.0967
1483.2423	1483.2809	1498.3035
1500.0683	1500.3210	1501.0506
1501.7614	1501.8097	1501.8288
1502.5142	1502.5748	1502.6657
1503.3222	1504.1314	1516.6329
1516.6810	1516.7075	1517.0051
1526.7994	1530.2335	1530.5973
1530.7833	1543.2001	1607.2435
1620.5338	1651.9207	1665.2939
1670.9928	1688.6580	3035.3233
3035.3659	3035.5035	3035.5456
3038.8767	3038.8874	3038.9509

3038.9965	3043.8684	3043.8718
3043.8856	3044.4057	3102.0185
3102.0230	3102.1285	3102.1657
3103.2126	3103.2276	3103.2956
3103.3552	3107.2739	3107.3244
3107.4482	3107.5931	3112.3924
3112.4455	3112.5693	3112.7835
3161.1241	3161.1271	3161.1617
3161.1654	3163.1833	3163.2076
3163.3936	3163.4088	3247.3688
3247.7214	3277.0432	3278.9769

DQH-

Zero-point correction= 0.631843

Thermal correction to Energy= 0.664217

Thermal correction to Enthalpy= 0.665161

Thermal correction to Gibbs Free Energy= 0.571353

Sum of electronic and zero-point Energies= -1241.484715

Sum of electronic and thermal Energies= -1241.452340

Sum of electronic and thermal Enthalpies= -1241.451396

Sum of electronic and thermal Free Energies= -1241.545205

Cartesian coordinates

C	2.804608	-1.255584	-0.010804
C	1.430361	-1.211804	-0.039657
C	0.685319	0.007700	-0.065609
C	1.432265	1.227075	-0.044056
C	2.806392	1.269104	-0.023520
C	3.490469	0.006369	-0.014340
H	0.896069	-2.146649	-0.027253
H	0.898257	2.162326	-0.035619

C	-0.737885	0.005218	-0.091821
C	-1.483899	1.242811	-0.095244
C	-1.479768	-1.234941	-0.113634
C	-2.837241	1.295377	-0.006124
H	-0.934974	2.167621	-0.166259
C	-2.833018	-1.294218	-0.031309
H	-0.928348	-2.156974	-0.198207
C	-3.590980	-0.001997	0.096232
O	-4.805442	-0.005998	0.280536
O	4.818746	0.077066	0.000745
C	-3.610549	2.614582	0.011465
C	-4.632248	2.637109	-1.153973
C	-4.347271	2.768658	1.367333
C	-2.674486	3.825701	-0.157784
H	-4.125524	2.524779	-2.118519
H	-5.377227	1.846803	-1.058629
H	-5.151990	3.600809	-1.156881
H	-3.634765	2.759694	2.199076
H	-4.871581	3.730022	1.382910
H	-5.077979	1.975464	1.525190
H	-3.272957	4.741272	-0.157658
H	-1.952652	3.907135	0.661828
H	-2.125017	3.791486	-1.104669
C	-3.601461	-2.616295	-0.047326
C	-4.344889	-2.804678	1.300219
C	-4.616591	-2.614257	-1.218806
C	-2.660558	-3.820097	-0.240844
H	-3.636961	-2.811241	2.135936
H	-5.079894	-2.018396	1.471788
H	-4.864638	-3.768596	1.291023

H	-4.104812	-2.477235	-2.177507
H	-5.133279	-3.579173	-1.248280
H	-5.364751	-1.828800	-1.108892
H	-3.255801	-4.737489	-0.262489
H	-2.109724	-3.762831	-1.185834
H	-1.939813	-3.917535	0.578084
C	3.564371	-2.600052	0.048428
C	4.369402	-2.692407	1.369849
C	2.593114	-3.798003	0.036540
C	4.482646	-2.771780	-1.189840
H	5.110736	-1.899213	1.507414
H	3.693491	-2.648173	2.229045
H	4.908198	-3.644102	1.404744
H	1.992307	-3.830134	-0.878108
H	3.173658	-4.723851	0.081317
H	1.920811	-3.792155	0.900296
H	4.979191	-3.745129	-1.139680
H	3.891852	-2.733977	-2.110119
H	5.275997	-2.024101	-1.293075
C	3.574435	2.608518	-0.011793
C	4.437394	2.721047	1.268286
C	4.461946	2.724717	-1.275077
C	2.606079	3.808685	-0.019244
H	3.812454	2.649347	2.164988
H	5.206026	1.949531	1.321899
H	4.937255	3.695217	1.283498
H	3.853598	2.658487	-2.183576
H	4.964180	3.697795	-1.276658
H	5.229381	1.951255	-1.317337
H	3.190053	4.733638	-0.011979

H	1.976387	3.827537	-0.915226
H	1.959268	3.824731	0.864576
H	5.239355	-0.797081	-0.006685

Vibrational frequencies

21.9696	29.6915	37.4482
47.2409	64.2446	69.4102
72.9543	77.1865	106.7472
128.2889	147.2738	160.0257
163.9392	165.6150	174.6238
192.8513	214.6397	223.7532
231.1025	236.9508	247.6277
259.6612	263.0601	267.3813
272.2339	280.1667	283.8562
291.7856	301.7266	313.6966
321.0627	327.9963	328.5767
339.9302	356.8651	370.0615
372.8284	375.7748	383.8438
385.1391	391.9453	396.5824
401.1984	408.5026	415.8437
421.1788	422.7312	453.3651
456.2836	457.0544	458.5069
471.6165	476.9323	529.9126
531.1446	544.5387	560.6251
584.2774	593.4497	621.1577
635.5625	653.8527	681.7710
711.5961	748.9749	760.1331
789.3813	790.4018	811.8646
827.6808	834.3438	852.5154
890.1755	896.0232	905.9082
919.3268	921.3810	936.8817

941.4027 942.3672 943.0508

944.1963 946.1984 948.4477

951.1600 954.0503 954.4711

975.6065 976.1151 979.9419

987.3550 1034.3902 1053.4506

1055.3793 1058.1268 1060.5702

1060.7726 1062.0266 1063.8520

1083.2399 1106.4524 1142.6556

1160.1012 1207.8580 1217.5205

1218.5070 1224.6503 1227.1514

1228.6974 1234.0123 1236.0415

1238.6940 1267.6536 1277.3954

1284.9185 1291.4445 1327.7086

1346.7200 1364.6190 1383.6119

1400.7852 1401.8922 1405.6213

1405.9607 1406.8950 1412.6055

1414.9818 1423.0122 1426.7316

1428.9934 1434.9756 1436.1420

1441.1739 1448.0773 1453.7498

1473.5503 1483.9888 1484.1761

1484.5028 1484.6177 1491.7382

1497.3824 1497.6598 1498.1743

1500.0434 1500.7947 1502.6526

1503.1332 1503.4403 1505.1531

1505.3339 1512.6543 1514.2245

1514.5411 1516.5538 1518.6598

1525.1485 1527.8593 1531.2350

1532.1226 1545.3266 1586.7297

1605.8884 1646.3547 1681.6206

1709.1110 3039.6623 3041.6349

3041.7483	3044.6272	3047.6722
3048.0542	3048.2644	3048.6271
3051.8870	3052.0064	3052.3229
3053.4917	3109.3981	3111.0611
3113.1726	3113.2472	3113.3461
3113.6695	3114.8529	3115.1058
3115.4934	3115.7001	3117.0630
3119.9445	3121.1742	3122.6546
3122.8893	3123.5570	3131.1006
3133.5747	3160.1664	3162.3122
3163.4664	3163.9842	3166.0726
3166.6432	3266.7084	3273.2396
3299.1780	3302.3286	3763.5490

DQH_2

Zero-point correction= 0.641903

Thermal correction to Energy= 0.674732

Thermal correction to Enthalpy= 0.675676

Thermal correction to Gibbs Free Energy= 0.652655

Sum of electronic and zero-point Energies= -1242.277493

Sum of electronic and thermal Energies= -1242.244664

Sum of electronic and thermal Enthalpies= -1242.243720

Sum of electronic and thermal Free Energies= -1242.337894

Cartesian coordinates

H	5.304745	-0.736374	0.365554
C	-3.548184	-0.006027	0.019270
C	-2.859126	1.183057	0.364166
C	-1.460793	1.143951	0.330426
C	-0.742782	0.001414	-0.039140
C	-1.471352	-1.140683	-0.396850
C	-2.867352	-1.183883	-0.377428

H	-0.900811	2.021364	0.623694
H	-0.919364	-2.014549	-0.715743
C	0.742759	-0.001475	-0.039134
C	1.460757	-1.144003	0.330481
C	1.471342	1.140617	-0.396842
C	2.859091	-1.183108	0.364241
H	0.900763	-2.021395	0.623776
C	2.867342	1.183800	-0.377445
H	0.919367	2.014502	-0.715717
C	3.548159	0.005930	0.019279
C	-3.627942	-2.466873	-0.784866
C	-2.665053	-3.601028	-1.193160
H	-2.002381	-3.894937	-0.372139
H	-3.248653	-4.483687	-1.475110
H	-2.045496	-3.329359	-2.054503
C	-4.467760	-2.990842	0.404717
H	-5.210335	-2.262019	0.730977
H	-4.992015	-3.909912	0.117319
H	-3.820935	-3.226225	1.257508
C	-4.543760	-2.184975	-1.999964
H	-5.294209	-1.426175	-1.776161
H	-3.953388	-1.841214	-2.856821
H	-5.063545	-3.103095	-2.297984
C	-3.598996	2.478350	0.779050
C	-4.406654	2.251127	2.082687
H	-5.166763	1.466032	2.015134
H	-3.734136	1.968585	2.898836
H	-4.924705	3.172428	2.370014
C	-2.620691	3.634325	1.073422
H	-2.011847	3.889068	0.200131

H	-3.191863	4.526689	1.349003
H	-1.950749	3.403405	1.907480
C	-4.518147	2.970114	-0.369630
H	-5.041159	3.883623	-0.067070
H	-3.920378	3.197030	-1.258181
H	-5.280240	2.248550	-0.677524
C	3.599070	-2.478309	0.779206
C	2.620970	-3.634446	1.073677
H	2.012009	-3.889210	0.200476
H	3.192324	-4.526750	1.349078
H	1.951141	-3.403712	1.907878
C	4.518318	-2.969925	-0.369443
H	5.280310	-2.248210	-0.677246
H	5.041456	-3.883362	-0.066877
H	3.920627	-3.196901	-1.258030
C	4.406775	-2.250839	2.082762
H	5.166745	-1.465618	2.015054
H	3.734279	-1.968328	2.898941
H	4.925018	-3.172019	2.370128
C	3.627859	2.466855	-0.784835
C	2.664811	3.601025	-1.192689
H	2.002354	3.894751	-0.371426
H	3.248287	4.483764	-1.474649
H	2.045014	3.329472	-2.053898
C	4.467886	2.990673	0.404664
H	4.991998	3.909841	0.117321
H	3.821220	3.225849	1.257635
H	5.210586	2.261856	0.730644
C	4.543416	2.185256	-2.000211
H	5.294021	1.426534	-1.776693

H	3.952903	1.841544	-2.856991
H	5.063013	3.103490	-2.298214
O	-4.919657	-0.086958	0.044395
O	4.919640	0.086715	0.044429
H	-5.304873	0.736146	0.365335

Vibrational frequencies

20.9037	34.6837	41.3183
49.8785	52.3590	73.5851
81.3416	101.0208	117.8703
125.3956	146.7942	162.4572
163.2017	173.4018	192.7194
202.0013	204.2139	212.3389
222.5424	232.7563	236.2366
239.6380	259.1852	259.4354
270.4194	282.7937	283.5500
288.2641	291.6023	311.0444
320.1460	320.2704	328.4193
339.9758	346.3069	351.8822
363.6611	365.9186	370.6271
371.2625	383.8868	385.8222
389.5521	398.0312	414.8246
416.7608	419.6881	430.6971
431.7270	453.7810	454.4132
461.1554	475.4111	477.7183
536.3721	537.9516	548.2924
558.5152	592.9926	628.2919
632.3998	635.9661	636.2459
670.3638	672.2346	763.4009
766.4033	769.2939	773.3402
774.5228	821.5685	825.4390

859.0179	893.5227	898.8170
904.8285	918.7280	925.3117
925.8674	938.2329	938.3931
941.1929	941.5761	943.3017
943.3349	950.2319	950.4725
963.5478	975.3729	975.4098
983.5741	983.5896	1048.0726
1050.9804	1055.7359	1056.2144
1059.7355	1059.7473	1060.6176
1060.7452	1139.3572	1145.9116
1148.6237	1176.6920	1177.5412
1220.8892	1222.1810	1224.9915
1225.0354	1228.4867	1228.5063
1233.1984	1235.2557	1261.2073
1267.4704	1270.9124	1279.3061
1292.6311	1296.3960	1312.0597
1323.7822	1347.3075	1357.1628
1360.1904	1401.0243	1401.0640
1409.8343	1409.8929	1416.0421
1416.2432	1422.4275	1422.5671
1431.9059	1433.4804	1433.8598
1446.6415	1446.7463	1464.8664
1482.2210	1483.9988	1484.9175
1485.2421	1485.2696	1487.4851
1489.8025	1492.7006	1496.9418
1497.4932	1499.3234	1499.8676
1500.8801	1500.9767	1504.8483
1505.6904	1513.4872	1513.5180
1514.1766	1514.2934	1518.6409
1522.6428	1526.5505	1527.0904

1527.6139	1529.8578	1620.1203
1632.9551	1650.3086	1650.9812
3034.4003	3034.4206	3035.2382
3035.2491	3041.2558	3041.2605
3042.4458	3042.5063	3043.6826
3043.6951	3050.1020	3050.1601
3096.9916	3097.0137	3098.3882
3098.3978	3108.3294	3108.4077
3110.1964	3110.2541	3110.3457
3110.3704	3112.1999	3112.2257
3116.6921	3116.7059	3119.2567
3119.2888	3120.2495	3120.2846
3121.6490	3121.6977	3156.6236
3156.6240	3158.0983	3158.1077
3233.5986	3234.1878	3242.0572
3242.6503	3855.3861	3855.9381

DDQH-

Zero-point correction= 0.073421

Thermal correction to Energy= 0.086120

Thermal correction to Enthalpy= 0.087065

Thermal correction to Gibbs Free Energy= 0.033599

Sum of electronic and zero-point Energies= -1485.838437

Sum of electronic and thermal Energies= -1485.825738

Sum of electronic and thermal Enthalpies= -1485.824793

Sum of electronic and thermal Free Energies= -1485.878259

Cartesian coordinates

C	1.075910	0.646273	-0.000207
C	-0.127731	1.393366	-0.000567
C	-1.330396	0.688095	-0.000418
C	-1.352265	-0.735943	-0.000687

C	-0.149279	-1.541245	-0.001484
C	1.077188	-0.738405	-0.000404
Cl	2.575629	-1.635893	0.000315
Cl	2.577350	1.571028	0.000694
O	-0.149003	-2.791108	0.000763
O	-0.174484	2.753432	-0.000536
C	-2.585618	-1.432169	-0.000308
N	-3.600104	-2.010266	0.000004
C	-2.550866	1.426303	0.000210
N	-3.554135	2.017340	0.000663
H	0.725274	3.116939	-0.000443

Vibrational frequencies

62.8596	80.1641	105.6042
127.5064	153.2061	164.1003
188.5906	208.1536	269.8920
276.5533	329.2902	341.4787
345.9198	367.7123	435.0495
447.6184	489.0516	502.9285
534.1983	546.6958	615.3086
694.5770	748.9976	752.9804
781.2880	862.8693	1004.5234
1065.8867	1209.7709	1227.0750
1295.0966	1394.3799	1433.3937
1533.6376	1593.2317	1650.3960
2302.5515	2332.6900	3753.0638

DDQ

Zero-point correction= 0.062962

Thermal correction to Energy= 0.075173

Thermal correction to Enthalpy= 0.076117

Thermal correction to Gibbs Free Energy= 0.023306

Sum of electronic and zero-point Energies= -1485.062371

Sum of electronic and thermal Energies= -1485.050160

Sum of electronic and thermal Enthalpies= -1485.049216

Sum of electronic and thermal Free Energies= -1485.102027

Cartesian coordinates

C	1.152841	0.677549	0.000006
C	-0.120462	1.457455	0.000019
C	-1.402660	0.678363	0.000007
C	-1.402660	-0.678363	0.000007
C	-0.120462	-1.457455	0.000017
C	1.152841	-0.677549	0.000006
Cl	2.592088	-1.623383	-0.000007
Cl	2.592088	1.623383	-0.000007
O	-0.141961	-2.672465	0.000005
O	-0.141961	2.672465	0.000002
C	-2.604700	-1.448954	-0.000004
N	-3.582845	-2.075197	-0.000012
C	-2.604700	1.448954	-0.000003
N	-3.582845	2.075197	-0.000011

Vibrational frequencies

55.5284	76.7798	101.2178
118.8877	147.5147	163.8717
210.4195	258.8484	262.4242
286.9286	318.0975	345.9817
382.6917	431.2030	473.1836
482.2612	502.9634	508.0007
528.6927	638.4921	755.2648
776.4025	791.8641	794.0574
885.0886	978.1717	1062.1172

1172.7904	1264.5130	1338.9493
1606.3880	1665.2837	1764.7188
1765.4427	2356.9685	2365.1642

CO_2

Zero-point correction= 0.011463

Thermal correction to Energy= 0.014122

Thermal correction to Enthalpy= 0.015067

Thermal correction to Gibbs Free Energy= -0.009263

Sum of electronic and zero-point Energies= -188.568440

Sum of electronic and thermal Energies= -188.565780

Sum of electronic and thermal Enthalpies= -188.564836

Sum of electronic and thermal Free Energies= -188.589166

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

627.7084	627.7084	1367.8066
2408.2997		

DBU

Zero-point correction= 0.246377

Thermal correction to Energy= 0.256074

Thermal correction to Enthalpy= 0.257019

Thermal correction to Gibbs Free Energy= 0.211341

Sum of electronic and zero-point Energies= -461.911276

Sum of electronic and thermal Energies= -461.901578

Sum of electronic and thermal Enthalpies= -461.900634

Sum of electronic and thermal Free Energies= -461.946311

Cartesian coordinates

C	1.951679	1.266737	0.576129
C	2.788683	-0.003006	0.370795
C	1.990236	-1.311481	0.326029
C	0.900339	1.535023	-0.523252
C	0.904107	-1.329502	-0.760493
C	-0.395650	0.764128	-0.354620
H	1.450579	1.234700	1.552466
H	3.343403	0.096462	-0.573335
H	1.514494	-1.504966	1.296416
H	1.310006	-0.937461	-1.701129
H	1.342956	1.332312	-1.507638
H	2.633614	2.124849	0.608052
H	3.541984	-0.067569	1.165895
H	2.682638	-2.142023	0.139524
H	0.615555	2.589156	-0.513137
H	0.605506	-2.360908	-0.965944
C	-1.480866	-1.432949	-0.048040
H	-1.132023	-2.291292	0.537683
H	-1.944149	-1.831354	-0.962552
C	-2.494414	-0.622523	0.751638
H	-3.427994	-1.186306	0.848738
H	-2.105188	-0.443480	1.761170
C	-2.715685	0.721572	0.055150
H	-3.401444	1.346876	0.639753
H	-3.206911	0.552248	-0.916728
N	-1.468925	1.459700	-0.139954
N	-0.318732	-0.608163	-0.398511

Vibrational frequencies

63.8029	73.9944	158.8771

237.3536	248.6634	311.9928
351.6311	367.2040	397.0086
430.0695	485.6335	513.2020
518.9296	646.3197	693.0206
697.0168	803.2402	847.6444
860.9638	872.6636	900.4724
903.1812	931.6651	969.1938
995.9944	1009.3260	1018.4993
1076.0031	1104.6452	1108.1476
1122.0195	1134.7779	1177.1291
1209.1493	1226.6981	1233.3212
1256.4094	1262.8459	1289.3517
1309.0208	1318.1535	1346.9444
1358.3417	1373.4289	1376.4241
1389.7231	1398.6362	1403.6449
1404.4396	1462.9214	1477.9088
1482.2413	1488.2548	1489.8727
1497.4774	1501.8092	1511.5536
1529.7688	1670.2161	2985.4942
3004.3685	3016.9827	3029.1955
3031.6653	3035.4577	3041.5839
3043.7969	3053.3188	3065.0004
3065.7415	3072.8609	3077.5548
3100.2251	3103.8310	3120.8681

TS

Zero-point correction= 0.638371

Thermal correction to Energy= 0.670124

Thermal correction to Enthalpy= 0.671068

Thermal correction to Gibbs Free Energy= 0.575211

Sum of electronic and zero-point Energies= -1514.456157

Sum of electronic and thermal Energies= -1514.424405

Sum of electronic and thermal Enthalpies= -1514.423461

Sum of electronic and thermal Free Energies= -1514.519318

Cartesian coordinates

C	-0.888653	0.641066	-0.306590
C	-2.404896	2.254790	-0.458141
C	-3.151998	-0.031740	-1.238388
H	-2.780566	-0.306359	-2.227392
N	-1.339703	2.851106	0.009198
N	-0.416837	1.824886	0.096594
N	-2.169055	0.914408	-0.656363
C	-3.749098	2.854670	-0.732288
H	-3.633985	3.836612	-1.196405
H	-4.290024	2.992332	0.214121
C	-4.543409	0.664165	-1.301762
O	-4.479375	2.042881	-1.643977
C	-4.606014	-1.021108	0.381891
C	-3.416592	-1.212012	-0.335608
C	-2.653173	-2.367373	-0.181418
C	-3.091381	-3.340948	0.721325
C	-4.276976	-3.155190	1.442798
C	-5.044206	-1.997795	1.275006
C	-5.246236	0.299857	0.031201
H	-1.733562	-2.503741	-0.741236
H	-4.609515	-3.923098	2.135402
H	-5.968515	-1.864413	1.829829
H	-5.040956	1.044392	0.809123
H	-6.331551	0.243731	-0.085317
C	0.928136	2.075461	0.536448

C	1.251854	1.868973	1.883167
C	1.866974	2.494538	-0.418421
C	2.589509	2.046878	2.257231
C	3.185652	2.669512	0.006985
C	3.567390	2.435499	1.335271
H	2.868830	1.882854	3.294574
H	3.932369	2.988239	-0.715680
C	1.458117	2.736686	-1.848421
H	0.686278	3.511537	-1.909432
H	1.039995	1.830935	-2.300293
H	2.312835	3.053103	-2.450016
C	5.010746	2.584733	1.747172
H	5.436734	3.520593	1.370473
H	5.617010	1.768192	1.336136
H	5.123575	2.569918	2.834505
C	0.198621	1.501199	2.896049
H	-0.426834	0.672161	2.554884
H	-0.471188	2.349698	3.079353
H	0.654799	1.217927	3.847348
H	-5.090592	0.198522	-2.124598
H	-2.514236	-4.250728	0.857398
C	2.996336	-0.443136	-2.332994
C	4.327046	-1.170771	-2.556768
C	4.812974	-2.003103	-1.365514
C	1.785039	-1.362256	-2.063641
C	3.815486	-3.086951	-0.938722
C	1.683438	-1.862715	-0.640732
H	3.095738	0.271019	-1.508175
H	4.225774	-1.832776	-3.428033
H	5.021557	-1.356668	-0.502972

H	3.418195	-3.607132	-1.817042
H	1.808958	-2.219944	-2.747849
H	2.767525	0.146685	-3.227212
H	5.094144	-0.431306	-2.815730
H	5.756661	-2.493271	-1.632486
H	0.857998	-0.825226	-2.277069
H	4.316739	-3.842702	-0.330160
C	2.793014	-2.851495	1.326251
H	3.827186	-2.661365	1.630873
H	2.584479	-3.914059	1.501636
C	1.830183	-1.972974	2.115396
H	1.760889	-2.336784	3.144227
H	2.197514	-0.941059	2.142522
C	0.471799	-2.000628	1.419258
H	-0.255670	-1.353990	1.917462
H	0.059341	-3.018138	1.432270
N	0.607754	-1.540980	0.039538
N	2.699478	-2.582190	-0.122107
H	-0.152473	-0.516359	-0.247486

Vibrational frequencies

-1246.9897	23.1834	29.2139
32.4486	37.7451	45.5159
54.7789	63.5469	69.4879
75.3265	82.6064	94.6328
98.2950	110.3954	123.5857
140.7082	168.2742	181.1983
185.0098	199.9723	204.9631
211.7021	222.9240	243.0607
247.3040	256.3383	269.0478
273.1534	288.1985	309.2507

320.5791	325.9916	342.0730
359.7176	361.5769	395.0869
395.8285	411.8276	417.7322
438.6176	452.7195	468.6410
494.9761	501.6310	516.1574
523.2451	528.2112	528.9284
530.4774	535.1184	568.5342
583.2665	596.8122	604.6672
619.8205	629.3179	648.7202
650.6599	696.2247	703.6984
706.9756	726.2488	732.6020
754.4758	770.7627	789.9728
808.2485	825.3727	841.3710
855.1359	869.5384	876.8332
879.2706	884.8079	887.3205
902.0816	904.2487	905.8838
916.7962	935.9417	958.4315
964.2431	975.1673	977.0135
982.0585	1001.3912	1005.4285
1008.1062	1016.6396	1023.0771
1028.0815	1037.1161	1043.0973
1049.2969	1052.4286	1057.6481
1064.4952	1066.1594	1069.4251
1069.9291	1076.5157	1085.0276
1107.6844	1117.3125	1124.9465
1126.5874	1135.1272	1136.2694
1166.4208	1184.4966	1186.1058
1186.5360	1198.3567	1221.5617
1226.5590	1229.9062	1233.3869
1245.7983	1250.1186	1257.0396

1268.7067	1276.7529	1287.3934
1290.2463	1293.9520	1297.9205
1314.8791	1318.6119	1321.0709
1324.1851	1335.6930	1343.8981
1348.6789	1351.7460	1357.3227
1360.6882	1370.6235	1377.7179
1381.7988	1387.4311	1397.7746
1402.4439	1406.5233	1407.7476
1415.5804	1416.7800	1418.0397
1418.6569	1423.9540	1446.0178
1450.6459	1471.8658	1472.7695
1479.3074	1481.2207	1483.2885
1485.2323	1488.0702	1488.7812
1489.6924	1490.7318	1495.0095
1498.1999	1498.6302	1501.3336
1502.8637	1506.9721	1516.5061
1519.8365	1523.1395	1528.5719
1544.6279	1590.7148	1619.2740
1636.8432	1640.2874	1654.2744
1662.2502	1670.5603	3024.0405
3034.5300	3034.9266	3036.2821
3040.8317	3042.6750	3049.3552
3049.8892	3051.2228	3055.5520
3064.1601	3065.2191	3067.9970
3074.2230	3084.4036	3094.5753
3100.9836	3103.2459	3104.2586
3107.8795	3109.2800	3116.4103
3116.9155	3117.8388	3123.3826
3124.0291	3124.4002	3130.9020
3132.3624	3144.0160	3146.5522

3184.1124	3186.2916	3186.8526
3196.9308	3205.8218	3214.3155

TS1

Zero-point correction= 0.525826

Thermal correction to Energy= 0.555667

Thermal correction to Enthalpy= 0.556611

Thermal correction to Gibbs Free Energy= 0.463895

Sum of electronic and zero-point Energies= -1474.913252

Sum of electronic and thermal Energies= -1474.883411

Sum of electronic and thermal Enthalpies= -1474.882467

Sum of electronic and thermal Free Energies= -1474.975183

Cartesian coordinates

C	-5.211528	-0.848797	-0.097341
C	-3.903847	-0.725153	-0.572705
C	-3.634911	-0.276183	-1.866626
C	-4.716876	0.057257	-2.686349
C	-6.032160	-0.061050	-2.217770
C	-6.288137	-0.516258	-0.921510
C	-5.237621	-1.361145	1.320298
C	-3.760545	-1.341790	1.794248
C	-2.897726	-1.137340	0.483636
H	-2.607909	-0.184074	-2.221286
H	-4.535900	0.411864	-3.697211
H	-6.861344	0.205286	-2.867416
H	-7.308694	-0.604406	-0.558855
H	-5.853181	-0.749810	1.988390
H	-3.481012	-2.279717	2.275421
H	-5.635491	-2.381666	1.363293
H	-2.385696	-2.063800	0.215098

N	-1.859708	-0.126803	0.700375
O	-3.523137	-0.353840	2.803332
C	-0.613625	-0.050357	0.165968
C	-2.071080	0.956149	1.521889
N	-0.137328	1.089305	0.687749
N	-1.024741	1.732458	1.550149
C	-3.334867	0.977035	2.314819
H	-4.182181	1.313029	1.701896
H	-3.241573	1.638282	3.177525
C	1.158199	1.664616	0.456805
C	1.298040	2.604491	-0.571605
C	2.231538	1.246482	1.257920
C	2.575632	3.132173	-0.793703
C	3.486081	1.802089	0.997822
C	3.676683	2.743962	-0.022687
H	2.710604	3.859741	-1.589797
H	4.335486	1.485387	1.597559
C	2.076716	-2.043190	-0.792552
C	1.467375	-0.965079	-1.310426
H	1.454712	-2.898746	-0.523362
C	3.510281	-2.205263	-0.514318
C	3.975333	-3.435500	-0.013281
C	4.448679	-1.170435	-0.703708
C	5.324111	-3.629981	0.285079
H	3.266507	-4.245038	0.142569
C	5.794717	-1.364958	-0.405349
H	4.120273	-0.206011	-1.075027
C	6.241169	-2.594987	0.090696
H	5.658140	-4.589499	0.669959
H	6.500161	-0.552573	-0.556830

H	7.291603	-2.741990	0.324611
C	-0.012396	-0.889687	-1.544597
H	-0.518388	-1.853725	-1.322623
O	-0.453576	-0.152232	-2.473968
C	0.120460	2.985505	-1.430854
H	-0.206213	2.115479	-2.013844
H	-0.728631	3.312633	-0.820892
H	0.383072	3.794388	-2.117517
C	2.038380	0.203014	2.326503
H	1.213329	0.463778	2.997735
H	1.796352	-0.766746	1.876685
H	2.945988	0.082212	2.922460
C	5.052389	3.305004	-0.286673
H	5.032103	4.073815	-1.063863
H	5.480478	3.747721	0.619702
H	5.740572	2.515589	-0.611781
H	2.020169	-0.081303	-1.617187

Vibrational frequencies

-225.9537	23.0992	24.3934
31.2353	43.6820	47.6950
51.4841	61.5264	71.7646
72.4013	82.3900	97.4027
106.1084	119.2239	134.0823
154.9878	162.9704	176.7695
191.5026	198.7540	209.2447
214.5613	239.6635	248.0505
263.3381	282.8493	288.5781
293.5716	322.9725	331.5091
335.5038	367.7652	383.3859
399.6943	416.2471	430.6427

450.9566	463.6993	487.0599
489.7092	498.9449	516.0333
528.6366	535.0971	543.5873
575.0002	582.6191	597.6503
601.3526	611.4300	615.8381
620.6140	625.4087	632.8250
702.5168	706.6923	713.1097
717.9012	736.6407	760.8250
766.8895	771.9667	793.3031
820.3277	841.3458	849.0945
856.1804	871.2254	873.0648
879.5153	881.6492	906.5671
910.8603	931.9046	948.8840
962.2213	967.6140	978.5278
980.1474	986.0641	991.0293
1000.2245	1011.0493	1012.5608
1028.8009	1033.7831	1039.3011
1044.1575	1049.8672	1055.7509
1056.4894	1056.9857	1068.1365
1070.4483	1075.2933	1079.2551
1093.3833	1095.9791	1114.9008
1116.5008	1129.2271	1182.2580
1187.9043	1188.0354	1196.0174
1199.1639	1213.5417	1225.5186
1227.7237	1238.4901	1249.2475
1266.1693	1271.4546	1279.1748
1286.0958	1289.6254	1311.3077
1319.3101	1329.7816	1330.8949
1341.1334	1345.5799	1356.3861
1367.5493	1368.3628	1374.0202

1378.4730	1399.8650	1405.1341
1420.9997	1423.2652	1427.7529
1440.5290	1448.3242	1452.3374
1468.0176	1481.5562	1483.1598
1484.0346	1486.6497	1489.3630
1496.6820	1497.3541	1502.5671
1511.0949	1528.4468	1533.7336
1536.1324	1546.3137	1626.4436
1639.3535	1640.4078	1642.1849
1654.1464	1655.5488	1658.2451
1708.0489	2859.3227	3029.8434
3040.8640	3041.0778	3042.8389
3054.5201	3097.7398	3098.2596
3099.5159	3103.1694	3109.6611
3124.7322	3126.5429	3128.1568
3130.6670	3131.1259	3139.1495
3147.7132	3176.0654	3180.0138
3180.7548	3182.5414	3183.3050
3189.0194	3190.4715	3193.4436
3203.4016	3205.8555	3216.4277

M1

Zero-point correction= 0.527031

Thermal correction to Energy= 0.557002

Thermal correction to Enthalpy= 0.557946

Thermal correction to Gibbs Free Energy= 0.465034

Sum of electronic and zero-point Energies= -1474.918567

Sum of electronic and thermal Energies= -1474.888597

Sum of electronic and thermal Enthalpies= -1474.887653

Sum of electronic and thermal Free Energies= -1474.980564

Cartesian coordinates

C	-5.159063	-0.671614	-0.107260
C	-3.910084	-0.468658	-0.697342
C	-3.764119	0.287792	-1.860550
C	-4.902441	0.878838	-2.412928
C	-6.158024	0.700427	-1.814857
C	-6.296126	-0.083315	-0.666185
C	-5.065869	-1.581365	1.090294
C	-3.547885	-1.843768	1.298299
C	-2.815645	-1.190137	0.057307
H	-2.779086	0.349083	-2.318040
H	-4.817869	1.472828	-3.318724
H	-7.035112	1.166256	-2.255844
H	-7.273540	-0.233208	-0.215411
H	-5.502533	-1.145976	1.996043
H	-3.328706	-2.911783	1.316638
H	-5.593113	-2.524725	0.910717
H	-2.306707	-1.910512	-0.582126
N	-1.756663	-0.261700	0.519049
O	-3.081447	-1.377084	2.569301
C	-0.615596	0.124491	-0.090945
C	-1.836686	0.406213	1.718170
N	-0.064592	1.015874	0.745497
N	-0.812439	1.194749	1.895485
C	-2.943490	0.040539	2.648885
H	-3.873570	0.561648	2.383973
H	-2.678610	0.298373	3.675531
C	1.185730	1.704885	0.578585
C	1.227483	2.831958	-0.251773
C	2.311640	1.207185	1.253784

C	2.469225	3.454588	-0.426526
C	3.525508	1.863470	1.043995
C	3.624603	2.981768	0.204109
H	2.530135	4.328548	-1.069481
H	4.416221	1.489085	1.541634
C	2.394562	-0.994473	-1.245890
C	1.105212	-1.316442	-1.060613
H	2.615742	-0.008711	-1.655566
C	3.576071	-1.795687	-0.894532
C	4.837600	-1.170872	-0.877252
C	3.508743	-3.158776	-0.544237
C	5.986434	-1.873706	-0.513866
H	4.908401	-0.119300	-1.142846
C	4.656524	-3.861162	-0.184614
H	2.552445	-3.672917	-0.564367
C	5.901864	-3.223261	-0.164477
H	6.947750	-1.367253	-0.504674
H	4.581591	-4.912894	0.078232
H	6.794715	-3.774752	0.115688
C	-0.068047	-0.410333	-1.454178
H	0.396014	0.509311	-1.900367
O	-1.000351	-1.021825	-2.177890
C	2.210611	0.006182	2.156630
H	3.199383	-0.304526	2.501480
H	1.590035	0.223101	3.032885
H	1.751318	-0.837927	1.633305
C	-0.012968	3.350451	-0.932917
H	-0.839640	3.460769	-0.223224
H	0.175990	4.323185	-1.393128
H	-0.351553	2.667201	-1.720123

C	4.954852	3.666290	0.011010
H	5.269895	4.174126	0.930566
H	5.738752	2.942935	-0.238637
H	4.912548	4.413504	-0.786091
H	0.805616	-2.275695	-0.640294

Vibrational frequencies

20.9802	25.1329	28.5429
35.1841	41.9753	49.6241
63.2931	80.4539	95.7080
96.4851	107.7310	112.2201
120.2260	128.8130	143.6674
158.1121	177.2085	187.5456
195.7153	215.3685	222.6908
235.7089	249.8378	269.7530
282.0614	285.9081	299.4042
308.9534	325.0717	336.2213
360.3915	366.6075	401.5923
416.9065	419.7137	449.7510
454.2783	480.4142	493.9129
511.1406	514.2948	524.9376
527.2442	533.5821	557.0960
578.5657	584.2092	599.3107
603.9070	615.8494	623.0343
625.1878	633.0748	683.6749
702.5214	708.6827	718.3429
730.0349	749.3923	755.9357
774.2271	789.5863	796.5204
827.2215	844.3521	854.2590
857.6193	870.7100	873.5977
878.1847	890.5512	900.1701

908.6398	929.9027	949.2528
959.1758	974.9772	978.0143
984.2957	990.2773	991.8359
1003.5534	1010.6742	1015.8018
1030.0835	1035.8315	1037.3592
1047.8749	1049.0826	1053.4474
1055.1315	1059.5303	1062.9358
1065.6831	1069.3948	1071.1933
1083.9478	1101.7897	1110.4886
1116.1246	1178.7849	1181.7653
1182.7981	1186.6208	1196.4275
1209.0283	1209.1870	1218.6030
1222.1416	1231.6873	1242.5989
1255.7691	1278.7147	1287.1045
1289.6068	1299.3651	1311.8192
1322.3959	1326.3578	1332.6022
1334.9280	1346.8437	1353.3009
1362.5416	1364.8381	1370.7976
1379.8576	1384.7641	1410.9358
1418.8975	1420.2212	1426.0660
1437.3512	1447.7813	1462.2879
1473.0257	1473.3461	1482.8794
1483.9527	1486.6856	1487.0740
1490.8123	1492.7425	1497.0963
1502.4174	1507.5565	1521.3582
1530.8680	1535.0851	1624.9497
1638.2261	1639.9661	1642.7007
1653.3542	1653.9576	1656.2045
1693.5068	2732.5036	3039.0477
3039.5523	3045.1798	3052.7291

3055.1414	3090.7743	3097.6733
3105.1827	3116.0658	3128.9386
3131.1990	3137.1462	3138.4054
3139.6880	3143.4680	3149.6096
3154.9879	3166.3447	3177.5381
3178.8508	3182.6367	3183.1335
3184.8986	3189.2086	3192.1152
3199.2793	3201.9133	3207.6899

TS2

Zero-point correction= 0.785286

Thermal correction to Energy= 0.826361

Thermal correction to Enthalpy= 0.827305

Thermal correction to Gibbs Free Energy= 0.710929

Sum of electronic and zero-point Energies= -1937.316330

Sum of electronic and thermal Energies= -1937.275255

Sum of electronic and thermal Enthalpies= -1937.274310

Sum of electronic and thermal Free Energies= -1937.390686

Cartesian coordinates

C	-5.256541	-1.714328	-0.529796
C	-4.028341	-1.048648	-0.514165
C	-3.953655	0.334046	-0.364130
C	-5.142018	1.056848	-0.233801
C	-6.377924	0.398141	-0.260680
C	-6.443193	-0.990525	-0.409244
C	-5.063745	-3.202040	-0.690220
C	-3.551736	-3.441640	-0.447292
C	-2.886562	-2.030973	-0.672939
H	-2.992385	0.833781	-0.335842
H	-5.107588	2.134941	-0.107567

H	-7.294883	0.971055	-0.156493
H	-7.403085	-1.499144	-0.417828
H	-5.658002	-3.798535	0.008474
H	-3.137917	-4.165534	-1.150765
H	-5.334695	-3.523057	-1.703290
H	-2.446467	-1.978312	-1.665372
N	-1.808805	-1.791058	0.300242
O	-3.290588	-4.014337	0.839814
C	-0.595224	-1.171336	0.196746
C	-1.938360	-2.253716	1.589273
N	-0.065108	-1.281214	1.437352
N	-0.890338	-1.974477	2.306142
C	-3.134718	-3.083827	1.911745
H	-4.024830	-2.456470	2.050866
H	-2.961685	-3.655180	2.824970
C	1.117294	-0.665106	1.972743
C	1.013748	0.656332	2.434196
C	2.284888	-1.428931	2.102423
C	2.159915	1.237872	2.982492
C	3.410161	-0.793961	2.638127
C	3.368390	0.535748	3.075408
H	2.108813	2.261273	3.343702
H	4.335972	-1.356547	2.724985
C	2.432886	-1.249504	-1.229638
C	1.134151	-1.318239	-1.566181
H	2.721921	-0.558006	-0.446785
C	3.538078	-2.054710	-1.764681
C	4.834173	-1.825407	-1.264452
C	3.373510	-3.056680	-2.741754
C	5.925679	-2.563807	-1.721133

H	4.978344	-1.061812	-0.504009
C	4.464487	-3.789906	-3.201252
H	2.385320	-3.268352	-3.138718
C	5.746435	-3.549255	-2.694109
H	6.915282	-2.369688	-1.316947
H	4.315575	-4.557884	-3.955248
H	6.593284	-4.127650	-3.051630
C	0.015548	-0.518136	-0.961091
H	0.530351	0.844217	-0.693100
O	-1.026068	-0.345231	-1.952808
C	2.316626	-2.882332	1.709708
H	3.342161	-3.257551	1.689423
H	1.745863	-3.484021	2.426674
H	1.872503	-3.043743	0.724544
C	-0.291661	1.404408	2.355293
H	-1.072063	0.888329	2.925725
H	-0.187079	2.414235	2.758608
H	-0.640355	1.487215	1.322646
C	4.589236	1.188948	3.673788
H	4.604357	1.058225	4.763035
H	5.511140	0.751332	3.279734
H	4.604012	2.264823	3.474705
H	0.805240	-1.989274	-2.362560
H	-0.681579	0.289848	-2.597387
C	-2.035794	3.685743	-0.346732
C	-2.203077	5.181456	-0.640983
C	-0.904929	5.996381	-0.620344
C	-1.122200	2.925878	-1.334694
C	0.148991	5.483924	-1.609031
C	0.355228	3.079096	-1.053552

H	-1.667448	3.537574	0.675418
H	-2.666761	5.291356	-1.631277
H	-0.467687	6.004491	0.386331
H	-0.311220	5.250971	-2.575050
H	-1.332589	3.255917	-2.359346
H	-3.023754	3.215445	-0.391073
H	-2.909417	5.607910	0.081116
H	-1.134770	7.037485	-0.875639
H	-1.353004	1.862755	-1.299508
H	0.895096	6.257509	-1.799837
C	2.278074	4.571611	-0.673862
H	2.280068	5.531248	-0.148650
H	2.927559	4.670901	-1.552263
C	2.764805	3.459215	0.242057
H	3.836859	3.570433	0.426133
H	2.248823	3.518822	1.205992
C	2.461644	2.111390	-0.399665
H	2.715730	1.300304	0.283130
H	3.053148	1.975450	-1.314660
N	1.035938	2.006551	-0.713817
N	0.898235	4.310952	-1.123187

Vibrational frequencies

-1361.7357	16.3506	19.8096
22.3661	25.4702	43.8222
45.8613	52.4386	56.8491
61.6447	69.8284	73.2423
83.6762	88.0962	95.6507
98.1190	106.6690	108.6636
122.1322	124.4296	133.8567
147.0832	151.2927	162.9294

172.8248	179.6068	183.9851
208.2599	217.8022	223.3264
241.6822	245.9094	254.0353
265.6976	266.6936	274.3679
289.0298	291.5714	307.1685
312.7840	322.3482	329.2327
337.1170	352.4178	365.3333
370.0296	375.0011	387.8297
404.5890	411.6675	413.0627
420.0204	440.6469	443.0875
444.5017	488.1793	492.1573
496.7819	514.5593	516.6670
522.4093	527.4329	532.7629
538.9277	544.3939	573.0241
584.0164	587.8111	600.2764
608.7917	616.8110	618.5482
632.5029	649.8115	652.3402
677.2060	704.1691	705.0285
711.6839	727.9431	733.6449
736.8263	754.8417	759.5866
765.3877	788.5712	799.4046
814.4563	832.7055	840.0312
852.6245	853.8052	859.8823
866.2637	870.2615	876.3281
881.2110	882.9612	895.8414
905.3997	906.3742	915.0836
919.4436	927.5480	940.3794
942.2520	960.7858	968.1488
975.4614	977.9253	984.7645
988.9493	996.6515	997.7795

999.1412	1002.9141	1010.9533
1014.6909	1020.0394	1026.3187
1031.1415	1044.3447	1046.0291
1049.3186	1053.1044	1053.3975
1057.2277	1065.4367	1068.2940
1073.1301	1075.6746	1090.2094
1095.0082	1102.1708	1108.8601
1109.6451	1116.9918	1119.3612
1124.0132	1126.4392	1135.2243
1178.0156	1185.6310	1185.8753
1186.3977	1193.7864	1205.6370
1211.8986	1214.1301	1220.6238
1228.6962	1235.4088	1246.0970
1247.2793	1249.0146	1263.4136
1269.6165	1271.5764	1276.4264
1289.9412	1290.1617	1297.5542
1300.8899	1304.5281	1313.6109
1315.7292	1325.9232	1330.6311
1336.4269	1338.5700	1341.4068
1342.6524	1356.7629	1365.7812
1370.6623	1370.8685	1372.6316
1378.1224	1380.7545	1381.8070
1383.5982	1398.2598	1400.7310
1408.9588	1412.2423	1419.2460
1420.5644	1424.1588	1427.4009
1432.9578	1445.4236	1463.0718
1466.1094	1471.8479	1474.1081
1478.4971	1485.6461	1485.8635
1486.8998	1487.6454	1489.7075
1491.3999	1492.1290	1496.1653

1498.5381	1500.1266	1500.3286
1507.4529	1508.9791	1518.8312
1521.3187	1524.0387	1531.8400
1536.5534	1540.1234	1625.3294
1634.7369	1637.4289	1641.2531
1652.0933	1653.6218	1656.5351
1658.8208	1684.9316	1711.0887
3023.9709	3032.8593	3038.7120
3040.2342	3044.1526	3044.4643
3050.9074	3051.6226	3051.9060
3054.8365	3063.2069	3068.2982
3071.2689	3076.6538	3087.6030
3099.1934	3102.8018	3106.0611
3109.1572	3118.9301	3119.5582
3119.6298	3124.4233	3124.6464
3127.8383	3129.8461	3136.5643
3143.8317	3149.7945	3151.1535
3170.3223	3173.3360	3175.8167
3183.1983	3183.9982	3185.8640
3186.0191	3192.0323	3195.4190
3200.6802	3207.3476	3209.0599
3222.8503	3227.4735	3784.6030

M2

Zero-point correction= 0.526828

Thermal correction to Energy= 0.557105

Thermal correction to Enthalpy= 0.558049

Thermal correction to Gibbs Free Energy= 0.464394

Sum of electronic and zero-point Energies= -1474.931670

Sum of electronic and thermal Energies= -1474.901393

Sum of electronic and thermal Enthalpies= -1474.900448

Sum of electronic and thermal Free Energies= -1474.994104

Cartesian coordinates

C	-5.047435	-0.954539	-0.271056
C	-3.717063	-1.074969	0.139251
C	-2.938365	-2.164836	-0.255309
C	-3.510436	-3.137279	-1.079116
C	-4.843577	-3.020256	-1.492724
C	-5.619570	-1.930247	-1.089694
C	-5.686723	0.294182	0.280671
C	-4.548806	1.060557	1.011440
C	-3.301497	0.088973	1.016021
H	-1.901764	-2.248469	0.055661
H	-2.918113	-3.989489	-1.399561
H	-5.277318	-3.783135	-2.133112
H	-6.653156	-1.840938	-1.413364
H	-6.125113	0.925580	-0.500003
H	-4.827267	1.286347	2.041345
H	-6.494386	0.052168	0.980392
H	-3.087805	-0.240295	2.030756
N	-2.099236	0.775160	0.529756
O	-4.287174	2.344677	0.440184
C	-0.755362	0.399794	0.646726
C	-2.177380	1.755971	-0.429022
N	-0.111557	1.278988	-0.222764
N	-1.023292	2.105230	-0.896143
C	-3.528585	2.296120	-0.765070
H	-4.016692	1.670548	-1.527104
H	-3.450114	3.312845	-1.154277
C	1.278420	1.552571	-0.361975

C	1.885431	1.304521	-1.608389
C	2.015893	2.041136	0.729382
C	3.259879	1.517448	-1.728510
C	3.394053	2.222949	0.563297
C	4.036187	1.953824	-0.648151
H	3.741586	1.310914	-2.681010
H	3.977421	2.584311	1.406885
C	1.842021	-1.359810	0.314153
C	1.077704	-1.161705	1.423829
H	1.390572	-1.169733	-0.655004
C	3.241673	-1.759019	0.273445
C	3.834607	-2.053887	-0.974770
C	4.069001	-1.827020	1.417282
C	5.175941	-2.415426	-1.075497
H	3.225709	-1.989526	-1.873219
C	5.407535	-2.197532	1.315541
H	3.664782	-1.563087	2.389818
C	5.974111	-2.493345	0.070409
H	5.601722	-2.633679	-2.051409
H	6.019564	-2.239646	2.212818
H	7.021600	-2.770088	-0.005433
C	-0.233676	-0.584290	1.467315
O	-1.067084	-1.004456	2.525590
C	1.364750	2.346225	2.052530
H	1.986852	3.024402	2.642797
H	0.381268	2.807355	1.919036
H	1.213477	1.430653	2.635666
C	1.081819	0.788186	-2.774087
H	0.387765	1.548665	-3.147271
H	1.736851	0.487779	-3.596056

H	0.471105	-0.074956	-2.486702
C	5.533612	2.078832	-0.780407
H	5.949037	2.768555	-0.039480
H	6.012519	1.103171	-0.627946
H	5.822637	2.429053	-1.776608
H	1.452082	-1.481214	2.397872
H	-1.217132	-1.958287	2.427290

Vibrational frequencies

15.9114	20.1994	30.5241
32.2299	42.1461	53.2314
58.3305	79.2440	90.0480
91.8173	100.0748	109.1841
128.8244	136.9033	144.6016
169.8659	190.3985	197.7999
208.0302	211.3150	218.9788
239.5347	243.0648	276.2850
287.6816	294.8277	306.9031
330.2806	332.6725	351.3788
365.0024	378.5178	388.3404
404.6727	414.4636	416.8287
443.1387	446.5351	465.9612
486.9351	503.3748	513.0384
521.8257	528.4836	532.9083
554.8660	578.4368	582.8794
593.7509	601.0138	609.7347
616.2667	631.2010	638.8705
651.1795	653.7979	704.7957
706.1493	713.2536	730.4550
757.2187	765.9707	769.1458
800.1665	824.1175	843.9661

850.2158	854.9033	870.0626
872.7942	874.8855	881.5730
899.3196	903.6167	913.0752
948.4333	957.9936	968.4012
971.6374	975.8405	977.7868
989.1893	992.6477	997.2521
1003.0866	1006.6268	1037.4468
1040.4537	1045.2265	1050.2857
1051.8114	1055.0374	1058.1369
1061.0338	1064.4613	1065.8975
1068.5487	1106.9292	1107.8562
1121.3200	1138.0058	1165.8067
1182.7115	1186.0355	1193.6458
1201.1145	1206.2137	1208.8906
1224.5661	1233.4048	1248.1981
1257.4168	1273.1969	1281.1582
1288.9997	1292.9293	1310.3081
1312.5351	1319.0021	1325.1436
1334.3727	1339.8272	1343.3640
1353.7976	1363.9084	1368.1429
1373.2403	1386.1196	1407.8566
1413.7375	1418.2443	1419.6162
1426.1798	1448.7209	1469.2083
1471.9432	1473.1646	1475.4092
1483.1536	1484.9966	1486.3940
1491.9078	1497.1590	1500.0540
1505.5610	1522.3522	1524.5925
1530.9781	1584.0665	1616.7034
1632.0039	1639.2079	1652.9803
1657.0261	1657.3895	1673.8550

1686.1489	3021.0869	3037.1682
3044.0750	3044.7729	3054.7572
3092.0216	3098.5772	3103.8527
3107.1404	3121.8848	3123.7462
3123.9175	3129.7140	3130.1116
3139.3961	3154.7087	3168.5605
3173.3167	3175.5768	3176.7532
3181.2339	3185.2557	3190.2135
3190.8307	3194.9588	3200.6066
3204.6299	3209.7416	3736.0776

pre-TS3

Zero-point correction= 1.147484

Thermal correction to Energy= 1.211065

Thermal correction to Enthalpy= 1.212009

Thermal correction to Gibbs Free Energy= 1.049318

Sum of electronic and zero-point Energies= -2716.019693

Sum of electronic and thermal Energies= -2715.956112

Sum of electronic and thermal Enthalpies= -2715.955168

Sum of electronic and thermal Free Energies= -2716.117859

Cartesian coordinates

C	-6.674844	-3.116852	0.052990
C	-5.658026	-2.276824	-0.410070
C	-5.271603	-2.280463	-1.750998
C	-5.914986	-3.154000	-2.631344
C	-6.934308	-3.998574	-2.173080
C	-7.322141	-3.982700	-0.830041
C	-6.915643	-2.923349	1.530028
C	-5.756723	-2.014638	2.022563
C	-5.093552	-1.437180	0.715843

H	-4.482323	-1.622198	-2.099124
H	-5.624539	-3.175543	-3.677675
H	-7.427195	-4.672836	-2.867795
H	-8.111296	-4.641312	-0.477329
H	-6.926876	-3.862895	2.092584
H	-6.125221	-1.195813	2.641640
H	-7.879378	-2.432734	1.708830
H	-5.371975	-0.389394	0.601873
N	-3.629469	-1.517780	0.807251
O	-4.833085	-2.700310	2.874759
C	-2.668706	-0.898661	0.000597
C	-3.064769	-2.669977	1.306350
N	-1.586241	-1.764592	0.066530
N	-1.849770	-2.853870	0.903076
C	-3.912825	-3.536647	2.182294
H	-4.427921	-4.299773	1.581243
H	-3.299253	-4.048250	2.926459
C	-0.333577	-1.768596	-0.622325
C	-0.290588	-2.143130	-1.976748
C	0.834588	-1.517805	0.115882
C	0.961052	-2.220016	-2.594579
C	2.064154	-1.636036	-0.538954
C	2.147864	-1.970537	-1.894116
H	1.010083	-2.500756	-3.644060
H	2.975627	-1.457457	0.022343
C	-4.400315	1.653705	0.645768
C	-3.746931	1.326536	-0.509883
H	-4.131006	1.125825	1.558871
C	-5.385064	2.713217	0.807288
C	-5.764060	3.107464	2.110487

C	-5.995714	3.381059	-0.279367
C	-6.688219	4.128444	2.319256
H	-5.314922	2.603711	2.963230
C	-6.914636	4.404751	-0.066928
H	-5.758868	3.083392	-1.296309
C	-7.268964	4.788116	1.231841
H	-6.956818	4.410753	3.333793
H	-7.368429	4.900652	-0.920970
H	-7.992167	5.582344	1.391969
C	-2.781509	0.291605	-0.709550
O	-1.853885	0.489238	-1.715595
H	-1.383518	1.343689	-1.575697
C	0.769823	-1.146134	1.575194
H	0.114612	-0.283997	1.733504
H	0.365517	-1.967932	2.175974
H	1.763120	-0.896115	1.956518
C	-1.551004	-2.448167	-2.742309
H	-2.241579	-3.058546	-2.152044
H	-2.070376	-1.519538	-2.997928
H	-1.325612	-2.983691	-3.668427
C	3.484001	-2.031467	-2.591783
H	4.295710	-2.225651	-1.885943
H	3.501046	-2.808515	-3.362598
H	3.703644	-1.078147	-3.088706
H	-3.877965	1.959926	-1.387406
C	1.776227	2.163161	-1.999307
C	2.951852	1.660419	-1.527068
C	3.250538	1.539483	-0.122891
C	2.325925	2.156320	0.794635
C	1.142254	2.706692	0.403507

C	0.748891	2.563706	-1.015756
H	3.678765	1.287564	-2.231651
H	2.611105	2.212585	1.834710
C	4.379312	0.826699	0.332101
C	4.507786	0.448924	1.717249
C	5.400688	0.360761	-0.571687
C	5.502148	-0.352511	2.188805
H	3.736097	0.772990	2.398404
C	6.451825	-0.412875	-0.183981
H	5.332951	0.664279	-1.605090
C	6.552179	-0.821900	1.243916
O	7.489148	-1.537635	1.637350
O	-0.435899	2.770890	-1.376308
C	5.554373	-0.802163	3.656562
C	5.477343	-2.346764	3.729297
C	6.864906	-0.306831	4.315167
C	4.376608	-0.236735	4.473596
H	4.547261	-2.709104	3.276674
H	6.317243	-2.812423	3.213118
H	5.489999	-2.669746	4.776449
H	6.919874	0.787478	4.293252
H	6.894232	-0.623262	5.364105
H	7.742054	-0.708404	3.807277
H	4.457702	-0.582890	5.508972
H	4.375804	0.858587	4.492475
H	3.407639	-0.575429	4.089940
C	7.530508	-0.873818	-1.176036
C	8.912653	-0.333958	-0.736123
C	7.564794	-2.420592	-1.235942
C	7.258450	-0.357944	-2.602552

H	8.909814	0.761647	-0.710904
H	9.188297	-0.702821	0.252203
H	9.678890	-0.651998	-1.452333
H	6.598567	-2.818478	-1.566183
H	8.324211	-2.745807	-1.956270
H	7.803089	-2.851227	-0.263258
H	8.048133	-0.715899	-3.270654
H	6.304066	-0.722114	-2.998072
H	7.257291	0.736459	-2.652741
C	1.490406	2.299790	-3.504334
C	1.137527	3.773937	-3.818302
C	2.722112	1.918120	-4.348609
C	0.322325	1.384741	-3.945030
H	0.254346	4.097696	-3.264751
H	1.970129	4.439895	-3.565226
H	0.930359	3.886559	-4.888535
H	2.980019	0.858657	-4.242070
H	2.501444	2.094506	-5.406034
H	3.602723	2.516728	-4.091404
H	0.249888	1.390877	-5.038939
H	0.486961	0.353040	-3.620870
H	-0.630746	1.720253	-3.541584
C	0.224867	3.460954	1.379551
C	-0.054576	4.874690	0.813036
C	-1.112146	2.712636	1.574629
C	0.879466	3.628087	2.763729
H	0.878561	5.433347	0.678147
H	-0.569916	4.824808	-0.147586
H	-0.685707	5.435998	1.510943
H	-0.945793	1.710100	1.982539

H	-1.743901	3.261089	2.282881
H	-1.655049	2.617595	0.638082
H	0.214030	4.212348	3.407287
H	1.047662	2.665354	3.258794
H	1.835812	4.159156	2.706626

Vibrational frequencies

12.4436	14.9091	19.8923
20.3938	22.6007	30.0993
35.1340	40.6933	43.4868
45.7498	49.2465	52.9300
57.7595	62.9601	65.8141
69.2573	71.8295	74.2927
78.1836	83.2361	88.0660
92.8053	109.6214	115.9260
123.9837	127.8511	130.1606
131.8700	137.4394	138.6227
151.0583	155.1114	161.8517
166.0400	175.8614	177.8274
183.9402	194.9266	196.7709
206.1808	213.6965	218.2900
227.8424	232.1550	236.5852
238.5993	247.1546	252.2450
266.2987	267.3579	268.8658
272.7890	275.0516	279.0774
282.6713	288.2313	289.3996
293.7056	296.3735	301.7775
305.1295	308.8117	312.1491
315.5037	321.2220	327.0435
327.5545	336.0838	341.8333
346.5090	361.8089	363.3918

366.3096	369.2164	372.5682
379.7006	385.7559	388.3368
389.9229	392.5544	399.6707
407.0945	408.3876	410.2715
414.0134	418.6737	421.5759
423.1026	442.5029	449.8891
451.9410	452.9383	463.6583
467.8186	473.5141	476.0317
490.2504	506.9591	515.8951
525.0575	528.1435	530.7745
532.3042	535.2066	536.2679
555.6581	558.9964	576.5683
581.4143	583.7197	591.5873
594.2304	595.0181	608.5878
616.1254	619.7459	625.9793
632.8854	639.2993	647.0307
668.0615	672.7640	685.0733
689.6579	694.3160	697.0709
708.3169	725.2602	734.3873
755.8263	758.3484	762.9788
765.7175	772.0421	794.6450
795.9874	816.0978	818.0068
825.3059	827.0104	831.5090
843.7355	852.7014	856.8710
859.8679	869.8307	872.0582
882.0575	887.1841	895.7937
897.5176	899.0284	900.7512
905.6099	913.3546	917.0468
918.7187	920.3432	925.9963
942.2372	942.5659	944.4636

945.6770	946.7688	947.5465
947.9147	949.5285	953.1620
960.1346	971.3014	975.3945
975.8931	976.1143	977.0599
978.1324	981.4003	984.4931
993.0598	998.4123	999.1471
1006.8819	1018.3973	1034.6472
1035.2226	1039.9143	1045.0034
1047.4881	1052.7875	1053.7331
1054.3583	1056.7033	1058.2084
1058.8242	1059.9261	1060.5772
1062.4380	1063.5581	1064.6592
1065.5171	1067.0072	1073.0767
1078.4574	1102.7428	1110.2802
1111.4134	1116.9085	1119.5988
1156.9486	1167.3574	1184.6819
1185.7827	1191.0874	1207.0923
1208.5670	1209.9101	1212.2458
1214.5962	1225.6270	1226.1602
1226.4998	1226.9985	1228.7159
1232.9681	1237.6255	1238.6637
1239.5376	1243.2092	1253.0068
1270.0721	1275.7356	1278.0838
1280.5532	1288.1973	1290.9958
1293.5477	1294.3772	1305.5134
1310.2633	1320.5326	1324.9030
1333.0794	1336.2527	1338.4408
1338.8675	1347.7563	1353.0541
1367.7948	1368.1807	1374.2085
1376.3137	1380.3073	1388.1851

1389.6712	1396.2205	1398.7341
1404.7170	1405.2397	1406.6968
1407.5873	1409.4433	1410.3024
1411.8730	1412.5801	1414.7664
1417.5930	1421.9828	1430.9311
1433.7245	1434.4709	1434.8021
1448.5139	1448.6100	1457.1935
1458.4993	1467.9903	1473.7531
1479.0707	1481.9206	1482.7987
1483.2200	1485.4193	1487.3594
1488.3503	1489.1322	1490.7422
1491.2919	1493.1763	1497.2149
1497.9189	1498.2909	1499.1475
1500.2313	1500.5789	1501.2332
1501.7334	1502.3851	1502.6358
1504.4985	1506.2651	1507.2867
1511.8454	1514.7321	1515.7097
1517.1622	1517.8197	1520.7687
1523.7691	1528.2742	1528.5651
1529.7607	1532.7560	1534.5380
1551.1064	1585.1080	1587.7482
1602.9685	1615.6321	1630.5448
1632.5381	1638.4762	1650.2800
1654.1904	1655.0204	1656.5762
1665.1571	1676.5023	1677.8927
3024.0487	3035.0857	3035.1804
3036.8261	3036.9245	3038.1292
3038.2781	3038.4175	3040.3718
3041.0663	3043.6590	3044.2509
3046.8468	3048.6434	3051.0497

3052.8457	3053.0035	3094.5691
3099.5714	3100.9266	3101.9073
3102.6275	3102.6351	3103.0149
3104.5528	3105.8797	3107.2968
3108.9229	3109.0349	3109.9614
3110.1614	3112.0834	3112.7628
3113.0989	3114.7640	3114.8009
3121.2138	3122.3253	3125.3816
3132.4720	3132.8239	3135.3823
3136.1851	3141.2441	3148.2685
3151.6904	3159.1784	3160.0985
3160.1755	3162.0651	3163.0951
3172.8405	3174.3677	3180.2158
3182.5874	3187.0218	3189.9437
3192.1708	3199.8514	3200.2720
3203.3461	3204.1823	3207.5076
3212.9381	3249.3821	3250.7252
3270.7191	3272.4638	3365.5071

TS3

Zero-point correction= 1.142957

Thermal correction to Energy= 1.205996

Thermal correction to Enthalpy= 1.206940

Thermal correction to Gibbs Free Energy= 1.043161

Sum of electronic and zero-point Energies= -2716.016749

Sum of electronic and thermal Energies= -2715.953711

Sum of electronic and thermal Enthalpies= -2715.952766

Sum of electronic and thermal Free Energies= -2716.116546

Cartesian coordinates

C	-0.176310	-3.990013	-1.575838

C	-0.754361	-2.921819	-0.882544
C	-0.186143	-1.647797	-0.933420
C	0.968388	-1.450008	-1.692795
C	1.547718	-2.516927	-2.390257
C	0.978767	-3.791282	-2.335055
C	-0.929145	-5.275423	-1.363605
C	-2.002897	-4.940974	-0.295666
C	-1.938954	-3.375733	-0.053973
H	-0.612679	-0.829514	-0.372642
H	1.429662	-0.467893	-1.718757
H	2.452026	-2.353880	-2.969618
H	1.433559	-4.621171	-2.868924
H	-1.398270	-5.628199	-2.289637
H	-1.753769	-5.420650	0.651444
H	-0.278572	-6.084427	-1.017513
H	-1.785165	-3.164504	1.000594
N	-3.224678	-2.724220	-0.405271
O	-3.298355	-5.444145	-0.611755
C	-3.734844	-1.492001	-0.035860
C	-4.168499	-3.338874	-1.180827
N	-4.980504	-1.460680	-0.611959
N	-5.241105	-2.613745	-1.321837
C	-3.935766	-4.729554	-1.664547
H	-3.338666	-4.726008	-2.586626
H	-4.889932	-5.215333	-1.874247
C	-6.060008	-0.526935	-0.452896
C	-6.484355	0.188919	-1.586715
C	-6.668393	-0.379749	0.802549
C	-7.516122	1.113725	-1.419670
C	-7.694654	0.565248	0.914581

C	-8.120372	1.330401	-0.174786
H	-7.846038	1.690150	-2.280014
H	-8.171336	0.701732	1.881664
C	-3.981325	1.637030	-0.020894
C	-3.453746	0.840820	0.950648
H	-4.136877	1.210604	-1.004702
C	-4.325752	3.040739	0.097040
C	-4.836812	3.704012	-1.040603
C	-4.179553	3.783293	1.290743
C	-5.188660	5.049965	-0.990219
H	-4.959484	3.145417	-1.964482
C	-4.525025	5.129253	1.334602
H	-3.793176	3.303623	2.184007
C	-5.033409	5.770225	0.197667
H	-5.583407	5.538322	-1.876494
H	-4.401861	5.684352	2.260096
H	-5.305652	6.820653	0.239941
C	-3.103163	-0.541187	0.829124
O	-2.118903	-1.005914	1.576616
C	-6.239489	-1.185055	2.000950
H	-7.025846	-1.189606	2.759850
H	-6.014943	-2.222279	1.734088
H	-5.337265	-0.763677	2.459857
C	-5.838738	-0.015067	-2.933651
H	-6.096628	-0.995250	-3.348141
H	-6.166557	0.751473	-3.639703
H	-4.745485	0.020435	-2.872032
C	-9.175481	2.395009	-0.012288
H	-9.796075	2.216446	0.870457
H	-8.705799	3.379638	0.106376

H	-9.828321	2.450687	-0.889129
H	-3.142256	1.273479	1.898012
H	-1.247890	-0.246117	1.689567
C	1.764317	-0.168615	2.133143
C	3.085206	-0.147180	1.723100
C	3.585928	0.730033	0.727920
C	2.665431	1.660516	0.179772
C	1.324477	1.683830	0.511871
C	0.829027	0.708998	1.463699
H	3.790398	-0.801763	2.213939
H	3.029899	2.352641	-0.565185
C	4.967691	0.683426	0.303796
C	5.583989	1.780368	-0.364803
C	5.768357	-0.473824	0.527983
C	6.894366	1.773301	-0.779899
H	4.993220	2.674414	-0.512429
C	7.080645	-0.574871	0.133494
H	5.294652	-1.326949	0.994333
C	7.716610	0.571879	-0.541916
O	8.921849	0.526349	-0.904897
O	-0.453258	0.684543	1.718689
C	7.527830	2.992952	-1.471237
C	8.716781	3.515862	-0.629460
C	8.021608	2.597179	-2.884346
C	6.529636	4.154973	-1.637254
H	8.376729	3.835095	0.362617
H	9.475652	2.743092	-0.503120
H	9.176933	4.381989	-1.120494
H	7.186160	2.246878	-3.501676
H	8.466605	3.465240	-3.385683

H	8.768090	1.804159	-2.829857
H	7.027118	4.990634	-2.141031
H	5.664106	3.872916	-2.247144
H	6.162857	4.525495	-0.673708
C	7.896081	-1.858125	0.367885
C	8.380585	-2.428603	-0.986842
C	9.116674	-1.546799	1.267724
C	7.070840	-2.956253	1.066767
H	7.527576	-2.676984	-1.629129
H	9.009504	-1.707845	-1.510071
H	8.957986	-3.346945	-0.824923
H	8.792446	-1.177333	2.247492
H	9.706356	-2.457042	1.430919
H	9.756770	-0.793584	0.807561
H	7.698655	-3.841322	1.215451
H	6.712109	-2.639691	2.052420
H	6.204763	-3.265291	0.470923
C	1.328507	-1.154291	3.242606
C	0.674752	-2.389516	2.583860
C	2.535528	-1.655011	4.068001
C	0.349696	-0.505658	4.250566
H	-0.182133	-2.112841	1.974308
H	1.392878	-2.907477	1.939544
H	0.332014	-3.094521	3.351178
H	3.090184	-0.827040	4.522811
H	2.173973	-2.300358	4.875256
H	3.235248	-2.251758	3.475020
H	0.159133	-1.203518	5.073604
H	0.782235	0.405672	4.678666
H	-0.605615	-0.243417	3.800768

C	0.376932	2.712249	-0.147302
C	-0.620599	1.989793	-1.079391
C	-0.391806	3.513847	0.930619
C	1.143278	3.737860	-1.007473
H	-0.091974	1.458771	-1.878378
H	-1.230235	1.276148	-0.530044
H	-1.294210	2.717058	-1.547825
H	0.306724	4.055161	1.579442
H	-1.044865	4.252394	0.452539
H	-1.003896	2.862341	1.552259
H	0.431501	4.461312	-1.418651
H	1.882695	4.296742	-0.423527
H	1.656210	3.271533	-1.855307

Vibrational frequencies

-1308.9235	7.4391	12.3552
15.6390	17.4249	23.4315
24.5050	25.8627	34.6350
37.9401	40.4837	44.0795
50.6633	57.2269	58.8354
61.2526	66.3577	67.9309
76.2326	77.8159	82.8572
88.8590	92.6789	99.7675
111.0260	117.4991	127.0666
134.3479	136.9809	142.5224
148.6763	158.3473	163.7607
167.8251	171.8963	178.2666
186.1509	192.3476	196.4438
199.8131	212.6890	215.8292
223.6056	226.1057	235.3566
241.0575	242.7881	245.8194

250.1480	257.3103	265.8959
267.5929	271.7014	276.9848
286.5068	290.5464	291.6064
295.9479	297.6199	304.4929
306.4131	310.9438	316.1445
322.6132	323.9474	325.6433
329.4030	337.7122	341.5015
347.3539	355.9489	357.6006
368.1664	372.6152	373.6300
374.5758	376.3862	385.4993
392.8157	395.0978	407.5989
408.8734	410.7271	413.1675
413.3410	420.3531	427.9950
432.6107	445.4037	448.6255
449.6115	459.6398	471.4638
474.5378	478.6989	481.7704
496.7030	510.1434	515.4012
516.3082	523.7115	529.9911
537.0114	538.4484	545.9122
553.7481	568.1412	576.8412
580.6579	588.0895	595.3121
604.5807	606.5151	615.8562
618.6018	623.9745	627.9575
631.5342	648.1544	654.6794
658.8519	671.9278	674.7422
683.5769	691.5023	694.5985
699.8934	716.8036	739.9608
755.8914	759.6582	762.7371
770.3566	774.8035	796.9733
800.1790	803.1972	808.5652

823.4933	828.3870	841.2556
848.4328	857.3598	862.6623
871.9189	876.4612	878.0262
884.0077	885.4490	899.2041
900.4657	901.8533	903.3657
906.5095	908.8868	911.7103
923.0759	929.5954	938.6758
940.0769	940.7599	942.9166
944.1910	944.9097	945.7730
946.3056	951.2079	958.3805
962.0299	972.5231	972.9648
973.7662	974.6504	976.8961
977.3786	981.2141	987.6742
996.4431	1004.0244	1005.7708
1009.3267	1029.3655	1044.2016
1044.9516	1048.6875	1049.5759
1049.8915	1053.9739	1055.5948
1058.1499	1058.6101	1060.0457
1060.2840	1061.7109	1062.8842
1062.9591	1063.6792	1066.8602
1069.5474	1070.2918	1101.3198
1108.2553	1114.2772	1118.2995
1119.8628	1126.5681	1137.7340
1168.3970	1184.5128	1187.7302
1189.6295	1195.2999	1197.8196
1208.2914	1209.4753	1212.7279
1224.4062	1225.0462	1227.0544
1228.0035	1228.8803	1231.9577
1235.9624	1237.3166	1237.7376
1238.3883	1240.7635	1244.6130

1260.3198	1268.9456	1276.4731
1284.2112	1288.7116	1290.0243
1292.8275	1294.1821	1301.2553
1307.7923	1321.3650	1326.8472
1335.2292	1342.1213	1342.6481
1345.2754	1348.6463	1349.9355
1353.9770	1368.9211	1369.3864
1369.6339	1380.1417	1381.2104
1394.4912	1395.4589	1400.5850
1402.5875	1403.0955	1404.3831
1407.5758	1408.6415	1410.6860
1414.8896	1419.6773	1426.3276
1427.5489	1427.9116	1429.7354
1432.2467	1433.0022	1433.8969
1439.1395	1448.0678	1449.3128
1456.2769	1470.8009	1472.5680
1477.3751	1479.8004	1481.0850
1481.9418	1482.4877	1482.9604
1486.8308	1488.8286	1489.9483
1490.2841	1493.2612	1495.5729
1496.2222	1497.4302	1498.0792
1498.4314	1499.0309	1499.9775
1500.6131	1501.3028	1501.8616
1503.0114	1503.4309	1504.4962
1505.6762	1507.6586	1510.0731
1514.4727	1514.8814	1517.0683
1518.4682	1523.0120	1524.8677
1528.6595	1530.3366	1532.1331
1534.0207	1540.7095	1545.6187
1548.3684	1562.6281	1579.9358

1615.1578	1627.8295	1635.3087
1636.8868	1638.8535	1642.4878
1654.9146	1658.0114	1658.1746
1660.9977	3030.0090	3030.6848
3031.3848	3031.8053	3034.6389
3034.6610	3035.7990	3037.3185
3037.3938	3038.0699	3038.2994
3038.7694	3043.9080	3045.2671
3046.3657	3046.5283	3056.2381
3092.4461	3093.7640	3094.1111
3095.5059	3096.2957	3098.2135
3099.5553	3099.5740	3100.8105
3101.8196	3103.4107	3104.1459
3104.8688	3105.0684	3105.8954
3108.3001	3109.2098	3109.3174
3109.4809	3112.9643	3127.7045
3128.7810	3137.0072	3139.2405
3146.4630	3155.3738	3157.1105
3157.9518	3159.5321	3169.6450
3173.6201	3176.8181	3181.0802
3181.7607	3183.7404	3183.8931
3185.5008	3190.6789	3194.6501
3195.6743	3198.0213	3198.7422
3208.1413	3210.1584	3215.2458
3226.6399	3227.2928	3232.7192
3248.6959	3249.7421	3276.7240

M3

Zero-point correction= 0.518718

Thermal correction to Energy= 0.548277

Thermal correction to Enthalpy= 0.549221

Thermal correction to Gibbs Free Energy= 0.457006

Sum of electronic and zero-point Energies= -1474.220507

Sum of electronic and thermal Energies= -1474.190949

Sum of electronic and thermal Enthalpies= -1474.190005

Sum of electronic and thermal Free Energies= -1474.282219

Cartesian coordinates

C	-2.196056	1.867643	-1.099276
C	-1.308280	1.027182	-0.510327
H	-1.894052	2.348960	-2.028111
C	-0.034487	0.733620	-1.136813
O	0.456536	1.313669	-2.102861
C	-3.533449	2.171114	-0.621650
C	-4.279075	3.164490	-1.288799
C	-4.125408	1.494775	0.468748
C	-5.568070	3.486063	-0.871735
H	-3.834733	3.683379	-2.133430
C	-5.414265	1.814174	0.876843
H	-3.584225	0.706445	0.981888
C	-6.138164	2.812108	0.210967
H	-6.128838	4.256704	-1.391415
H	-5.862415	1.284442	1.711998
H	-7.145911	3.056909	0.533046
C	0.759012	-0.421934	-0.559216
C	2.409301	-1.763556	-0.041778
C	3.148968	0.405817	-1.024656
H	2.725170	0.980852	-1.845770
N	1.327522	-2.400165	0.332165
N	0.304605	-1.546266	0.014320
N	2.101316	-0.552433	-0.602196

C	3.837704	-2.196053	-0.050246
H	3.904254	-3.283082	0.010709
H	4.380616	-1.758986	0.798685
C	4.451017	-0.370591	-1.481766
O	4.371376	-1.786577	-1.305928
C	4.981009	1.195769	0.308853
C	3.597831	1.273319	0.130742
C	2.802375	2.073784	0.950975
C	3.416436	2.805134	1.969110
C	4.803825	2.734201	2.152388
C	5.593256	1.933283	1.324075
C	5.622848	0.272912	-0.693524
H	1.727103	2.128427	0.805816
H	5.270008	3.307777	2.948196
H	6.668067	1.879695	1.471657
H	6.232861	-0.505435	-0.222944
H	6.280712	0.821352	-1.375983
C	-1.060622	-1.937324	0.273864
C	-1.848329	-2.382088	-0.796421
C	-1.530559	-1.827913	1.591703
C	-3.182129	-2.690803	-0.513855
C	-2.870573	-2.151414	1.815676
C	-3.712463	-2.568735	0.775620
H	-3.820931	-3.031615	-1.323766
H	-3.266243	-2.068635	2.824109
C	-0.639370	-1.338991	2.703729
H	-0.300573	-0.312977	2.515504
H	0.255826	-1.960904	2.802849
H	-1.171790	-1.347560	3.656878
C	-5.172323	-2.839484	1.033995

H	-5.754423	-1.917300	0.910748
H	-5.340437	-3.199046	2.053233
H	-5.574831	-3.576283	0.333047
C	-1.295118	-2.500622	-2.193323
H	-0.304874	-2.967222	-2.196182
H	-1.196555	-1.515871	-2.665486
H	-1.958409	-3.101928	-2.818937
H	4.574934	-0.246225	-2.557074
H	2.816436	3.433542	2.620274
H	-1.543196	0.524609	0.417318

Vibrational frequencies

17.8051	26.0273	31.9314
37.1321	45.9872	52.2193
59.6023	78.8304	82.9641
83.6348	96.4290	117.2010
123.4129	134.3451	153.2143
170.1637	192.7426	195.2652
204.3693	223.9072	226.2485
246.2938	258.1612	275.9044
283.4836	292.9475	296.4095
319.4220	333.8441	353.7385
378.6183	388.2074	410.4135
419.3852	438.6643	449.2911
465.9018	489.2678	492.7046
505.3273	513.8064	522.3911
530.4214	546.8000	573.9553
579.3265	583.0919	598.9353
611.6068	622.0118	628.7547
637.7001	685.0253	696.2985
699.9762	715.5876	736.0735

747.5293	756.0698	766.9418
782.0545	798.7507	801.4266
827.1710	851.3772	858.2276
870.3607	876.0780	877.8037
896.0416	901.3054	909.1687
911.2032	949.5761	949.6957
960.6376	971.0009	975.3064
989.5152	992.5687	1005.5018
1011.0943	1015.3663	1028.1736
1034.2960	1037.8301	1042.2435
1047.1685	1055.1019	1058.1245
1060.0721	1065.3647	1066.3906
1067.3033	1072.5380	1101.5521
1106.1435	1120.6925	1127.3510
1151.0914	1186.1395	1191.3032
1192.2981	1204.0379	1205.8500
1216.8073	1219.7517	1233.0766
1249.0725	1255.0918	1272.1879
1293.3387	1297.1362	1305.5537
1317.8239	1324.5776	1332.3057
1337.9709	1344.2239	1346.2178
1355.6516	1369.8679	1374.5713
1376.6208	1386.4499	1408.2007
1418.1758	1420.7123	1426.1852
1436.6476	1445.4037	1465.4519
1472.4577	1481.2254	1485.7757
1487.1485	1487.3306	1491.5971
1492.9852	1495.2881	1499.5165
1506.3111	1515.3216	1529.9455
1532.0973	1538.0222	1616.3213

1624.8863	1633.2673	1638.9435
1641.0295	1650.8051	1656.8922
1660.0970	1729.5491	3039.7789
3043.0038	3045.9841	3050.5738
3062.6688	3101.0706	3104.2603
3105.6448	3112.1712	3134.3306
3140.5227	3142.3839	3145.4597
3157.9612	3161.1561	3176.2590
3188.0282	3189.4041	3191.0202
3191.3249	3194.9699	3195.7680
3203.4712	3203.5082	3211.1795
3213.5566	3218.1477	3265.4023

pre-TS4

Zero-point correction= 0.729796

Thermal correction to Energy= 0.776665

Thermal correction to Enthalpy= 0.777610

Thermal correction to Gibbs Free Energy= 0.647436

Sum of electronic and zero-point Energies= -5135.065936

Sum of electronic and thermal Energies= -5135.019066

Sum of electronic and thermal Enthalpies= -5135.018122

Sum of electronic and thermal Free Energies= -5135.148296

Cartesian coordinates

C	1.719423	-0.399370	1.262572
C	0.424458	0.005632	1.017156
H	2.393007	0.437848	1.424336
C	-0.784041	-0.735621	0.824944
O	-0.970115	-1.964644	0.777894
C	2.374560	-1.680699	1.476137
C	3.691519	-1.633640	1.990927

C	1.822337	-2.946638	1.179445
C	4.420068	-2.796616	2.213307
H	4.140578	-0.668668	2.205811
C	2.559899	-4.105102	1.396697
H	0.817790	-3.002566	0.783638
C	3.857794	-4.038993	1.913846
H	5.432002	-2.732494	2.601959
H	2.121984	-5.069669	1.155289
H	4.427749	-4.949410	2.076079
C	-2.032370	0.097949	0.646315
C	-4.015610	0.745395	-0.032624
C	-3.380012	-1.500949	-0.863709
H	-2.424236	-1.930247	-1.152265
N	-3.611306	1.699835	0.763318
N	-2.374124	1.278757	1.192226
N	-3.089671	-0.261984	-0.114201
C	-5.201750	0.669087	-0.937448
H	-5.613910	1.665664	-1.102000
H	-5.984785	0.028434	-0.511040
C	-4.230224	-1.170088	-2.148999
O	-4.720319	0.177134	-2.185975
C	-5.361476	-2.846762	-0.794247
C	-4.243885	-2.445935	-0.057452
C	-4.021182	-2.913413	1.237908
C	-4.950890	-3.791981	1.798693
C	-6.074726	-4.197293	1.066592
C	-6.284666	-3.731416	-0.234008
C	-5.372052	-2.219281	-2.165636
H	-3.137314	-2.604480	1.785656
H	-6.790328	-4.880790	1.514741

H	-7.157603	-4.047252	-0.798474
H	-6.324421	-1.738458	-2.412293
H	-5.182277	-2.968434	-2.942524
C	-1.666549	2.062222	2.172144
C	-1.153239	3.307258	1.775351
C	-1.536103	1.555535	3.473889
C	-0.451709	4.041764	2.734334
C	-0.825383	2.334515	4.391769
C	-0.274056	3.572140	4.041618
H	-0.030703	5.002203	2.449186
H	-0.703917	1.963536	5.405870
C	-2.117114	0.224404	3.879690
H	-1.488869	-0.605966	3.537225
H	-3.119279	0.074890	3.465585
H	-2.186035	0.154911	4.967732
C	0.468217	4.401432	5.059490
H	1.276742	4.973084	4.593929
H	0.895930	3.777679	5.849635
H	-0.206049	5.122539	5.538092
C	-1.344292	3.830309	0.376895
H	-2.373595	4.171318	0.221736
H	-1.148353	3.063312	-0.375718
H	-0.674990	4.671168	0.186277
H	-3.583365	-1.239548	-3.021290
H	-4.799986	-4.166161	2.807047
H	0.304183	1.079159	0.945245
C	-0.180974	1.854429	-2.631113
C	0.560491	3.053807	-2.513633
C	0.029430	4.299411	-2.841312
C	-1.292151	4.363816	-3.290068

C	-2.052730	3.191513	-3.405110
C	-1.511307	1.946578	-3.089934
C	0.560928	0.687427	-2.193208
C	1.895255	0.993604	-1.752023
H	0.623907	5.202469	-2.737736
H	-1.727316	5.325482	-3.545305
H	-3.082618	3.250017	-3.746701
H	-2.103193	1.044689	-3.172158
S	2.176211	2.760996	-1.862639
C	0.024980	-0.637929	-2.189775
O	-1.085767	-0.977107	-2.646744
H	0.668292	-1.415959	-1.739876
C	2.847601	0.083067	-1.320720
H	2.575422	-0.952159	-1.475644
C	4.186535	0.275538	-0.813475
C	5.112895	-0.801138	-0.750786
C	4.660517	1.499319	-0.272091
C	6.400886	-0.663722	-0.241844
C	5.944190	1.648193	0.239359
H	3.984024	2.343337	-0.217097
C	6.830988	0.568213	0.251411
H	7.062556	-1.522793	-0.225821
H	6.248441	2.610423	0.641080
H	7.836750	0.673615	0.645678
Br	4.621224	-2.558623	-1.358917

Vibrational frequencies

14.4357	19.6537	23.0486
27.0729	35.3269	40.1539
44.4694	45.5984	48.2282
54.5604	63.8233	66.5387

70.0788	77.0618	77.8486
80.4134	83.2500	93.6516
109.7854	112.1583	118.4695
127.6179	129.0910	136.3237
144.9022	148.1790	165.3908
180.8354	182.6007	188.3774
191.5395	202.2741	207.7009
214.2493	219.0011	221.1245
228.0843	237.2572	238.4549
249.5521	256.2273	289.0913
291.8961	293.1473	306.2613
318.8153	334.5287	338.7447
359.2114	373.1156	380.9677
389.8799	394.6239	405.3800
413.0883	418.8129	427.6091
447.1475	448.2909	449.1735
461.8919	478.3566	492.9414
497.4669	510.5895	514.7915
519.0110	526.8690	530.8660
537.1706	541.8793	543.5430
549.8375	578.6024	583.5005
593.4183	604.7354	609.5446
610.0269	615.2376	618.9373
633.3451	643.2844	664.7589
677.3417	678.7054	697.7550
705.5652	707.9774	717.0567
734.6319	739.9719	743.2865
749.1226	751.7407	758.6610
761.9703	763.9154	766.3030
781.5228	787.4948	798.6598

810.3998	813.1694	824.8795
833.3883	844.0377	858.1168
868.2353	874.6136	875.3006
875.8749	882.6582	901.3328
903.0150	905.5439	906.9137
939.1629	943.7995	949.8461
956.3034	962.7568	973.5563
975.1269	981.8792	984.9587
989.8174	991.5037	992.2929
993.0888	1001.0139	1001.1396
1010.2603	1019.3397	1020.4303
1037.5352	1043.7873	1046.2737
1049.5941	1051.4630	1054.4502
1057.3363	1061.9070	1063.8899
1065.0321	1066.4429	1070.6523
1076.5548	1090.9228	1100.8767
1110.1663	1112.5376	1116.9504
1132.6609	1142.0604	1152.8778
1183.0424	1183.3897	1184.0442
1188.6621	1189.9722	1190.8382
1200.3342	1211.9607	1214.6593
1220.7552	1223.6213	1227.0154
1240.4407	1270.2637	1273.5303
1290.1023	1291.6416	1297.1686
1303.0560	1305.8697	1310.5025
1319.7840	1330.0306	1332.6828
1334.7226	1343.1352	1351.2826
1354.0132	1358.5084	1368.1051
1372.0647	1378.0384	1381.1290
1404.6354	1416.4078	1420.2937

1421.9874	1426.7724	1442.2112
1446.0467	1457.7547	1462.4834
1465.1482	1468.8519	1472.4390
1480.8468	1482.5223	1484.3952
1487.0261	1489.9555	1492.3918
1494.6672	1496.7278	1497.6911
1498.4959	1503.8622	1506.1865
1511.8991	1519.7672	1524.0964
1533.8317	1547.3226	1575.4662
1595.3760	1603.5446	1622.5468
1627.3860	1631.0147	1632.6982
1639.4791	1639.7668	1647.4451
1651.9989	1653.6458	1656.9703
1668.2098	2960.5818	3041.0693
3044.6718	3047.4302	3057.8873
3057.8951	3099.4758	3103.7483
3109.9171	3125.4124	3131.1588
3138.4087	3150.5572	3155.6195
3161.2755	3173.4813	3176.7469
3181.0023	3181.1497	3183.2543
3185.0337	3186.8123	3188.1286
3188.2704	3190.4246	3192.4937
3197.7004	3201.6099	3204.0434
3204.5532	3208.7697	3213.6351
3213.9376	3220.5355	3221.5366
3221.7166	3244.8158	3247.7971

TS4-chemo

Zero-point correction= 0.731006

Thermal correction to Energy= 0.776373

Thermal correction to Enthalpy= 0.777317

Thermal correction to Gibbs Free Energy= 0.652498

Sum of electronic and zero-point Energies= -5135.047208

Sum of electronic and thermal Energies= -5135.001842

Sum of electronic and thermal Enthalpies= -5135.000897

Sum of electronic and thermal Free Energies= -5135.125717

Cartesian coordinates

C	-2.408541	1.451230	-1.061799
C	-1.681232	0.596246	-0.328525
H	-1.991861	1.796610	-2.005908
C	-0.301722	0.171181	-0.712876
O	0.231742	0.570389	-1.812941
C	-3.767854	1.892275	-0.731923
C	-4.620839	2.324066	-1.764136
C	-4.268602	1.875080	0.584727
C	-5.939196	2.694674	-1.497995
H	-4.244310	2.353118	-2.783344
C	-5.584188	2.247312	0.849712
H	-3.616924	1.587490	1.403895
C	-6.428521	2.654059	-0.189552
H	-6.583356	3.017047	-2.311317
H	-5.950855	2.230616	1.872354
H	-7.453082	2.946740	0.021090
C	-0.131753	-1.362712	-0.638961
C	0.782733	-3.334277	-1.052417
C	2.420077	-1.536530	-0.803021
H	2.381355	-0.453030	-0.918322
N	-0.500682	-3.557365	-1.099105
N	-1.064048	-2.320244	-0.831222
N	1.044633	-2.019197	-0.766789
C	1.948093	-4.189147	-1.429233

H	1.602429	-5.101834	-1.916533
H	2.539348	-4.459257	-0.545692
C	3.178768	-2.146213	-2.026088
O	2.713279	-3.457933	-2.392332
C	4.544373	-2.310321	-0.053712
C	3.258025	-1.976303	0.384043
C	2.905164	-2.069078	1.728333
C	3.877288	-2.476394	2.647040
C	5.173519	-2.783843	2.219348
C	5.513891	-2.707944	0.864386
C	4.647472	-2.173059	-1.554386
H	1.896541	-1.852872	2.064488
H	5.918051	-3.100284	2.944070
H	6.514389	-2.969978	0.531891
H	5.196778	-2.985182	-2.037963
H	5.137372	-1.229142	-1.826088
C	-2.496778	-2.186930	-0.944503
C	-3.011994	-1.653606	-2.142172
C	-3.314120	-2.620722	0.103852
C	-4.388705	-1.453432	-2.212863
C	-4.692230	-2.392099	-0.018999
C	-5.241594	-1.788737	-1.150143
H	-4.809688	-1.018932	-3.115586
H	-5.343750	-2.701094	0.794424
C	-2.793717	-3.367191	1.305511
H	-1.705737	-3.424105	1.331307
H	-3.175268	-4.394413	1.289025
H	-3.138198	-2.904945	2.234337
C	-6.715082	-1.483504	-1.238716
H	-6.884257	-0.403139	-1.155793

H	-7.278487	-1.973897	-0.440112
H	-7.130924	-1.801935	-2.200654
C	-2.111762	-1.319095	-3.302907
H	-1.524462	-2.195297	-3.602061
H	-1.400493	-0.525325	-3.053494
H	-2.701218	-0.995573	-4.163978
H	3.031481	-1.531022	-2.915752
H	3.620455	-2.557471	3.698950
H	-2.085470	0.163959	0.578628
C	3.210141	3.135670	-1.029728
C	4.209028	2.545563	-0.219366
C	5.564468	2.859484	-0.357809
C	5.928837	3.785071	-1.331229
C	4.953860	4.383156	-2.148957
C	3.606993	4.068394	-2.007826
C	1.878759	2.653650	-0.699874
C	1.869949	1.711127	0.313858
H	6.311837	2.393165	0.276859
H	6.975732	4.044289	-1.458962
H	5.258221	5.101087	-2.905078
H	2.853400	4.520750	-2.639448
S	3.505342	1.416443	0.925713
C	0.650626	3.125032	-1.352932
O	0.626000	3.851863	-2.342577
H	-0.284026	2.844117	-0.850024
C	0.769330	0.912142	0.883716
H	1.173189	0.011186	1.338522
C	-0.124161	1.585129	1.867015
C	-0.880881	0.846546	2.797288
C	-0.285650	2.983483	1.938118

C	-1.757977	1.424151	3.710034
C	-1.156049	3.586476	2.842320
H	0.297655	3.610962	1.274776
C	-1.901591	2.811888	3.732301
H	-2.321293	0.798310	4.393219
H	-1.247586	4.668444	2.851509
H	-2.584332	3.273433	4.438528
Br	-0.788158	-1.080979	2.781306

Vibrational frequencies

-161.6671	23.2332	26.4945
28.6141	31.2201	31.7963
43.2394	49.7830	54.1062
58.7069	64.6730	65.1990
72.6173	76.6207	78.1561
88.3094	98.7834	102.0016
104.4320	116.5568	121.4497
129.8786	133.5467	141.7800
147.6420	156.8729	159.3802
173.2594	178.4152	198.8646
207.4934	210.7025	216.3368
220.9298	228.4192	233.6515
246.2330	256.0511	265.5962
277.7013	286.5715	293.5261
303.3458	317.7212	335.6111
337.5892	347.5177	348.9263
362.4579	370.2113	376.8178
383.4627	403.0403	407.9574
418.4706	424.3718	433.0350
438.9503	445.7894	451.2359
464.9117	473.4104	496.4618

499.6691	503.1572	512.7852
514.1578	519.6006	525.5987
529.3716	534.4400	539.9842
557.6232	566.1107	580.4611
590.6845	601.7530	603.9040
611.7645	622.0084	626.2801
632.1675	644.6668	665.2596
679.3994	698.1619	711.4967
712.3264	716.0171	732.1261
735.1910	741.5919	744.2370
748.6722	755.6947	763.9506
767.8055	769.9579	774.4032
775.7765	787.3055	793.6345
826.0388	838.3907	843.9634
861.1707	870.6125	874.6169
876.6024	879.0710	882.8357
888.5363	896.0702	903.8360
905.4102	914.8875	940.2964
951.3292	959.5129	959.9270
964.3571	971.0338	979.8499
985.9177	987.0981	988.4224
998.3840	999.5802	1002.4346
1011.6812	1017.7470	1028.1592
1029.4138	1034.4411	1036.3757
1041.3933	1042.6897	1045.6013
1048.0194	1049.4952	1053.4675
1054.9373	1056.3406	1058.7261
1064.3107	1071.3110	1075.1197
1076.6114	1082.7455	1085.7552
1091.9671	1095.9247	1110.2805

1117.1559	1142.7587	1151.6202
1178.2495	1179.2034	1183.1212
1185.1742	1190.3108	1192.5822
1195.5801	1203.8438	1209.8513
1219.3082	1232.2175	1239.2150
1240.5951	1245.6010	1272.6541
1288.4416	1293.8477	1294.8422
1298.4454	1303.9067	1305.2239
1312.5413	1321.1129	1328.6085
1335.5962	1342.0575	1348.8291
1354.2310	1357.8894	1360.6863
1364.0262	1368.2153	1372.1359
1381.2697	1408.0226	1412.9518
1417.7039	1421.0642	1424.2053
1430.3435	1437.7667	1450.0393
1451.8741	1466.4694	1470.4821
1472.2488	1474.2391	1481.4455
1483.6020	1484.9302	1491.1793
1494.5240	1495.1377	1496.9324
1498.4624	1499.2612	1499.9114
1506.8834	1507.1588	1521.6983
1527.6908	1534.8533	1549.8414
1606.1861	1607.4823	1624.2614
1638.2055	1640.6158	1641.7157
1641.7852	1646.4208	1653.7066
1654.4079	1660.8300	1704.0343
1732.9926	3041.4063	3041.7911
3048.1348	3051.0826	3056.1355
3058.4473	3102.4817	3105.5515
3116.3676	3116.8999	3119.1485

3129.4209	3136.9574	3140.0791
3153.7280	3163.7859	3169.8387
3171.4886	3177.7713	3180.5468
3183.2647	3183.7307	3186.4460
3187.1634	3192.7650	3194.2561
3196.3506	3197.6753	3201.1048
3206.2965	3207.3766	3208.5550
3209.5097	3215.5607	3218.8892
3221.7902	3223.3704	3242.9124

M4-chemo

Zero-point correction= 0.732516

Thermal correction to Energy= 0.777999

Thermal correction to Enthalpy= 0.778943

Thermal correction to Gibbs Free Energy= 0.653582

Sum of electronic and zero-point Energies= -5135.049375

Sum of electronic and thermal Energies= -5135.003892

Sum of electronic and thermal Enthalpies= -5135.002948

Sum of electronic and thermal Free Energies= -5135.128309

Cartesian coordinates

C	-2.436995	1.448752	-0.978851
C	-1.704913	0.661219	-0.184734
H	-2.010703	1.732022	-1.938786
C	-0.286047	0.233706	-0.534862
O	0.142243	0.526002	-1.760081
C	-3.806994	1.898130	-0.698993
C	-4.626335	2.306485	-1.766774
C	-4.349819	1.914266	0.600545
C	-5.950858	2.688876	-1.551919
H	-4.218331	2.307640	-2.774243

C	-5.671838	2.296451	0.815256
H	-3.727372	1.638556	1.446409
C	-6.481389	2.681732	-0.259326
H	-6.567725	2.992745	-2.393037
H	-6.071895	2.302674	1.825444
H	-7.511039	2.982265	-0.088142
C	-0.212607	-1.328329	-0.529644
C	0.609324	-3.328264	-1.016783
C	2.322957	-1.598911	-0.818621
H	2.311619	-0.516945	-0.953617
N	-0.681480	-3.495786	-1.041332
N	-1.187254	-2.241378	-0.722651
N	0.934832	-2.033981	-0.704697
C	1.724524	-4.228616	-1.433167
H	1.327410	-5.127564	-1.906610
H	2.332351	-4.521685	-0.567966
C	3.002964	-2.233023	-2.075430
O	2.489864	-3.531700	-2.420295
C	4.464656	-2.411326	-0.170312
C	3.210821	-2.041088	0.328252
C	2.928644	-2.098807	1.690972
C	3.938861	-2.511785	2.565002
C	5.202672	-2.859092	2.075171
C	5.472284	-2.815164	0.702942
C	4.492910	-2.296727	-1.676328
H	1.945816	-1.848948	2.076531
H	5.977325	-3.180019	2.765534
H	6.447890	-3.105667	0.323357
H	4.993566	-3.130449	-2.175716
H	4.995185	-1.371269	-1.985989

C	-2.617121	-2.070497	-0.821602
C	-3.128823	-1.581568	-2.039708
C	-3.436908	-2.459627	0.240942
C	-4.505666	-1.391541	-2.125447
C	-4.816651	-2.246399	0.101583
C	-5.363687	-1.696627	-1.057113
H	-4.923692	-0.991466	-3.045338
H	-5.470164	-2.525447	0.924342
C	-2.914889	-3.126545	1.487867
H	-1.838558	-3.297779	1.454271
H	-3.402097	-4.098881	1.617852
H	-3.139951	-2.529234	2.375968
C	-6.840189	-1.414185	-1.169817
H	-7.025008	-0.334305	-1.122053
H	-7.405646	-1.887645	-0.362373
H	-7.241786	-1.767713	-2.125592
C	-2.219009	-1.283739	-3.202303
H	-1.703606	-2.195143	-3.529533
H	-1.445795	-0.554608	-2.933083
H	-2.790553	-0.895899	-4.049134
H	2.828689	-1.611655	-2.956024
H	3.737085	-2.566274	3.630515
H	-2.109399	0.289056	0.750368
C	3.289363	2.977640	-1.171594
C	4.221755	2.488870	-0.224846
C	5.573078	2.848631	-0.255096
C	5.999887	3.713718	-1.257514
C	5.091369	4.210262	-2.209949
C	3.749339	3.851762	-2.175878
C	1.946800	2.479004	-0.926605

C	1.879019	1.614471	0.139754
H	6.269810	2.462145	0.482311
H	7.045020	4.005127	-1.303898
H	5.445555	4.882675	-2.985872
H	3.047397	4.224395	-2.911179
S	3.447135	1.411195	0.923351
C	0.760663	2.903804	-1.702984
O	0.824038	3.424594	-2.811882
H	-0.194643	2.850072	-1.162645
C	0.718883	0.835574	0.695758
H	1.142537	-0.035956	1.195685
C	-0.013205	1.604318	1.786932
C	-0.638420	0.944105	2.855700
C	-0.100691	3.005539	1.793921
C	-1.324054	1.610117	3.868648
C	-0.782186	3.696923	2.793347
H	0.383218	3.563621	1.001018
C	-1.394652	3.002598	3.837015
H	-1.795015	1.050090	4.668644
H	-0.829680	4.780803	2.755977
H	-1.924370	3.532153	4.622561
Br	-0.657440	-0.982980	2.906823

Vibrational frequencies

20.3719	25.2071	26.9594
30.4425	31.4979	39.1020
43.3325	52.6693	57.0432
60.0887	64.8594	69.9307
74.6652	85.9552	95.7934
99.0846	109.5752	109.7203
115.1076	125.2102	129.0652

135.9166	143.3899	147.5604
156.5398	160.6104	168.4419
178.7074	194.2252	209.8581
212.0111	217.3433	218.9803
223.1878	239.7522	250.9539
251.7847	262.2434	277.1630
281.8830	291.9425	301.6864
321.8364	328.8124	336.7764
347.6970	351.9191	361.7442
370.5008	372.7429	378.6153
401.0106	408.2297	418.6436
422.4009	434.6435	439.2480
444.5534	459.0013	467.4281
479.3608	496.1473	497.8849
504.0015	512.3672	513.9079
515.2648	521.5862	527.2732
529.9565	542.3117	547.5646
563.9546	580.6673	589.7027
598.8779	604.2048	613.3010
625.9934	629.1868	630.9477
634.6869	650.5184	681.7578
695.8760	710.2116	711.2834
713.1693	723.7402	736.0423
740.3840	743.5389	745.3939
754.9334	758.9744	764.8632
769.9481	773.7583	779.2774
787.4053	794.7504	801.0323
823.9627	835.7181	842.5394
861.0377	874.4037	877.6204
879.5715	880.7508	890.7392

893.7927	904.5791	905.8071
915.0558	927.4305	946.2573
953.6271	960.9170	965.1036
968.9509	972.7488	979.9061
983.8765	985.9592	987.6060
999.6062	1002.4457	1007.5395
1011.6406	1021.6719	1025.9165
1028.3646	1033.9872	1035.9448
1040.7452	1045.7177	1046.9837
1049.6690	1053.1410	1054.8813
1055.7010	1059.1119	1062.9271
1068.1739	1071.6520	1074.9352
1076.9457	1081.3270	1085.9904
1095.4914	1111.1684	1117.5653
1140.5861	1150.5238	1174.6127
1178.4605	1182.4397	1185.7253
1190.0316	1192.7262	1194.7923
1202.1044	1210.8030	1213.5743
1219.1379	1226.1301	1227.5315
1236.6215	1241.3785	1261.9786
1264.9601	1290.3710	1292.7851
1293.4596	1299.1425	1302.7903
1311.2331	1314.2153	1319.1335
1323.8283	1342.1480	1347.0055
1348.7001	1354.0576	1357.9953
1360.9905	1361.9716	1366.3918
1372.1413	1378.4112	1383.8017
1410.5037	1421.2609	1424.9056
1431.0649	1435.5191	1451.0603
1459.5116	1465.6249	1469.4212

1473.4277	1476.0589	1478.7507
1482.3956	1485.4566	1487.8359
1493.1125	1493.8980	1496.8554
1499.2445	1500.4426	1503.0198
1507.6434	1516.8277	1522.1217
1531.1591	1535.9720	1570.6923
1608.3960	1615.8263	1625.7285
1640.5601	1640.9399	1642.6337
1642.9851	1650.2909	1654.5271
1655.3943	1661.3359	1721.0363
1735.8079	3024.8650	3041.8705
3044.7375	3048.6389	3050.1923
3057.3001	3087.8302	3102.5996
3102.9106	3115.1306	3116.5228
3116.7527	3128.3350	3131.0741
3132.9858	3153.5674	3162.2055
3173.6764	3177.6446	3179.2084
3182.4514	3183.1738	3186.6271
3187.9691	3191.7391	3196.1729
3197.0056	3198.5396	3198.6887
3204.5344	3206.6828	3208.2320
3209.8538	3210.5623	3215.7956
3222.3685	3226.8365	3239.1568

TS4RR

Zero-point correction= 0.729632

Thermal correction to Energy= 0.775826

Thermal correction to Enthalpy= 0.776770

Thermal correction to Gibbs Free Energy= 0.647751

Sum of electronic and zero-point Energies= -5135.061044

Sum of electronic and thermal Energies= -5135.014849

Sum of electronic and thermal Enthalpies= -5135.013905

Sum of electronic and thermal Free Energies= -5135.142924

Cartesian coordinates

C	1.505441	0.120908	-1.266853
C	0.535363	0.970172	-0.706949
H	1.115277	-0.663273	-1.907504
C	-0.816447	0.570583	-0.725496
O	-1.242307	-0.575908	-1.018149
C	2.855666	0.603185	-1.599119
C	3.561305	0.008737	-2.660748
C	3.493759	1.617211	-0.858055
C	4.862010	0.405129	-2.966703
H	3.084224	-0.777456	-3.238009
C	4.792014	2.012487	-1.166032
H	2.975743	2.087696	-0.027881
C	5.484723	1.405474	-2.218926
H	5.391776	-0.075165	-3.784524
H	5.269758	2.792155	-0.579038
H	6.500742	1.711077	-2.452011
C	-1.876317	1.620608	-0.504890
C	-3.842004	2.615577	-0.547575
C	-3.889443	0.326597	-1.490287
H	-3.149525	-0.233028	-2.057279
N	-3.040683	3.494306	-0.009955
N	-1.817764	2.862908	0.014360
N	-3.175235	1.463602	-0.871601
C	-5.269444	2.739681	-0.962127
H	-5.569514	3.788208	-0.976903
H	-5.927972	2.191469	-0.274852
C	-5.062559	0.839804	-2.417377

O	-5.340144	2.238566	-2.295000
C	-5.915595	-0.730534	-0.764240
C	-4.568277	-0.536673	-0.450036
C	-3.996934	-1.101296	0.689758
C	-4.810839	-1.862005	1.532250
C	-6.163987	-2.057854	1.226683
C	-6.723900	-1.498854	0.075020
C	-6.286248	-0.040629	-2.052115
H	-2.944043	-0.956886	0.907552
H	-6.784301	-2.651272	1.892568
H	-7.773539	-1.653092	-0.159743
H	-7.183680	0.580856	-1.968563
H	-6.475508	-0.770197	-2.847846
C	-0.701388	3.563637	0.593479
C	0.104956	4.347218	-0.243085
C	-0.495248	3.436241	1.972202
C	1.193117	4.993144	0.350001
C	0.605724	4.102501	2.514719
C	1.462547	4.873564	1.719868
H	1.846370	5.598376	-0.272757
H	0.806235	3.998823	3.576177
C	-1.423579	2.600716	2.811944
H	-1.391723	1.552499	2.501337
H	-2.458924	2.945256	2.712651
H	-1.139713	2.642713	3.863640
C	2.673244	5.535268	2.329488
H	3.469990	4.799804	2.496489
H	2.438420	5.979853	3.301952
H	3.075239	6.318426	1.680547
C	-0.165158	4.437987	-1.722043

H	-1.207227	4.706334	-1.924876
H	0.024275	3.473225	-2.207336
H	0.480309	5.184432	-2.190312
H	-4.776274	0.719433	-3.462461
H	-4.387205	-2.303948	2.427484
H	0.809113	1.944175	-0.334388
C	-1.022036	-3.366459	1.001297
C	-0.470325	-4.459717	0.292167
C	-1.126722	-5.686861	0.185554
C	-2.369905	-5.830830	0.802682
C	-2.937670	-4.759904	1.510420
C	-2.277410	-3.538439	1.616838
C	-0.153983	-2.201920	0.981119
C	1.054987	-2.420591	0.287135
H	-0.680645	-6.510977	-0.362731
H	-2.896256	-6.778245	0.733410
H	-3.904666	-4.887046	1.988882
H	-2.701761	-2.715402	2.175948
S	1.113664	-4.072008	-0.369633
C	-0.441114	-0.968859	1.680821
O	-1.429453	-0.766489	2.395790
H	0.310812	-0.167188	1.565905
C	2.128431	-1.493725	0.169253
H	2.151392	-0.777458	0.978601
C	3.451247	-1.814966	-0.369028
C	4.645109	-1.351517	0.228311
C	3.605824	-2.510171	-1.591123
C	5.902942	-1.602318	-0.316880
C	4.854828	-2.773250	-2.143952
H	2.712649	-2.807553	-2.130543

C	6.013255	-2.325709	-1.504044
H	6.789153	-1.229527	0.184677
H	4.922114	-3.312676	-3.084040
H	6.993672	-2.522292	-1.926700
Br	4.594795	-0.310434	1.844740

Vibrational frequencies

-208.4712	12.3533	15.5716
25.7476	31.2357	36.0742
38.9353	43.3858	45.6665
49.0167	53.0701	60.1046
65.9028	69.3479	74.2338
80.9014	86.1605	89.7997
94.2784	104.7530	111.8474
123.1257	132.4763	136.0614
142.1808	146.6741	155.1901
156.1016	166.8213	184.4289
190.3323	198.7156	207.3432
214.2347	219.7081	228.9541
237.8209	242.3138	244.8777
251.4898	262.0551	281.1620
289.2122	293.2424	298.9356
317.1074	321.9802	338.3769
352.9727	365.1348	379.5869
387.7554	394.8334	403.8347
416.8073	425.0893	431.5293
446.3680	448.7096	450.2528
459.0370	474.0542	491.9508
502.8251	510.6432	515.0915
525.7786	528.5518	533.0460
539.4535	542.2291	546.3143

569.4488	581.6274	584.1235
593.8291	600.8926	606.1971
615.7412	617.5036	631.1695
633.1128	641.5175	667.7693
684.2557	698.0839	701.9906
708.5458	710.7353	715.7935
731.7656	736.4076	743.2846
752.2536	754.2961	759.6688
765.4402	766.8630	770.0360
774.7041	785.7582	789.4175
801.6853	812.0792	828.0516
846.1580	865.0100	868.8701
871.0297	872.3680	878.7759
882.6378	886.8982	902.1987
905.8908	909.5029	928.5141
943.3534	948.2570	950.6204
954.4387	959.0205	976.2974
978.8577	985.1724	988.9195
992.0617	993.1580	1007.7426
1008.0156	1010.4287	1013.3495
1016.3800	1033.2165	1037.2643
1040.5824	1047.6241	1050.4366
1052.2465	1053.7676	1057.1522
1058.4114	1061.3919	1064.6418
1067.3714	1069.3916	1070.5137
1080.6212	1085.6666	1099.1163
1110.3563	1112.8942	1116.2761
1141.5721	1154.5037	1156.3352
1180.9569	1184.0949	1186.5932
1186.9083	1192.9453	1193.1948

1202.2388	1213.6224	1214.6268
1218.1539	1223.6103	1234.8494
1244.1337	1272.9329	1273.9313
1278.5053	1288.9818	1291.3018
1296.9663	1301.1264	1309.4597
1321.3927	1327.7819	1329.5249
1332.1652	1337.7676	1343.9877
1350.5510	1362.1545	1368.1339
1369.0945	1375.9164	1380.6343
1382.7816	1402.9792	1406.6096
1415.8835	1421.4404	1426.1430
1438.4181	1447.7323	1450.0784
1458.9884	1468.8655	1469.2085
1471.8233	1478.2842	1480.9989
1481.8651	1484.2883	1487.6676
1490.0845	1494.2153	1496.6509
1496.9096	1503.5297	1504.3693
1507.8074	1520.4757	1528.2190
1533.2702	1536.2396	1558.8454
1602.3989	1606.3026	1613.2516
1629.2259	1635.5560	1636.8408
1639.1513	1639.8519	1640.7820
1652.8111	1653.1123	1656.9409
1702.3797	2952.0394	3041.3236
3046.5049	3048.2611	3048.9185
3059.4297	3100.6152	3101.6475
3106.9062	3113.5564	3128.9716
3132.4101	3142.2330	3143.6950
3152.0319	3155.4733	3178.9408
3182.2832	3182.3001	3183.1596

3185.6131	3189.5564	3190.0811
3193.7079	3193.8854	3194.9949
3198.9868	3205.0731	3205.5341
3206.6926	3207.3932	3213.0499
3219.5944	3219.9724	3224.1151
3241.0830	3244.5122	3254.7340

TS4RS

Zero-point correction= 0.729640

Thermal correction to Energy= 0.775720

Thermal correction to Enthalpy= 0.776664

Thermal correction to Gibbs Free Energy= 0.648864

Sum of electronic and zero-point Energies= -5135.060256

Sum of electronic and thermal Energies= -5135.014176

Sum of electronic and thermal Enthalpies= -5135.013232

Sum of electronic and thermal Free Energies= -5135.141032

Cartesian coordinates

C	1.398079	0.590294	-0.915956
C	0.048353	0.885403	-0.725213
H	1.624456	-0.395660	-1.304628
C	-0.932002	-0.127773	-0.800222
O	-0.720213	-1.364764	-0.873042
C	2.396560	1.628773	-1.193402
C	3.539985	1.294843	-1.944286
C	2.249004	2.962728	-0.760497
C	4.491454	2.260595	-2.270438
H	3.672893	0.269223	-2.275460
C	3.203708	3.923220	-1.081555
H	1.398410	3.238626	-0.148608
C	4.326740	3.579751	-1.843106
H	5.362647	1.980943	-2.855920

H	3.073284	4.945245	-0.736352
H	5.067470	4.333231	-2.094732
C	-2.375732	0.292433	-0.904473
C	-4.547805	0.184130	-1.257144
C	-3.410343	-2.019141	-1.456575
H	-2.444321	-2.260813	-1.891613
N	-4.317603	1.444263	-1.006674
N	-2.962801	1.501921	-0.782288
N	-3.395653	-0.555728	-1.209156
C	-5.806398	-0.482892	-1.697532
H	-6.521363	0.259183	-2.055164
H	-6.262346	-1.045346	-0.871460
C	-4.598103	-2.412841	-2.427293
O	-5.449974	-1.323568	-2.791313
C	-4.764931	-3.657431	-0.338361
C	-3.666947	-2.806299	-0.189659
C	-2.939136	-2.762193	0.999876
C	-3.343965	-3.578188	2.057874
C	-4.450902	-4.425872	1.920647
C	-5.164161	-4.474936	0.720800
C	-5.364887	-3.560570	-1.716345
H	-2.069689	-2.121640	1.092828
H	-4.753474	-5.054689	2.753237
H	-6.017914	-5.138229	0.612846
H	-6.438447	-3.342931	-1.699575
H	-5.241033	-4.498263	-2.268945
C	-2.388538	2.785747	-0.468715
C	-1.896876	3.573255	-1.520836
C	-2.366438	3.186297	0.870537
C	-1.331224	4.803133	-1.182200

C	-1.794482	4.430561	1.155530
C	-1.266008	5.243776	0.147732
H	-0.925636	5.428778	-1.972874
H	-1.752058	4.761935	2.189171
C	-2.915303	2.290830	1.947984
H	-2.410372	1.320499	1.942298
H	-3.984126	2.102677	1.796741
H	-2.779558	2.738430	2.934210
C	-0.597865	6.554597	0.479567
H	-0.850146	7.328286	-0.252529
H	0.493612	6.443185	0.467992
H	-0.883092	6.912496	1.472703
C	-1.919422	3.071791	-2.939747
H	-2.917968	2.728966	-3.230553
H	-1.235167	2.222497	-3.053104
H	-1.606499	3.854100	-3.634550
H	-4.176593	-2.744279	-3.376323
H	-2.789692	-3.559328	2.990440
H	-0.257808	1.904978	-0.565186
C	4.773652	-2.617082	-0.566110
C	5.765248	-1.684790	-0.173615
C	7.115477	-1.851471	-0.487189
C	7.492715	-2.982966	-1.208850
C	6.528173	-3.920931	-1.610778
C	5.182286	-3.748265	-1.299992
C	3.435634	-2.218270	-0.159346
C	3.417602	-1.015758	0.574442
H	7.853420	-1.118359	-0.175405
H	8.538195	-3.135968	-1.459988
H	6.836272	-4.797080	-2.174538

H	4.435244	-4.465889	-1.613051
S	5.056663	-0.350785	0.726214
C	2.224751	-2.881415	-0.612471
O	2.196188	-3.940994	-1.249676
H	1.279257	-2.363307	-0.382157
C	2.369909	-0.224389	1.132979
H	2.676459	0.783857	1.393250
C	1.271679	-0.708746	1.957120
C	0.368276	0.186346	2.582713
C	1.082093	-2.075143	2.284640
C	-0.644506	-0.234885	3.445368
C	0.071799	-2.509654	3.129444
H	1.777343	-2.803621	1.885377
C	-0.809064	-1.591207	3.712889
H	-1.290311	0.499134	3.913526
H	-0.021271	-3.569351	3.347501
H	-1.599166	-1.919648	4.380310
Br	0.571658	2.093135	2.382586

Vibrational frequencies

-118.6718	20.7338	24.8197
25.6552	28.6827	35.8550
38.0595	45.7290	47.5293
49.1991	54.3490	61.5773
63.4537	71.1424	77.1457
83.5250	84.7155	87.6446
97.9962	104.2413	118.2816
122.8600	125.8662	141.6085
141.7645	152.2275	154.1553
158.5384	178.8342	185.3630
193.7447	199.1519	209.0227

214.4779	218.0379	218.8017
239.3537	244.7380	257.4138
264.0514	279.4398	286.7929
289.3956	296.9223	310.8244
320.3758	323.9084	339.2756
356.3478	367.5755	381.6853
387.8100	389.7662	392.3995
410.5457	417.3436	435.0274
445.6087	449.4309	453.2823
462.6181	476.9879	492.4936
500.0238	508.7197	514.9375
522.6648	527.1303	530.4862
531.3779	537.5070	555.3021
555.3469	569.8566	583.4582
588.0658	598.9240	605.1041
609.9985	620.6238	631.6145
635.3790	645.4598	661.0121
671.9487	683.6975	694.7100
703.4964	708.6411	713.8613
729.7053	735.9681	746.7015
750.2320	752.6230	761.5269
764.8833	767.8660	772.4992
772.7791	781.8198	794.8147
801.0277	826.1684	831.2306
850.2887	851.8049	857.1328
870.6189	873.0815	879.4369
880.6883	882.3592	900.2147
903.2578	908.5753	918.4219
921.3524	948.9962	952.9565
960.3231	962.4445	972.3472

973.1496	977.1200	992.6980
996.9628	997.6017	999.4293
1003.3292	1007.5124	1013.6772
1021.6823	1037.2524	1039.4484
1041.5045	1045.1231	1047.0740
1053.5013	1054.5499	1055.1575
1057.0700	1058.2144	1060.2005
1065.4490	1067.8641	1075.2521
1076.6818	1090.9147	1102.5982
1107.1679	1112.5675	1121.6874
1144.7749	1150.9400	1153.3350
1180.9588	1183.7898	1185.5502
1185.8029	1192.4031	1195.6761
1199.8087	1201.6191	1212.2075
1213.6534	1223.3704	1239.9193
1243.1220	1254.3234	1274.7642
1286.4144	1288.4653	1291.0772
1295.3001	1305.0932	1310.8796
1317.1567	1326.9574	1328.2293
1331.0781	1337.5310	1344.0105
1347.6882	1357.5910	1366.9726
1367.1924	1369.8103	1379.1301
1382.5598	1408.5786	1415.5715
1419.2056	1425.1023	1426.3383
1436.6434	1447.4543	1448.8428
1455.2781	1469.2088	1471.5146
1472.1712	1475.2158	1481.0943
1482.8437	1486.8319	1488.3216
1492.4397	1493.4454	1494.6432
1496.3126	1498.8972	1507.7500

1510.2318	1513.8093	1520.5918
1526.2099	1533.6522	1570.0199
1593.9875	1604.2718	1608.3527
1628.1144	1633.5016	1635.6009
1638.0356	1640.5177	1641.6640
1651.8555	1654.1201	1657.7457
1692.8628	3019.9613	3040.6556
3043.5648	3044.4588	3051.6470
3058.1872	3095.2991	3101.8199
3105.9039	3115.2192	3131.4513
3131.9794	3142.5224	3149.6223
3155.4919	3171.7788	3173.5647
3180.3159	3183.2067	3184.0055
3184.8983	3188.1440	3191.4465
3192.1824	3193.2916	3198.1016
3198.4620	3205.9064	3206.4779
3207.6041	3212.3427	3214.2885
3219.5819	3220.4311	3225.3239
3226.6464	3243.9319	3295.0148

TS4SR

Zero-point correction= 0.729078

Thermal correction to Energy= 0.775532

Thermal correction to Enthalpy= 0.776476

Thermal correction to Gibbs Free Energy= 0.646500

Sum of electronic and zero-point Energies= -5135.064743

Sum of electronic and thermal Energies= -5135.018289

Sum of electronic and thermal Enthalpies= -5135.017345

Sum of electronic and thermal Free Energies= -5135.147321

Cartesian coordinates

C	-1.374471	0.242145	-0.567843

C	-0.070459	0.725080	-0.306302
H	-1.411641	-0.633307	-1.211193
C	1.060980	-0.047459	-0.590776
O	1.114100	-1.224357	-1.041015
C	-2.499328	1.182827	-0.720404
C	-3.517996	0.908564	-1.649173
C	-2.606276	2.349907	0.061690
C	-4.592386	1.783670	-1.815476
H	-3.461699	0.001942	-2.244561
C	-3.678653	3.222164	-0.103564
H	-1.863680	2.547499	0.827396
C	-4.675175	2.945699	-1.047174
H	-5.369633	1.549346	-2.537047
H	-3.745891	4.113579	0.513782
H	-5.513764	3.624737	-1.170036
C	2.394373	0.608084	-0.342408
C	4.538635	0.864332	0.076638
C	3.775955	-1.496097	0.174104
H	2.826861	-1.940009	0.469878
N	4.105903	2.072512	-0.166538
N	2.765806	1.897617	-0.439929
N	3.529045	-0.057475	-0.029104
C	5.857421	0.383193	0.583341
H	6.438229	1.215597	0.982698
H	6.435624	-0.102753	-0.213230
C	4.879559	-1.707556	1.283370
O	5.564922	-0.506827	1.660281
C	5.509830	-2.864573	-0.761978
C	4.348183	-2.150452	-1.065234
C	3.839269	-2.103980	-2.362895

C	4.529110	-2.780310	-3.371464
C	5.698264	-3.494556	-3.077014
C	6.193066	-3.545530	-1.771109
C	5.838051	-2.781546	0.707170
H	2.919446	-1.564863	-2.562272
H	6.224712	-4.014984	-3.872126
H	7.098771	-4.101726	-1.545579
H	6.877865	-2.502491	0.905181
H	5.665162	-3.743941	1.202587
C	1.946333	3.031484	-0.779656
C	1.559426	3.897881	0.254312
C	1.530189	3.185493	-2.108325
C	0.689473	4.938633	-0.078257
C	0.658149	4.242813	-2.385314
C	0.214525	5.114200	-1.384558
H	0.360773	5.616400	0.705114
H	0.309396	4.378349	-3.405518
C	1.961505	2.226195	-3.187133
H	1.392416	1.291053	-3.125309
H	3.022674	1.970724	-3.103419
H	1.789070	2.655915	-4.176683
C	-0.791060	6.194636	-1.692300
H	-1.807366	5.832480	-1.491574
H	-0.751882	6.495752	-2.743047
H	-0.631930	7.081097	-1.070850
C	2.014471	3.674098	1.672955
H	3.105476	3.640919	1.748055
H	1.628630	2.723630	2.057076
H	1.647951	4.469677	2.325919
H	4.405004	-2.038695	2.206964

H	4.154589	-2.756190	-4.390662
H	0.057617	1.711516	0.109906
C	-5.394435	-1.952961	-0.271607
C	-4.703217	-3.020013	-0.889495
C	-5.334026	-3.935799	-1.732964
C	-6.697086	-3.775939	-1.977099
C	-7.405297	-2.720661	-1.379999
C	-6.771355	-1.814518	-0.534837
C	-4.528840	-1.149026	0.572466
C	-3.193887	-1.592105	0.590816
H	-4.777696	-4.748050	-2.190895
H	-7.209922	-4.471949	-2.634236
H	-8.467005	-2.608435	-1.580884
H	-7.314210	-0.998669	-0.075920
S	-2.997545	-3.016525	-0.451030
C	-4.991843	-0.003918	1.336050
O	-6.125628	0.476484	1.280200
H	-4.253447	0.444667	2.026252
C	-2.082969	-0.884272	1.157920
H	-2.406596	0.003444	1.685090
C	-0.871714	-1.455769	1.753150
C	-0.025828	-0.659670	2.563144
C	-0.432922	-2.785370	1.561647
C	1.157251	-1.134093	3.129518
C	0.740279	-3.277009	2.118622
H	-1.038849	-3.461728	0.973029
C	1.549989	-2.451185	2.904050
H	1.757982	-0.479332	3.750921
H	1.021284	-4.310860	1.942022
H	2.465397	-2.827190	3.349778

Br -0.523480 1.143711 3.050100

Vibrational frequencies

-222.4169	12.4502	19.5133
25.2670	27.8998	31.6972
37.9942	43.8131	44.3278
49.7673	53.7133	56.8564
63.2406	66.6486	72.0944
75.9576	77.4647	83.6505
94.5022	103.7145	109.0850
125.5546	128.8235	132.6946
138.8823	147.5881	152.0086
155.8981	157.7786	166.6051
177.9965	193.3379	203.8578
213.3960	221.6703	223.5092
227.7584	230.4832	235.6516
254.9551	262.1841	278.8998
286.2440	293.2369	309.4579
319.4811	327.1002	331.2845
353.0714	366.9527	375.2918
389.4962	396.5405	403.9321
409.5478	417.5078	429.2377
442.2737	445.5403	449.0725
453.4591	479.9078	494.0215
501.7242	508.7848	513.0900
525.3894	529.3899	533.1532
536.8834	544.7156	547.7443
559.3308	577.8189	581.2701
588.3054	599.8222	606.9182
616.9897	619.8376	631.1834
640.0170	642.9765	669.4476

673.0015 696.4839 703.3488

706.8808 708.8646 717.5470

729.7980 730.7078 744.5665

746.1768 748.0216 757.9146

765.2733 769.8609 770.5310

772.3626 782.9204 790.1717

799.7088 809.1517 828.7658

846.8704 855.2283 868.0667

870.7781 875.7037 880.7263

882.4046 887.7870 905.1797

906.6455 912.7661 928.8738

949.0683 953.4553 954.1534

959.3428 960.1201 974.7850

977.1485 978.7205 990.7480

993.4151 995.2590 998.2522

999.1417 1005.8139 1012.7257

1020.3924 1036.0131 1039.6175

1042.8608 1044.2494 1049.3298

1052.1630 1053.1384 1055.5343

1057.2151 1060.4422 1063.1615

1066.2787 1067.3945 1069.8490

1077.9470 1093.1132 1100.6855

1104.6624 1109.2284 1117.5868

1143.4549 1152.9223 1156.4750

1184.1394 1184.6762 1184.9446

1186.2428 1192.6987 1193.1695

1202.5532 1210.9422 1214.0093

1216.5841 1224.9341 1233.8118

1243.9477 1268.0165 1273.7081

1273.9834 1290.5104 1291.1125

1293.5519	1303.3529	1309.7814
1316.3416	1321.8128	1323.2563
1331.2675	1339.2215	1342.5005
1348.9619	1360.1629	1366.6371
1369.4154	1373.7752	1377.6083
1382.5626	1399.9832	1412.5920
1416.0865	1419.5694	1425.0504
1439.0726	1446.6863	1450.5654
1463.5786	1467.5382	1469.5720
1471.7150	1479.6596	1483.7719
1485.6612	1486.6526	1488.2643
1489.9109	1494.5377	1497.0901
1498.0371	1499.6602	1504.1693
1506.6651	1520.5739	1526.5433
1528.1613	1532.0225	1555.2905
1600.6879	1607.3483	1611.6731
1628.3083	1635.3686	1636.5339
1637.4392	1640.4241	1641.8130
1652.3979	1653.2197	1658.1844
1710.1442	2960.8815	3038.7868
3046.0659	3049.7036	3053.5158
3059.0275	3102.2251	3102.4568
3108.3487	3120.2770	3130.7423
3137.9904	3141.0419	3141.1375
3155.1652	3155.7180	3164.0467
3180.8465	3183.2951	3183.5146
3185.5534	3187.3173	3187.4171
3192.6881	3193.9508	3196.4686
3196.6894	3205.3749	3205.8207
3206.2564	3206.9340	3208.8986

3212.8330	3218.3848	3222.2347
3229.7673	3244.4323	3274.2918

TS4SS

Zero-point correction= 0.729731

Thermal correction to Energy= 0.775850

Thermal correction to Enthalpy= 0.776794

Thermal correction to Gibbs Free Energy= 0.647854

Sum of electronic and zero-point Energies= -5135.057418

Sum of electronic and thermal Energies= -5135.011299

Sum of electronic and thermal Enthalpies= -5135.010355

Sum of electronic and thermal Free Energies= -5135.144015

Cartesian coordinates

C	-1.581143	0.318498	-1.538333
C	-0.376877	0.741865	-0.954985
H	-1.516858	-0.515856	-2.228778
C	0.810892	-0.002942	-1.032784
O	1.010779	-1.102840	-1.618812
C	-2.705592	1.236813	-1.779266
C	-3.771489	0.812208	-2.598549
C	-2.769068	2.531870	-1.228526
C	-4.857815	1.643243	-2.855350
H	-3.740376	-0.186615	-3.026404
C	-3.859409	3.363385	-1.485820
H	-1.961912	2.902383	-0.607478
C	-4.908283	2.925720	-2.297564
H	-5.666176	1.293153	-3.491091
H	-3.886579	4.358233	-1.049869
H	-5.755047	3.575987	-2.497176
C	2.009915	0.592223	-0.345649

C	3.930481	0.776301	0.707109
C	3.333068	-1.564601	0.139971
H	2.376741	-2.077159	0.093505
N	3.522022	2.006995	0.552634
N	2.327936	1.881597	-0.122955
N	3.046026	-0.116413	0.158467
C	5.075702	0.225750	1.490869
H	5.442709	0.972275	2.196732
H	5.901878	-0.072158	0.831477
C	4.124285	-1.981752	1.439887
O	4.554973	-0.871770	2.237445
C	5.352919	-2.658241	-0.552130
C	4.244951	-1.939572	-1.008067
C	4.065193	-1.661445	-2.362948
C	5.032131	-2.104869	-3.267776
C	6.148763	-2.822398	-2.818357
C	6.313376	-3.107796	-1.460308
C	5.307793	-2.852859	0.942298
H	3.180651	-1.127234	-2.692861
H	6.892896	-3.162269	-3.533187
H	7.178708	-3.667300	-1.115730
H	6.234708	-2.555559	1.444036
H	5.132411	-3.904544	1.195498
C	1.615095	3.065965	-0.527282
C	0.982347	3.825815	0.466867
C	1.566808	3.392433	-1.891239
C	0.241398	4.935826	0.048928
C	0.813992	4.512185	-2.252070
C	0.133444	5.284261	-1.302195
H	-0.268956	5.534668	0.798413

H	0.751835	4.783228	-3.302602
C	2.263613	2.557781	-2.934838
H	1.700788	1.640010	-3.140901
H	3.269013	2.264156	-2.616804
H	2.349560	3.110783	-3.873193
C	-0.726985	6.442896	-1.738414
H	-1.686348	6.078884	-2.127041
H	-0.250189	7.015325	-2.540464
H	-0.941735	7.121719	-0.908400
C	1.079260	3.449839	1.920984
H	2.099504	3.582527	2.295590
H	0.814996	2.401290	2.083541
H	0.409708	4.064560	2.524649
H	3.449928	-2.531643	2.092905
H	4.915124	-1.897273	-4.327486
H	-0.369115	1.641437	-0.357891
C	-0.495759	-0.002376	2.899660
C	-1.474923	1.006423	3.062595
C	-1.381388	1.989258	4.048367
C	-0.268713	1.982322	4.889323
C	0.730226	1.009969	4.729972
C	0.626748	0.023800	3.751245
C	-0.816779	-0.928420	1.821867
C	-2.022985	-0.608968	1.154418
H	-2.152821	2.746295	4.152620
H	-0.174235	2.739346	5.662129
H	1.599698	1.022772	5.381184
H	1.399797	-0.722960	3.627529
S	-2.762526	0.838910	1.876916
C	-0.021184	-2.091213	1.518690

O	1.037147	-2.400534	2.086355
H	-0.411490	-2.748123	0.729191
C	-2.653975	-1.061048	-0.029798
H	-3.626627	-0.603140	-0.183009
C	-2.629020	-2.440386	-0.585725
C	-3.753698	-3.277744	-0.437050
C	-1.560528	-2.969906	-1.337959
C	-3.825441	-4.555731	-0.988980
C	-1.612086	-4.249354	-1.888587
H	-0.675237	-2.359392	-1.493696
C	-2.744980	-5.046436	-1.720741
H	-4.713264	-5.160279	-0.841045
H	-0.764450	-4.617362	-2.459244
H	-2.795359	-6.041023	-2.153336
Br	-5.272693	-2.686782	0.594301

Vibrational frequencies

-182.3997	13.9051	20.2968
20.8758	26.4845	30.2354
37.6701	39.1869	43.4106
49.0596	51.8313	58.4545
63.1879	68.7943	75.2378
81.8528	87.6955	94.1802
94.9404	104.0597	114.6282
128.8613	138.4134	144.8500
148.2635	152.4847	170.9264
175.6671	183.6931	187.2762
197.2923	202.8334	205.5948
211.1427	217.8023	221.3940
228.0608	232.2846	240.7115
252.6504	263.6149	273.4250

285.0612	290.8818	299.5042
319.9183	326.4909	330.1111
365.4318	371.0670	379.0708
393.2364	402.9642	407.6802
415.3266	420.9798	435.6586
441.4310	445.4146	452.3360
468.8114	475.1564	491.0179
499.9509	509.7561	512.4988
514.5471	527.9999	529.1155
532.9971	541.2700	543.6308
561.5727	578.1048	582.5476
588.8427	599.3843	607.7709
613.1021	619.8482	630.6478
638.4521	642.2700	647.5022
670.4603	672.1553	701.2655
705.0121	710.2324	712.8262
729.2255	747.2683	747.9309
749.6138	760.5598	762.9572
770.7352	773.6229	775.3651
780.1076	788.1226	798.8713
806.6289	827.5567	831.3823
844.9650	855.0246	868.9195
878.1190	880.0066	881.5386
887.7314	900.9255	906.2758
907.5129	912.6092	927.8501
942.8878	946.9431	952.3946
962.4625	973.6376	976.6817
978.0620	985.9097	989.9840
992.5665	998.7114	1001.4834
1003.5135	1012.0421	1013.1200

1023.9014	1037.0480	1040.4486
1042.4341	1046.0011	1047.8857
1048.6252	1050.7307	1052.1013
1055.6502	1059.8489	1061.2202
1066.1584	1068.1236	1070.4769
1077.2475	1095.6986	1097.6239
1101.8051	1112.3249	1116.6028
1144.3479	1149.9960	1152.6411
1183.2363	1183.7071	1184.3908
1186.1559	1192.1845	1195.4835
1199.2764	1199.6522	1210.6248
1213.0087	1221.2239	1235.0231
1241.0861	1245.7922	1271.7120
1272.7467	1286.0127	1291.6228
1297.3868	1303.9001	1309.8800
1316.8923	1330.5613	1331.4940
1332.7081	1336.7636	1342.8089
1349.1877	1357.3769	1367.7749
1368.2359	1373.9890	1378.3945
1379.3934	1414.3040	1418.8540
1420.3880	1425.4121	1428.1789
1438.7042	1447.1860	1454.0161
1463.7561	1466.0579	1467.9217
1470.3470	1480.2878	1482.4241
1484.5997	1485.5187	1489.4691
1490.9166	1493.7669	1495.9399
1497.4966	1500.1431	1505.7077
1508.4076	1518.5739	1520.4573
1525.1861	1532.2663	1574.7883
1603.2973	1605.9664	1607.8836

1626.8027	1634.5812	1634.8470
1637.1998	1639.5767	1641.2641
1650.9606	1652.5338	1657.0192
1680.7742	3039.2611	3040.9188
3048.1232	3052.5142	3056.5634
3059.6156	3096.9283	3101.8152
3111.4255	3123.8395	3131.3877
3139.0586	3151.2319	3153.9489
3163.1842	3166.9552	3168.3486
3178.1756	3182.4427	3182.9484
3184.3827	3184.5938	3186.9051
3187.0473	3191.2392	3192.2408
3193.9252	3193.9645	3196.2973
3204.4735	3205.1903	3206.6649
3207.5597	3218.1466	3218.6439
3221.7662	3244.9879	3249.2859

TS4RR'

Zero-point correction= 0.733348

Thermal correction to Energy= 0.778813

Thermal correction to Enthalpy= 0.779758

Thermal correction to Gibbs Free Energy= 0.653516

Sum of electronic and zero-point Energies= -4812.085745

Sum of electronic and thermal Energies= -4812.040280

Sum of electronic and thermal Enthalpies= -4812.039335

Sum of electronic and thermal Free Energies= -4812.165577

Cartesian coordinates

C	1.618150	-0.640842	-1.076429
C	0.519892	0.228453	-0.857951
H	1.457645	-1.392695	-1.844095
C	-0.728674	0.036097	-1.453238

O	-1.140759	-0.879107	-2.213800
C	3.008285	-0.153614	-0.966873
C	4.058439	-0.909846	-1.521976
C	3.340231	1.043092	-0.302546
C	5.381961	-0.485721	-1.428022
H	3.825918	-1.846176	-2.018551
C	4.665171	1.467466	-0.206418
H	2.563336	1.660443	0.132673
C	5.692901	0.706796	-0.767193
H	6.172097	-1.087679	-1.867915
H	4.892351	2.391941	0.316671
H	6.724873	1.035738	-0.687788
C	-1.737461	1.131330	-1.185458
C	-3.662809	2.162257	-0.921988
C	-3.798596	-0.307960	-0.767868
H	-3.244250	-1.105344	-1.265749
N	-2.788769	3.126739	-1.035744
N	-1.584225	2.465737	-1.190905
N	-3.061262	0.935330	-1.018940
C	-5.152280	2.176545	-0.798263
H	-5.556623	3.127833	-1.147557
H	-5.455803	2.029707	0.246978
C	-5.269562	-0.191481	-1.315804
O	-5.648754	1.149848	-1.655673
C	-5.292855	-0.844766	1.027870
C	-3.963873	-0.550915	0.717001
C	-2.976505	-0.505761	1.700095
C	-3.337460	-0.783933	3.020444
C	-4.666578	-1.093582	3.339506
C	-5.651614	-1.123834	2.348107

C	-6.160673	-0.808770	-0.206073
H	-1.948603	-0.270702	1.443163
H	-4.934915	-1.307931	4.369994
H	-6.682419	-1.353213	2.603209
H	-7.071955	-0.215960	-0.078898
H	-6.471127	-1.819015	-0.496846
C	-0.360790	3.209755	-1.345210
C	0.205586	3.317238	-2.622469
C	0.226433	3.753766	-0.194272
C	1.429890	3.983358	-2.722289
C	1.447707	4.414742	-0.350616
C	2.068989	4.525918	-1.600586
H	1.898439	4.071989	-3.698821
H	1.931361	4.835247	0.526872
C	-0.407922	3.575871	1.160405
H	-0.481989	2.513695	1.417929
H	-1.422367	3.986823	1.187777
H	0.185525	4.063486	1.936620
C	3.426635	5.168335	-1.731381
H	4.210683	4.400925	-1.704718
H	3.623067	5.868040	-0.914008
H	3.528796	5.704553	-2.679811
C	-0.461351	2.710638	-3.829890
H	-1.523539	2.973097	-3.874739
H	-0.398245	1.616390	-3.807947
H	0.017163	3.055026	-4.749382
H	-5.360845	-0.734539	-2.256785
H	-2.582480	-0.765259	3.800671
H	0.639616	1.086620	-0.212488
C	2.320972	0.191614	3.199252

C	0.926058	0.200058	3.048526
C	0.070702	1.028455	3.757104
C	0.673200	1.906383	4.666825
C	2.068158	1.927871	4.838519
C	2.906393	1.076863	4.114177
C	2.813010	-0.807413	2.274673
C	1.692273	-1.327706	1.614290
H	-1.002282	1.002426	3.601686
H	0.049949	2.582189	5.244364
H	2.502841	2.623504	5.550622
H	3.982577	1.090772	4.238439
C	4.188663	-1.171541	2.058206
O	5.145550	-0.633984	2.621648
H	4.360946	-1.991991	1.333979
C	1.605610	-2.166836	0.469122
H	2.563768	-2.601970	0.209027
C	0.450022	-2.999252	0.111070
C	0.504341	-3.909124	-0.970490
C	-0.792834	-2.931492	0.778121
C	-0.592892	-4.648343	-1.397338
C	-1.900977	-3.666304	0.367459
H	-0.882486	-2.291761	1.641914
C	-1.814476	-4.517417	-0.734164
H	-0.495794	-5.320487	-2.242579
H	-2.834253	-3.565087	0.913042
H	-2.674643	-5.087901	-1.070404
Br	2.149467	-4.182737	-1.946518
O	0.547112	-0.716792	2.089686

Vibrational frequencies

-226.4012	18.0449	21.7452

26.9345	33.8129	37.3718
41.8611	45.7075	49.0102
52.6714	59.5321	61.7425
70.0940	72.2814	78.9491
82.9061	88.3985	93.5798
101.1561	115.7664	117.8449
130.0095	135.3152	138.4434
142.1912	151.9510	159.7954
162.5760	169.1833	174.0750
187.5628	195.0274	201.0946
213.6454	218.9628	223.8458
229.0792	241.9378	254.5355
261.2863	275.0961	289.3171
293.5874	307.8134	319.0289
323.1604	330.5590	341.6449
363.4073	369.7510	380.2071
394.7614	411.0355	413.6546
418.2522	423.5231	431.6395
449.5351	461.6802	470.4461
488.1603	492.3900	506.1917
515.2956	517.3380	527.1676
531.1280	534.7066	541.5040
546.1026	565.7536	579.9328
584.8269	589.2779	591.9642
597.3854	611.9553	617.1407
621.2516	629.9226	633.2400
654.0878	679.5733	684.6327
704.1132	706.7284	715.7699
721.0260	735.2773	745.8328
749.4581	754.8700	757.7282

758.5799	761.4920	765.8637
768.4167	773.4388	778.0379
786.9514	794.8234	799.7415
829.2064	842.5527	844.8204
863.2098	870.1923	879.6263
880.9194	882.5749	884.8662
887.1217	904.4716	909.8385
913.0874	925.4660	943.1535
946.4700	952.7852	961.2546
963.5039	976.0803	981.6502
984.6798	985.7604	990.1234
991.2736	1002.0930	1005.6944
1007.7688	1014.4207	1019.7599
1024.6009	1033.1392	1036.9940
1038.7606	1043.7683	1049.4433
1055.5378	1058.5470	1059.4866
1061.6696	1066.5152	1068.6186
1068.9467	1077.3759	1082.0499
1086.6795	1099.6253	1114.4807
1114.9109	1121.0654	1139.5789
1150.1427	1154.9154	1175.6292
1184.4269	1188.2961	1189.6811
1194.1337	1200.4017	1206.0384
1207.3596	1216.2702	1224.5296
1231.8731	1236.5021	1237.3486
1255.1000	1268.7696	1270.1019
1290.3233	1292.4850	1296.4396
1308.5209	1313.4864	1317.1107
1319.6505	1325.2847	1328.3523
1329.5618	1341.2632	1343.9119

1345.3429	1369.9738	1370.5861
1376.6386	1377.1272	1380.7159
1389.5430	1408.6056	1419.1258
1420.0203	1420.3447	1425.4581
1439.4925	1448.2127	1457.3470
1465.9258	1468.0964	1472.9666
1478.0075	1479.2789	1484.4664
1485.8253	1488.1991	1490.6411
1492.0584	1498.3510	1499.7989
1504.7245	1508.4114	1511.6575
1514.2724	1527.5873	1528.7605
1535.4024	1561.7105	1578.8898
1603.5302	1625.0027	1629.0488
1633.2658	1636.3486	1640.2127
1640.7225	1644.1695	1653.3393
1653.9568	1658.7163	1662.6687
1711.7477	2937.9364	3039.8801
3044.8573	3045.6495	3051.3284
3057.7432	3103.5812	3103.6244
3105.7869	3112.3327	3124.0011
3130.8565	3133.7153	3141.5129
3144.1209	3150.1215	3181.7850
3182.6956	3185.4001	3186.9432
3187.3464	3187.9933	3190.0470
3192.9362	3197.7154	3200.1246
3203.1900	3204.2625	3206.4374
3206.8741	3214.2413	3214.9081
3218.6650	3220.6759	3225.8794
3231.4499	3249.9996	3278.2128

TS4SR'

Zero-point correction= 0.729754

Thermal correction to Energy= 0.775734

Thermal correction to Enthalpy= 0.776678

Thermal correction to Gibbs Free Energy= 0.649160

Sum of electronic and zero-point Energies= -5135.063362

Sum of electronic and thermal Energies= -5135.017382

Sum of electronic and thermal Enthalpies= -5135.016437

Sum of electronic and thermal Free Energies= -5135.143956

Cartesian coordinates

C	1.072841	-0.209559	1.589352
C	0.080583	0.659518	1.055897
H	0.693209	-1.052236	2.160019
C	-1.267707	0.290817	1.016760
O	-1.821584	-0.672738	1.617936
C	2.385962	0.286252	2.034100
C	2.870664	1.565142	1.700159
C	3.218256	-0.557933	2.795055
C	4.139168	1.978881	2.106507
H	2.256370	2.250622	1.127731
C	4.483857	-0.144446	3.202566
H	2.860720	-1.547809	3.064066
C	4.953069	1.126802	2.855190
H	4.491275	2.968996	1.831139
H	5.107724	-0.814243	3.787499
H	5.942397	1.448351	3.167405
C	-2.163603	1.080623	0.098452
C	-3.869756	1.571274	-1.209557
C	-4.036842	-0.672042	-0.161671
H	-3.262942	-1.388958	0.101143
N	-3.079610	2.606293	-1.301639

N	-2.023392	2.294715	-0.474319
N	-3.351357	0.619203	-0.369543
C	-5.089504	1.219886	-1.991727
H	-5.194947	1.887315	-2.848060
H	-5.994839	1.286334	-1.374102
C	-4.808463	-1.109222	-1.469482
O	-4.867379	-0.101134	-2.483826
C	-6.324890	-1.071023	0.437295
C	-5.101878	-0.586192	0.906065
C	-4.953012	-0.125391	2.213387
C	-6.069525	-0.132625	3.052259
C	-7.303841	-0.605197	2.585980
C	-7.438300	-1.082662	1.279443
C	-6.215569	-1.551077	-0.987962
H	-3.981461	0.210453	2.560380
H	-8.164440	-0.603900	3.248961
H	-8.395372	-1.454354	0.923875
H	-6.986128	-1.136117	-1.646017
H	-6.304686	-2.642067	-1.040778
C	-0.896719	3.185612	-0.397010
C	0.058794	3.111647	-1.423324
C	-0.747005	3.989713	0.738097
C	1.229346	3.853985	-1.260556
C	0.437097	4.726907	0.845416
C	1.440309	4.652639	-0.127958
H	2.018576	3.755301	-1.998962
H	0.590846	5.345341	1.725787
C	-1.782343	3.990285	1.832067
H	-1.757331	3.041184	2.380912
H	-2.794056	4.109939	1.431200

H	-1.595039	4.796510	2.544837
C	2.735587	5.408087	0.032618
H	2.931879	5.648793	1.081289
H	2.712922	6.352239	-0.525724
H	3.576504	4.823666	-0.353594
C	-0.144115	2.213591	-2.615508
H	-1.014070	2.524664	-3.204057
H	-0.320884	1.176758	-2.309884
H	0.734427	2.226750	-3.263929
H	-4.264429	-1.923482	-1.947715
H	-5.980086	0.224414	4.074089
H	0.406941	1.528376	0.510168
C	5.127149	-0.666498	-0.910862
C	5.420749	-1.952503	-0.401329
C	6.724386	-2.443694	-0.314872
C	7.767580	-1.624793	-0.744447
C	7.501363	-0.341872	-1.249776
C	6.199268	0.141459	-1.336939
C	3.706530	-0.376065	-0.888159
C	2.931225	-1.429943	-0.366891
H	6.921929	-3.435696	0.080095
H	8.790811	-1.983484	-0.684602
H	8.325742	0.285254	-1.577318
H	5.989273	1.130014	-1.723946
O	3.957732	-2.796631	0.093607
C	3.129179	0.874187	-1.340565
O	3.760126	1.824001	-1.815991
H	2.032206	0.956261	-1.247014
C	1.514580	-1.405723	-0.148651
H	1.033402	-0.694960	-0.803337

C	0.684548	-2.604695	0.076136
C	-0.524853	-2.827917	-0.615614
C	1.003204	-3.558695	1.066282
C	-1.340199	-3.930393	-0.376663
C	0.203524	-4.669356	1.318212
H	1.883205	-3.395010	1.678636
C	-0.972591	-4.863572	0.593644
H	-2.257258	-4.063012	-0.939741
H	0.493319	-5.372895	2.092725
H	-1.607240	-5.723739	0.781832
Br	-1.155416	-1.581351	-1.955361

Vibrational frequencies

-267.7363	19.9051	21.5411
24.9952	26.9711	37.7721
40.3088	44.8327	46.1275
49.1826	54.8580	59.4108
65.0007	68.2717	76.0793
80.7061	89.5476	94.7041
102.5500	105.5244	129.2006
130.1534	131.8883	133.8263
152.2090	154.9513	163.6358
172.3546	177.2854	190.9627
193.7268	205.3300	208.6731
214.3231	223.5440	227.1884
235.4683	241.2472	244.0755
253.8299	267.5073	282.9334
288.1004	294.2585	308.0495
314.1710	321.1779	329.1596
363.2479	371.4982	382.6352
384.3852	394.1245	406.5250

418.2838	422.8613	431.7279
441.0231	448.8186	449.0065
464.0368	467.4547	495.1538
501.0847	505.4318	512.2164
522.2228	523.6248	530.9855
537.8743	544.6667	547.1858
564.4374	572.5836	582.7645
591.0936	601.0356	608.8537
615.8345	617.8837	632.0055
633.0333	647.5680	662.4513
670.7373	689.7879	702.3193
705.8284	709.5030	716.3307
731.1370	741.7387	744.8522
747.6368	755.9072	760.3321
763.6601	769.7860	771.2744
771.5699	779.8901	792.5141
799.5160	809.3139	827.8005
847.7116	855.3261	870.0252
871.9271	877.5518	879.2545
886.6575	900.8532	902.6922
903.5943	909.9153	928.7534
949.4269	951.5265	958.9216
960.6601	962.5840	974.4217
975.6919	978.2728	989.3561
996.5251	997.5345	998.6986
1004.1244	1010.4639	1013.8408
1019.4609	1037.0325	1037.6509
1041.2122	1045.6041	1049.2078
1052.0329	1054.0139	1057.8943
1060.1151	1061.5239	1065.3136

1065.8421	1066.9204	1070.4200
1076.9427	1095.6812	1104.1126
1108.9308	1114.1827	1118.3060
1139.1436	1142.4220	1156.2214
1182.4389	1184.0974	1185.6370
1188.3569	1189.7138	1194.7528
1201.7618	1212.9006	1215.6198
1216.4631	1224.9046	1230.5136
1244.6925	1253.3951	1268.2754
1272.3464	1286.2916	1289.1261
1295.6894	1303.4291	1309.5538
1313.9700	1318.2867	1325.9724
1328.3867	1336.1544	1340.1199
1349.0169	1360.9228	1368.1197
1368.7570	1373.3655	1374.9971
1382.7981	1400.6480	1412.2543
1412.9065	1417.7156	1423.5802
1432.3024	1441.6673	1448.8101
1453.0285	1466.1692	1467.2772
1469.6679	1478.6254	1484.2672
1485.7656	1486.6803	1487.7727
1489.5055	1496.3972	1498.3649
1498.6342	1502.8180	1504.5730
1507.7847	1522.0276	1525.6063
1529.0932	1534.0433	1550.6076
1604.9559	1607.6192	1610.6266
1628.6656	1636.3660	1637.2242
1637.7125	1640.8006	1641.1340
1652.5663	1652.8815	1659.2718
1695.6098	2998.9847	3040.8722

3042.9377	3044.3115	3051.3324
3055.3066	3097.9710	3103.7958
3105.0303	3109.8082	3131.7875
3133.3720	3139.7119	3146.1409
3152.1300	3162.5082	3178.9246
3181.4497	3182.8107	3184.3147
3184.3960	3188.3584	3193.1043
3193.9161	3193.9252	3196.7979
3204.1218	3205.0426	3206.3086
3206.8482	3207.2384	3212.5144
3215.8793	3217.0673	3220.7541
3231.3537	3243.8866	3283.9880

M4RR

Zero-point correction= 0.732854

Thermal correction to Energy= 0.778884

Thermal correction to Enthalpy= 0.779828

Thermal correction to Gibbs Free Energy= 0.649844

Sum of electronic and zero-point Energies= -5135.069632

Sum of electronic and thermal Energies= -5135.023602

Sum of electronic and thermal Enthalpies= -5135.022658

Sum of electronic and thermal Free Energies= -5135.152642

Cartesian coordinates

C	0.605999	1.714721	0.175602
C	-0.439647	0.733706	0.596755
H	0.334287	1.997733	-0.844151
C	-1.090279	0.009560	-0.365993
O	-0.910995	-0.021230	-1.635604
C	0.657526	3.003077	0.991163
C	1.227736	4.147367	0.407203
C	0.210052	3.095156	2.316512

C	1.349107	5.339106	1.120493
H	1.579263	4.099466	-0.619241
C	0.330681	4.288473	3.035511
H	-0.242791	2.236513	2.800305
C	0.901346	5.415018	2.442336
H	1.791418	6.209413	0.643391
H	-0.024453	4.333504	4.061539
H	0.993983	6.342278	3.000621
C	-2.285000	-0.782703	0.097921
C	-4.339409	-1.310104	0.684880
C	-3.852571	1.138414	0.694231
H	-2.956589	1.671589	1.016706
N	-3.778590	-2.449605	0.379720
N	-2.496518	-2.097719	0.000419
N	-3.458658	-0.269846	0.529725
C	-5.689464	-0.989727	1.236788
H	-6.128452	-1.867489	1.713201
H	-6.361872	-0.647008	0.438451
C	-5.015311	1.264494	1.756521
O	-5.497909	0.006235	2.239843
C	-5.687628	2.264982	-0.364510
C	-4.424189	1.712335	-0.584346
C	-3.823934	1.733040	-1.844830
C	-4.521335	2.328567	-2.898349
C	-5.786862	2.891950	-2.686272
C	-6.377247	2.864597	-1.420254
C	-6.118285	2.118009	1.072710
H	-2.846643	1.282077	-2.004519
H	-6.315469	3.353011	-3.515840
H	-7.360748	3.298207	-1.261144

H	-7.091723	1.626700	1.176416
H	-6.202086	3.092739	1.565435
C	-1.560077	-3.112454	-0.402896
C	-0.787837	-3.732597	0.585720
C	-1.500498	-3.457497	-1.761256
C	0.079570	-4.748610	0.172413
C	-0.612610	-4.472924	-2.120451
C	0.179906	-5.129544	-1.169293
H	0.697699	-5.241532	0.915109
H	-0.541500	-4.761846	-3.166031
C	-2.352308	-2.743834	-2.776802
H	-2.092311	-1.679501	-2.784398
H	-3.417470	-2.825526	-2.531186
H	-2.199020	-3.158400	-3.776204
C	1.133056	-6.216639	-1.599765
H	1.539879	-6.758166	-0.742104
H	1.977279	-5.795224	-2.157929
H	0.638445	-6.937512	-2.259855
C	-0.875111	-3.312778	2.030367
H	-1.914863	-3.258049	2.369675
H	-0.426187	-2.325165	2.181174
H	-0.340416	-4.017401	2.670417
H	-4.630503	1.754880	2.650854
H	-4.078186	2.355675	-3.889550
H	-0.717017	0.600095	1.635731
C	2.614459	-2.372374	1.429736
C	3.044900	-2.731960	0.132397
C	3.536091	-4.006924	-0.162989
C	3.598376	-4.940991	0.866542
C	3.168165	-4.606761	2.163117

C	2.674894	-3.339017	2.451280
C	2.216047	-0.976797	1.494604
C	2.345329	-0.310550	0.289779
H	3.864381	-4.260990	-1.165695
H	3.981562	-5.936363	0.663551
H	3.222526	-5.350921	2.952399
H	2.340956	-3.078901	3.447521
S	2.914311	-1.378489	-0.980054
C	1.736059	-0.312759	2.703471
O	1.404563	-0.891744	3.735037
H	1.688970	0.789785	2.657694
C	2.128599	1.165193	0.041133
H	2.683915	1.656054	0.841441
C	2.728854	1.618277	-1.280177
C	3.910802	2.364016	-1.380353
C	2.073388	1.294581	-2.483876
C	4.432204	2.770982	-2.609506
C	2.584090	1.685077	-3.719419
H	1.140538	0.735731	-2.425479
C	3.766069	2.425525	-3.784107
H	5.347220	3.351468	-2.644814
H	2.055377	1.417338	-4.629156
H	4.170179	2.741645	-4.741045
Br	4.880581	2.894628	0.197482

Vibrational frequencies

8.4141	13.4557	18.7298
25.6825	28.3653	32.0359
38.6547	44.1841	48.4451
53.7625	57.9297	62.4652
68.3620	77.5337	81.7017

83.9884	91.5205	98.1581
104.5089	113.1269	118.3968
129.7174	141.3516	148.4522
161.3972	172.7686	174.6994
185.0255	186.7483	192.9566
205.2768	210.3745	214.1491
217.0271	219.5943	228.7766
242.8282	255.0096	260.8390
274.9499	281.6264	288.8977
296.5873	298.0038	318.3116
321.0107	325.1936	348.0395
372.0872	381.5166	387.0808
397.9010	418.9341	421.3848
432.7277	441.7382	445.3077
450.5281	455.3782	479.2639
483.1226	495.3813	501.7999
504.9951	510.8282	516.4330
519.4621	524.0561	526.7193
536.9782	556.6448	576.9105
582.1919	589.3502	594.1753
603.2493	611.7985	614.0915
623.5483	626.3505	632.8925
639.3532	677.5209	689.1119
698.0236	707.2548	710.7169
714.4316	718.7083	724.1361
738.3082	746.5260	748.1671
754.1983	766.0404	771.0719
772.7724	777.1499	781.6931
787.3550	796.2721	803.4857
816.3544	829.9221	850.8743

864.6098	867.0200	873.0156
880.7203	881.4344	882.3850
904.5549	906.7687	911.4665
911.5328	914.5366	942.6145
955.8002	958.6344	961.9018
976.9926	981.8926	982.8692
990.1387	990.3283	998.2587
1001.7484	1014.6169	1016.8315
1024.1428	1037.0310	1037.2328
1038.9027	1039.5184	1043.4935
1047.7005	1048.8391	1055.2224
1057.2321	1058.8927	1061.0427
1063.4496	1066.3253	1074.1054
1075.4621	1077.3542	1079.5813
1088.9245	1101.8583	1104.1387
1120.9520	1128.8817	1146.4490
1153.5432	1178.1392	1183.6645
1185.4361	1189.6044	1191.5962
1195.4087	1197.1154	1199.6855
1204.3868	1212.3081	1218.0628
1224.5603	1228.4855	1232.6982
1250.2158	1251.1206	1276.5631
1289.9397	1293.4438	1295.7346
1298.2695	1303.2756	1310.0801
1319.0213	1331.0931	1333.7446
1340.6484	1343.2805	1346.8883
1352.3534	1358.0691	1363.2432
1365.0037	1368.4521	1380.8100
1382.8550	1398.2943	1409.0795
1416.0630	1417.3187	1423.0917

1435.7036	1448.8514	1458.5612
1464.6280	1469.3506	1469.7037
1471.8950	1474.2038	1480.0849
1481.5878	1484.9133	1487.8675
1489.2235	1492.0252	1495.7505
1498.2327	1499.6882	1509.8201
1520.1072	1520.7243	1529.1385
1536.7935	1540.6888	1557.1199
1607.7452	1614.9105	1632.0548
1633.0921	1640.7661	1642.0359
1643.4110	1644.0197	1653.4920
1655.8081	1656.5869	1658.8335
1732.4582	2996.4345	3036.9095
3038.0011	3041.7899	3051.7489
3059.6060	3081.9834	3097.2517
3100.0667	3103.1494	3105.0613
3113.8417	3120.9191	3133.8332
3135.1606	3135.2542	3143.5676
3150.5243	3152.6547	3168.7705
3178.8230	3182.3514	3183.2780
3185.8457	3188.5821	3194.0320
3194.4247	3197.1077	3200.4390
3200.8799	3206.1683	3206.5479
3207.4157	3207.7954	3211.4292
3216.6475	3219.6056	3242.6897

M4RS

Zero-point correction= 0.732969

Thermal correction to Energy= 0.779000

Thermal correction to Enthalpy= 0.779944

Thermal correction to Gibbs Free Energy= 0.648271

Sum of electronic and zero-point Energies= -5135.072045

Sum of electronic and thermal Energies= -5135.026015

Sum of electronic and thermal Enthalpies= -5135.025071

Sum of electronic and thermal Free Energies= -5135.156744

Cartesian coordinates

C	1.203956	0.645800	0.615393
C	-0.247337	0.336295	0.828413
H	1.262883	1.026420	-0.403372
C	-1.029867	0.075277	-0.263216
O	-0.702901	-0.043255	-1.498717
C	1.708830	1.745079	1.535555
C	2.246920	2.922752	0.999986
C	1.659547	1.607925	2.931846
C	2.716813	3.941065	1.833363
H	2.298918	3.040074	-0.079337
C	2.127478	2.622362	3.767159
H	1.257636	0.695421	3.361509
C	2.657480	3.795054	3.220579
H	3.130586	4.846149	1.397146
H	2.080115	2.496976	4.845504
H	3.022706	4.585086	3.870661
C	-2.517996	0.068938	-0.021203
C	-4.580335	0.790083	0.257960
C	-2.820904	2.540654	0.530886
H	-1.842594	2.475697	1.009632
N	-4.710375	-0.469397	-0.061068
N	-3.409139	-0.902083	-0.247748
N	-3.258779	1.154711	0.297590
C	-5.588068	1.813927	0.665938

H	-6.507075	1.336125	1.008275
H	-5.827780	2.477118	-0.176891
C	-3.862444	3.299788	1.444959
O	-5.024180	2.526824	1.765664
C	-3.523637	4.509653	-0.645828
C	-2.765898	3.341525	-0.752120
C	-2.059060	3.029735	-1.915337
C	-2.125068	3.922613	-2.987334
C	-2.877618	5.100586	-2.888058
C	-3.581343	5.401103	-1.719020
C	-4.196468	4.620085	0.698373
H	-1.487857	2.106638	-1.990451
H	-2.916546	5.786105	-3.730007
H	-4.168170	6.312668	-1.647472
H	-5.282362	4.741241	0.617710
H	-3.823806	5.481196	1.263484
C	-3.168137	-2.270577	-0.624828
C	-3.066411	-3.234779	0.384397
C	-3.107250	-2.577287	-1.993175
C	-2.898404	-4.564528	-0.017523
C	-2.927341	-3.917720	-2.338370
C	-2.823211	-4.922172	-1.366430
H	-2.812419	-5.333844	0.745011
H	-2.867778	-4.183953	-3.390670
C	-3.214714	-1.493766	-3.032289
H	-2.392739	-0.781023	-2.900494
H	-4.155617	-0.940138	-2.933461
H	-3.168192	-1.913328	-4.040044
C	-2.605303	-6.356369	-1.779789
H	-3.386517	-6.694419	-2.469907

H	-2.599037	-7.029105	-0.917800
H	-1.648250	-6.468127	-2.303070
C	-3.096642	-2.858890	1.842757
H	-3.902873	-2.152713	2.064608
H	-2.152798	-2.390610	2.143431
H	-3.238331	-3.744785	2.466770
H	-3.405989	3.496679	2.415082
H	-1.585765	3.702478	-3.904068
H	-0.685333	0.390202	1.817315
C	5.154062	0.533711	-1.537797
C	5.953340	0.224945	-0.411982
C	7.339257	0.406474	-0.401352
C	7.941686	0.913453	-1.548235
C	7.169302	1.229782	-2.679308
C	5.791213	1.046445	-2.684720
C	3.741821	0.254366	-1.304010
C	3.498654	-0.241970	-0.033765
H	7.927149	0.160964	0.477585
H	9.016641	1.066124	-1.566361
H	7.656984	1.626597	-3.564940
H	5.196719	1.292597	-3.554271
S	4.966224	-0.385000	0.905819
C	2.693576	0.474441	-2.315825
O	2.903109	0.987252	-3.411897
H	1.671438	0.146309	-2.056398
C	2.211116	-0.595311	0.677523
H	2.465255	-0.704711	1.735468
C	1.615613	-1.939697	0.271358
C	0.877879	-2.710558	1.186934
C	1.792092	-2.504120	-0.999755

C	0.339816	-3.954853	0.866704
C	1.255470	-3.742721	-1.346820
H	2.382259	-1.975025	-1.735607
C	0.524656	-4.473186	-0.413139
H	-0.221261	-4.508510	1.609900
H	1.415998	-4.133826	-2.346628
H	0.098848	-5.437420	-0.669234
Br	0.592928	-2.117685	3.001238

Vibrational frequencies

2.5228	14.5832	18.9506
25.7681	30.8228	32.9483
36.4192	39.0810	42.3788
48.0733	50.7402	54.8862
63.7204	65.7919	73.3511
77.6075	90.8284	95.5225
100.8914	113.8525	121.0666
125.0556	136.5142	149.0464
155.1728	158.6562	188.5925
195.0258	198.1760	208.4341
212.4512	215.3330	221.6550
225.0690	232.3511	238.1119
247.2266	255.1229	263.9728
270.3679	285.4687	289.7437
293.5184	315.3630	325.4029
326.7194	335.9509	343.9190
376.4602	380.0895	386.8455
395.6227	409.4867	418.7911
433.7400	438.1091	451.0133
455.8843	459.2356	466.6432
481.4095	493.6311	503.4862

505.6405 508.7648 515.1074

525.4348 529.3311 535.8560

538.0515 550.0365 563.7849

581.7633 587.4207 591.2312

598.6202 613.2766 616.4897

621.5858 633.7455 640.6002

651.5413 675.7707 684.5981

695.6197 698.5243 706.0218

713.1737 715.2360 721.5421

732.5297 739.6732 747.8048

752.0486 766.3008 768.1086

772.9898 775.8363 776.0954

782.0892 795.1168 801.5602

826.3664 841.9107 852.5645

870.8668 872.5308 873.8873

880.7762 884.3669 885.2628

898.0442 901.0423 910.0463

913.1513 937.3197 957.0545

958.2722 962.0594 964.2760

971.3589 975.9332 983.7242

990.5361 992.1716 1000.9295

1003.9716 1013.6386 1015.8216

1022.1105 1024.9178 1033.9643

1038.3152 1038.5219 1042.4131

1048.4277 1054.1036 1056.3218

1057.6994 1059.3107 1063.7023

1069.0704 1073.1232 1073.7547

1073.9572 1077.6496 1081.5008

1085.1785 1102.8819 1104.0584

1120.0700 1122.3581 1142.2056

1151.9415	1173.6009	1181.3901
1184.0917	1186.0099	1189.4380
1193.5362	1195.6594	1199.6856
1203.7540	1212.1732	1216.0666
1219.0513	1221.2887	1231.5626
1249.0694	1259.3848	1273.5692
1286.7445	1287.4415	1294.5533
1296.1191	1305.1914	1309.3922
1317.8025	1323.4670	1328.4015
1341.7536	1343.1774	1350.6698
1355.1384	1359.8190	1362.6197
1363.1803	1368.3557	1378.8774
1379.5633	1401.6484	1405.9772
1416.2812	1420.0460	1430.8201
1432.3545	1449.5447	1454.5937
1464.1889	1470.4720	1471.3917
1474.4415	1474.8313	1477.5443
1480.7613	1484.0888	1490.9490
1493.1626	1493.6802	1496.5818
1497.7133	1498.7708	1508.0244
1513.9846	1526.3076	1530.2695
1536.1646	1537.4037	1552.4669
1608.1655	1619.9272	1632.4073
1634.4152	1640.4386	1641.8197
1643.5282	1643.7127	1652.2858
1654.9558	1656.8895	1659.1392
1728.6770	2990.6539	3035.3705
3038.0234	3039.8595	3050.2032
3059.8246	3069.5636	3096.8559
3097.7049	3101.5584	3114.9238

3117.3128	3125.4153	3127.6144
3132.9026	3135.1885	3135.9782
3149.5737	3168.5205	3175.9904
3181.1465	3181.5844	3183.2288
3185.8540	3189.3135	3191.1027
3194.7228	3196.9786	3200.1970
3200.6523	3206.3905	3207.2406
3211.7663	3213.6037	3215.4902
3228.0530	3246.2301	3250.1682

M4SR

Zero-point correction= 0.732848

Thermal correction to Energy= 0.778777

Thermal correction to Enthalpy= 0.779721

Thermal correction to Gibbs Free Energy= 0.650813

Sum of electronic and zero-point Energies= -5135.077518

Sum of electronic and thermal Energies= -5135.031588

Sum of electronic and thermal Enthalpies= -5135.030644

Sum of electronic and thermal Free Energies= -5135.159553

Cartesian coordinates

C	-1.391363	-0.156286	1.534764
C	-0.201789	-0.792467	0.876221
H	-1.096143	0.184002	2.534954
C	1.061959	-0.258850	0.978981
O	1.421652	0.815699	1.570350
C	-2.488443	-1.201377	1.686836
C	-2.994397	-1.902887	0.580160
C	-2.937386	-1.573420	2.962609
C	-3.936848	-2.919033	0.742263
H	-2.633994	-1.669620	-0.415851

C	-3.877989	-2.592283	3.130896
H	-2.539052	-1.061147	3.834811
C	-4.386510	-3.266850	2.018992
H	-4.313685	-3.444482	-0.130799
H	-4.207133	-2.861331	4.130763
H	-5.119023	-4.059060	2.144858
C	2.130614	-0.972610	0.200015
C	3.957514	-1.330786	-0.976721
C	3.595936	1.050649	-0.388111
H	2.685825	1.627561	-0.239261
N	3.411143	-2.509895	-0.858560
N	2.275220	-2.275366	-0.110053
N	3.211549	-0.369117	-0.344811
C	5.111529	-0.873899	-1.803400
H	5.402850	-1.651885	-2.510404
H	5.976512	-0.619420	-1.176554
C	4.282619	1.391805	-1.769674
O	4.637247	0.244986	-2.551386
C	5.725504	2.050672	0.076648
C	4.637543	1.392761	0.654303
C	4.578268	1.141468	2.024463
C	5.656035	1.539858	2.818757
C	6.759898	2.185855	2.245616
C	6.798752	2.452445	0.874091
C	5.520649	2.251626	-1.403971
H	3.697128	0.668282	2.445842
H	7.592245	2.487666	2.875338
H	7.652555	2.961409	0.435187
H	6.381077	1.948910	-2.009283
H	5.325496	3.306799	-1.628301

C	1.372152	-3.359243	0.168777
C	0.527665	-3.787848	-0.866980
C	1.333993	-3.892267	1.462965
C	-0.402373	-4.783960	-0.559078
C	0.383740	-4.885263	1.717675
C	-0.498488	-5.331409	0.726607
H	-1.080038	-5.125828	-1.336803
H	0.323202	-5.309611	2.716388
C	2.246780	-3.377372	2.544846
H	1.934847	-2.376940	2.867541
H	3.282032	-3.300437	2.196781
H	2.224421	-4.033781	3.417879
C	-1.566811	-6.345919	1.047429
H	-2.491059	-5.838035	1.350846
H	-1.266921	-7.000935	1.870815
H	-1.805791	-6.967439	0.179145
C	0.597359	-3.167405	-2.239151
H	1.525809	-3.443635	-2.751233
H	0.576592	-2.073309	-2.192475
H	-0.242877	-3.496221	-2.855345
H	3.575365	1.929788	-2.400323
H	5.637183	1.352222	3.888500
H	-0.367547	-1.682527	0.291999
C	-2.146384	0.391534	-2.898992
C	-3.540614	0.507528	-2.681759
C	-4.470850	0.257378	-3.695132
C	-3.993853	-0.126039	-4.945497
C	-2.612886	-0.250687	-5.179596
C	-1.689145	0.006015	-4.172727
C	-1.386592	0.725472	-1.707224

C	-2.187882	1.024275	-0.622668
H	-5.536336	0.355171	-3.511536
H	-4.697937	-0.331581	-5.746228
H	-2.263051	-0.553112	-6.162342
H	-0.623986	-0.087207	-4.345492
S	-3.893393	0.995705	-1.027550
C	0.069017	0.850632	-1.651374
O	0.850376	0.426271	-2.505050
H	0.452257	1.441597	-0.803926
C	-1.739244	1.222048	0.793853
H	-0.750352	1.691098	0.766406
C	-2.634830	2.203532	1.534895
C	-2.527244	3.583258	1.282435
C	-3.608572	1.812147	2.463939
C	-3.319901	4.529453	1.926104
C	-4.415551	2.743842	3.119194
H	-3.743755	0.759556	2.672336
C	-4.270095	4.104402	2.855808
H	-3.198558	5.583320	1.702120
H	-5.157913	2.400276	3.833061
H	-4.890936	4.837540	3.361616
Br	-1.263244	4.230945	-0.020174

Vibrational frequencies

15.4014	17.0381	22.0493
24.1370	27.9811	33.1327
39.9081	44.2451	48.6723
50.8922	57.4560	59.1947
71.9941	77.5379	81.2437
83.3633	87.5139	101.1923
110.8087	112.9198	124.3443

131.7228	138.3886	144.7055
161.5502	173.1967	175.7462
179.2875	182.9302	184.7060
196.2042	208.5275	213.9906
221.0021	223.5587	233.9781
240.7839	254.0870	259.3676
270.8507	290.4006	292.9530
305.2318	316.5941	319.6943
330.4564	343.3639	361.1141
378.9896	389.8300	390.6861
402.3401	407.4339	418.7553
428.8332	437.7467	440.5009
445.0974	447.9038	459.9369
490.4559	499.2542	502.3547
504.7006	514.0621	520.8769
525.8979	531.9559	536.9848
542.7627	561.7481	576.8085
581.1357	581.8654	601.4630
608.6071	613.4387	619.3504
622.7663	636.2784	645.9125
648.4816	671.2562	683.8019
696.1329	706.6277	709.5080
719.6121	722.3811	732.4509
735.7361	747.2709	751.1242
753.8580	764.7711	767.0145
768.6451	771.0356	775.5065
779.0155	792.4518	801.5767
823.8820	830.0702	843.0100
862.3140	869.8152	874.4649
879.6830	882.5752	890.6993

893.5919	903.8109	906.6516
919.3216	935.1537	944.2429
949.3215	959.7146	960.9887
974.1646	974.6948	976.4309
987.4005	989.3837	1001.4947
1002.0593	1002.9212	1003.1057
1009.2464	1015.1542	1030.9423
1030.9821	1038.7698	1042.9793
1044.7405	1047.7105	1050.9175
1054.6115	1058.0966	1059.9831
1062.7209	1065.8511	1067.5925
1069.7139	1076.7571	1080.2542
1090.4684	1097.7846	1101.3904
1115.8949	1116.7748	1148.8315
1149.7308	1179.2327	1183.2332
1184.6543	1186.1120	1191.8436
1195.1555	1195.6039	1200.1322
1201.1665	1210.2591	1215.5188
1222.2439	1223.6060	1229.7131
1246.3675	1250.5326	1271.5943
1274.9881	1287.2134	1289.0079
1294.7805	1301.8876	1310.2707
1314.5649	1324.7592	1331.6515
1334.9394	1337.3817	1343.1081
1357.2536	1360.0481	1364.0322
1369.0600	1375.4936	1381.1619
1388.3172	1399.5540	1409.3271
1417.8821	1421.3629	1428.4396
1437.7216	1448.2756	1459.0292
1467.9798	1469.8414	1472.5678

1473.1413	1478.1316	1480.2931
1482.2372	1484.6580	1486.8738
1492.3461	1494.7406	1498.2691
1498.8472	1502.6264	1505.3768
1507.4265	1509.9251	1521.3677
1527.6931	1535.0737	1558.2370
1607.7828	1618.5836	1631.4318
1635.0714	1640.0972	1640.6883
1643.1099	1643.3181	1645.0762
1653.7012	1655.2617	1658.1901
1710.1766	3014.1016	3036.0742
3041.4090	3041.6376	3042.6286
3048.5879	3054.9853	3057.6054
3100.7097	3100.9390	3104.8310
3110.2926	3129.4012	3136.3762
3137.8693	3138.4458	3153.0644
3162.5973	3176.2538	3181.6071
3182.8060	3183.2095	3185.5029
3188.3986	3191.6488	3192.7038
3194.8964	3199.1919	3202.5484
3204.0455	3208.8096	3210.4251
3211.2610	3212.4867	3223.2060
3234.8250	3249.7053	3280.0066

M4SS

Zero-point correction= 0.733165

Thermal correction to Energy= 0.779140

Thermal correction to Enthalpy= 0.780084

Thermal correction to Gibbs Free Energy= 0.650715

Sum of electronic and zero-point Energies= -5135.068023

Sum of electronic and thermal Energies= -5135.022049

Sum of electronic and thermal Enthalpies= -5135.021104

Sum of electronic and thermal Free Energies= -5135.150473

Cartesian coordinates

C	-1.372775	0.446632	-0.992254
C	0.031136	0.902381	-0.721832
H	-1.328669	-0.307520	-1.784495
C	1.072381	0.030643	-0.935268
O	1.021457	-1.141888	-1.449053
C	-2.258206	1.576652	-1.469624
C	-2.341193	2.799910	-0.783907
C	-3.005800	1.424114	-2.647090
C	-3.175265	3.821139	-1.241552
H	-1.756355	2.954559	0.116091
C	-3.839511	2.444259	-3.109241
H	-2.944317	0.488403	-3.196487
C	-3.932704	3.645327	-2.403350
H	-3.232478	4.755912	-0.690328
H	-4.416717	2.298688	-4.018006
H	-4.584135	4.439365	-2.757037
C	2.397588	0.432939	-0.366555
C	4.374708	0.256112	0.596129
C	3.333352	-1.929943	0.021557
H	2.284770	-2.223051	0.013968
N	4.148981	1.539774	0.552878
N	2.917099	1.639878	-0.064870
N	3.339255	-0.454098	0.043208
C	5.447524	-0.511344	1.290984
H	5.992132	0.135612	1.979874
H	6.156486	-0.947224	0.574756
C	4.112349	-2.504813	1.273281

O	4.775563	-1.510159	2.059123
C	5.061887	-3.384246	-0.792728
C	4.068316	-2.482282	-1.177603
C	3.823793	-2.193103	-2.519707
C	4.619504	-2.810304	-3.487150
C	5.629292	-3.706211	-3.109521
C	5.852105	-4.004554	-1.762552
C	5.094808	-3.564139	0.703550
H	3.011447	-1.522507	-2.781003
H	6.241375	-4.178732	-3.872694
H	6.630169	-4.706267	-1.474668
H	6.091565	-3.420967	1.134073
H	4.769084	-4.571514	0.985737
C	2.307630	2.931625	-0.218324
C	1.764812	3.534283	0.926152
C	2.224438	3.497953	-1.497558
C	1.096352	4.750078	0.753027
C	1.549044	4.714943	-1.614736
C	0.967819	5.345886	-0.507323
H	0.653265	5.232260	1.620353
H	1.460164	5.172760	-2.596501
C	2.789172	2.792244	-2.701926
H	2.145722	1.950694	-2.984840
H	3.787391	2.388628	-2.504667
H	2.852599	3.469860	-3.556554
C	0.178548	6.618470	-0.684844
H	-0.825644	6.392811	-1.065472
H	0.654974	7.287761	-1.408248
H	0.061622	7.157046	0.259801
C	1.870279	2.878094	2.278923

H	2.888116	2.956516	2.676922
H	1.630894	1.812143	2.227474
H	1.186283	3.346224	2.989916
H	3.400343	-2.954028	1.967062
H	4.451165	-2.600631	-4.539571
H	0.180266	1.846424	-0.223978
C	-5.135398	-2.370088	-0.366834
C	-4.332635	-3.491436	-0.055015
C	-4.828193	-4.798962	-0.061776
C	-6.165664	-4.990502	-0.391144
C	-6.985125	-3.892897	-0.706313
C	-6.487044	-2.595152	-0.697521
C	-4.392187	-1.114279	-0.289034
C	-3.064550	-1.295722	0.068184
H	-4.186251	-5.639710	0.182269
H	-6.576618	-5.995484	-0.404908
H	-8.027273	-4.060681	-0.962011
H	-7.120256	-1.753125	-0.941027
S	-2.694415	-2.994662	0.317377
C	-5.024975	0.186082	-0.546080
O	-6.193978	0.332618	-0.888763
H	-4.387384	1.068146	-0.409767
C	-1.850097	-0.402683	0.276358
H	-1.017117	-1.106136	0.342225
C	-1.851950	0.338807	1.612394
C	-0.810772	0.201631	2.549620
C	-2.895360	1.200231	1.988842
C	-0.796411	0.883007	3.768067
C	-2.898643	1.898592	3.193758
H	-3.730986	1.330847	1.317194

C	-1.842170	1.744682	4.089897
H	0.026954	0.738167	4.458044
H	-3.729738	2.556176	3.428783
H	-1.830375	2.276710	5.036028
Br	0.694435	-0.977181	2.260016

Vibrational frequencies

15.5367	15.7759	21.3848
26.7436	27.7177	33.8484
38.7342	41.6186	46.2882
48.1598	57.3116	60.9673
65.8517	78.9784	80.6233
82.9174	88.2714	96.6042
99.1929	113.8472	122.3704
129.8969	135.4514	137.5466
149.5148	153.6979	157.0730
184.4058	189.1749	195.3688
201.2945	209.2952	216.8728
221.4629	229.6940	231.8635
243.4883	261.2527	270.7178
286.8132	288.1924	294.0324
300.3744	320.1676	325.0847
327.7875	345.3752	364.7228
377.7622	380.5735	401.5915
404.0896	409.0579	418.6873
429.8324	434.2437	443.4416
447.1720	452.7014	468.5628
488.0256	500.1045	503.8903
511.8886	517.7169	520.1671
528.0514	528.5319	530.3751
542.3591	551.3675	577.2088

580.3957	582.7037	591.5070
600.3355	609.0079	620.7599
631.5392	644.4640	648.5687
657.7980	672.9534	688.2623
696.6544	700.7152	708.0037
713.3157	714.5607	725.3046
731.2869	742.0226	748.4501
751.9746	757.7329	765.9957
768.9446	770.8537	777.7614
785.6235	796.3263	799.8177
811.5119	830.8642	848.1610
869.0386	870.8402	878.4376
882.9377	886.2813	886.6849
895.8003	905.5197	905.6561
907.4791	941.4898	948.5514
952.9364	960.5221	966.7924
969.4666	974.8340	976.6618
987.6404	987.7865	1002.6874
1004.7638	1005.9823	1006.6755
1014.5501	1022.4961	1024.3427
1034.9250	1041.3252	1042.2343
1044.7751	1045.4263	1050.1005
1052.2916	1056.2510	1057.1137
1059.1169	1065.8475	1068.7242
1071.1940	1071.6812	1083.7921
1090.4427	1097.7290	1101.5347
1116.7533	1118.6018	1143.7344
1148.2992	1173.2492	1180.4120
1183.1329	1185.5976	1192.5500
1192.9488	1196.1889	1199.6896

1203.2905	1209.6467	1213.8809
1218.1198	1221.3324	1222.4300
1243.0410	1257.6812	1270.3185
1281.4612	1288.7986	1289.8011
1295.0633	1305.6647	1311.0625
1316.4792	1323.0515	1331.6549
1337.5236	1342.7201	1352.3579
1355.7803	1357.9005	1364.1746
1366.5369	1369.9076	1378.2549
1403.8029	1404.7812	1413.4980
1417.8834	1419.7591	1428.3919
1436.9489	1447.1655	1458.9300
1463.9229	1467.1224	1471.0428
1471.3627	1475.1600	1477.1861
1481.1205	1483.2280	1486.7993
1488.6582	1491.6516	1494.8325
1495.6893	1497.5337	1501.2307
1508.8619	1510.0691	1520.9343
1526.9728	1536.5569	1549.7472
1607.6410	1617.3468	1630.8869
1636.4893	1638.9692	1641.0318
1641.9820	1643.3303	1645.0004
1653.9422	1655.3702	1657.5602
1734.3805	3037.5449	3042.3413
3046.9511	3053.2177	3058.0904
3064.5390	3075.7849	3078.7780
3096.6105	3100.5729	3104.5006
3117.4015	3119.4808	3130.5958
3138.7943	3147.1953	3149.9059
3153.3630	3177.8701	3181.6463

3183.0412	3183.0950	3185.5159
3189.0826	3191.8973	3193.4068
3196.6823	3201.0185	3202.5490
3205.4246	3210.0691	3210.9517
3212.9661	3216.2233	3222.8129
3255.1957	3264.7599	3282.3032

M4SR'

Zero-point correction= 0.347475

Thermal correction to Energy= 0.372275

Thermal correction to Enthalpy= 0.373220

Thermal correction to Gibbs Free Energy= 0.289742

Sum of electronic and zero-point Energies= -4082.969719

Sum of electronic and thermal Energies= -4082.944920

Sum of electronic and thermal Enthalpies= -4082.943975

Sum of electronic and thermal Free Energies= -4083.027453

Cartesian coordinates

C	1.177609	1.411715	1.108051
C	0.530501	1.507700	2.485271
H	2.262627	1.448009	1.242333
C	1.231033	1.407038	3.592326
O	1.869326	1.330220	4.575624
C	0.775509	2.632107	0.286073
C	-0.569394	2.946612	0.036978
C	1.761392	3.514245	-0.178485
C	-0.913696	4.088633	-0.686171
H	-1.355978	2.300985	0.413685
C	1.420088	4.659855	-0.900931
H	2.807354	3.302578	0.027979
C	0.079772	4.948017	-1.162490

H	-1.960802	4.308323	-0.873664
H	2.201969	5.326759	-1.252819
H	-0.189575	5.837450	-1.724628
H	-0.539364	1.654348	2.589382
C	-2.843190	-0.634640	0.052596
C	-2.632057	-0.303009	-1.306450
C	-3.677802	-0.256319	-2.233365
C	-4.962865	-0.545831	-1.785948
C	-5.194915	-0.879668	-0.439814
C	-4.152397	-0.928396	0.478200
C	-1.601431	-0.619062	0.810513
C	-0.510381	-0.256210	0.044067
H	-3.492543	0.000578	-3.271486
H	-5.792686	-0.513071	-2.485533
H	-6.205888	-1.102638	-0.111818
H	-4.327573	-1.183295	1.515469
S	-0.934794	0.015490	-1.631199
C	-1.486579	-1.031940	2.211596
O	-2.439343	-1.271779	2.945082
H	-0.457192	-1.146918	2.594944
C	0.911596	-0.031116	0.497684
H	1.069922	-0.684007	1.357765
C	1.901077	-0.505140	-0.561712
C	2.166102	-1.877759	-0.716505
C	2.555682	0.364523	-1.444790
C	3.047739	-2.366323	-1.676966
C	3.441207	-0.105317	-2.415697
H	2.360823	1.426603	-1.382737
C	3.692640	-1.470919	-2.531053
H	3.225856	-3.432651	-1.758474

H	3.928825	0.600320	-3.081077
H	4.380827	-1.847227	-3.281526
Br	1.277622	-3.172123	0.401082

Vibrational frequencies

19.6606	25.0667	25.9128
36.4106	40.1053	54.7262
69.3205	75.1139	100.8541
109.2407	129.7461	133.1016
150.6127	167.2883	200.2129
203.0059	212.2305	230.4043
241.7245	254.4382	287.2716
316.4273	334.6702	362.5515
375.5935	381.5047	424.5315
428.0169	443.5542	455.5068
488.4931	504.0788	509.1753
519.1123	530.9149	541.2203
557.8571	584.6323	617.1606
620.6468	634.0784	653.2351
655.0085	683.3080	709.0349
721.0220	734.2772	747.2833
752.9495	765.3419	775.5317
778.1168	781.3627	818.2288
849.2230	872.2030	884.8577
892.3208	911.1946	945.7937
962.2327	965.5267	976.9133
994.1524	998.1365	1003.8472
1010.2599	1013.7069	1014.7046
1029.0384	1034.6991	1048.7335
1059.1251	1060.7671	1079.5573
1087.2124	1115.0263	1149.5575

1150.3516	1156.7321	1178.7519
1187.2051	1195.6710	1196.6378
1206.4693	1217.7519	1219.8602
1254.3966	1270.0698	1292.9172
1312.4407	1322.2773	1335.2175
1359.3636	1365.2885	1367.8099
1383.5582	1384.2836	1431.8629
1448.3655	1471.4109	1475.5388
1493.2622	1498.3878	1508.9171
1536.3414	1556.3459	1608.8557
1619.4336	1635.8147	1643.2132
1644.0415	1655.9219	1740.6919
2195.1575	2985.1801	3079.0969
3094.9026	3178.5698	3186.0436
3190.8015	3195.0550	3197.4151
3202.3876	3204.1356	3210.3983
3211.3512	3213.2820	3213.5275
3220.7835	3244.1972	3246.7011

TS5SR'

Zero-point correction= 0.347885

Thermal correction to Energy= 0.371158

Thermal correction to Enthalpy= 0.372103

Thermal correction to Gibbs Free Energy= 0.293586

Sum of electronic and zero-point Energies= -4082.919017

Sum of electronic and thermal Energies= -4082.895744

Sum of electronic and thermal Enthalpies= -4082.894800

Sum of electronic and thermal Free Energies= -4082.973316

Cartesian coordinates

C	-0.557094	1.233435	-0.600923

C	0.319441	2.006074	0.397164
H	-0.265985	1.584042	-1.596174
C	0.170794	3.401282	0.519917
O	0.001877	4.522975	0.364384
C	-2.051599	1.434315	-0.449943
C	-2.838761	1.586654	-1.598177
C	-2.675536	1.455264	0.805358
C	-4.220330	1.748084	-1.499547
H	-2.364004	1.570091	-2.575675
C	-4.058138	1.613784	0.905971
H	-2.083853	1.336504	1.707836
C	-4.834859	1.758244	-0.245689
H	-4.815433	1.865005	-2.400676
H	-4.527620	1.623590	1.885420
H	-5.910980	1.882679	-0.165689
H	0.363589	1.574086	1.397103
C	3.700341	0.204529	-0.231850
C	3.817833	-1.168252	-0.559680
C	5.063690	-1.798704	-0.634779
C	6.201980	-1.040722	-0.370347
C	6.101824	0.321783	-0.032425
C	4.863189	0.947455	0.040580
C	2.325401	0.648680	-0.214876
C	1.436042	-0.342437	-0.510304
H	5.143260	-2.851019	-0.889719
H	7.179006	-1.512187	-0.422024
H	7.004490	0.888173	0.177362
H	4.759381	1.990790	0.319403
S	2.235767	-1.892149	-0.829542
C	1.931934	2.105377	0.014421

C	-0.075933	-0.272632	-0.520219
H	-0.440128	-0.734796	-1.442224
C	-0.686828	-1.035322	0.654889
C	-1.890911	-1.749676	0.553017
C	-0.070885	-1.014200	1.917315
C	-2.472048	-2.387028	1.649224
C	-0.639026	-1.638562	3.025899
H	0.885122	-0.511422	2.022348
C	-1.846799	-2.323651	2.893456
H	-3.404192	-2.927297	1.528582
H	-0.133593	-1.595566	3.985544
H	-2.300418	-2.817775	3.747071
Br	-2.818129	-1.898900	-1.124877
O	2.467256	2.804968	0.999456
H	1.938182	2.584783	-0.996552

Vibrational frequencies

-438.9968	22.5161	37.9834
44.0628	54.7476	58.4784
63.0546	73.7213	107.0677
116.3015	127.7357	142.7704
153.9249	171.2169	178.7141
215.7899	219.9651	249.9530
274.7456	289.9869	313.1901
321.3083	343.1672	359.8933
384.6533	415.4129	421.7812
441.0187	462.2672	487.9051
502.7565	505.4294	520.6733
533.0923	559.8505	568.0946
579.3566	623.0162	630.5630
642.1817	662.8260	683.1544

706.4931	714.5934	717.4603
728.9538	748.7414	755.8030
771.2906	776.8887	788.6710
794.5806	800.9456	856.1206
861.6902	888.8389	900.5744
910.1936	929.9957	965.2912
969.1522	978.4464	986.4382
1001.3388	1004.9273	1013.1195
1014.6614	1015.9071	1019.5411
1032.3827	1045.4780	1059.2225
1074.5909	1079.0337	1087.9723
1117.9254	1132.2529	1138.1395
1150.5900	1167.4337	1188.1514
1189.7517	1195.4315	1202.5578
1219.0726	1229.7321	1240.0159
1260.4726	1277.8275	1294.9941
1297.7331	1313.9783	1318.6300
1326.1137	1344.9322	1362.7240
1364.3950	1367.7062	1371.8565
1396.8505	1401.5663	1472.4921
1473.5535	1494.6575	1496.8720
1509.6906	1539.9089	1584.7069
1611.5660	1617.6682	1638.5213
1641.8036	1642.7780	1659.4572
2200.5607	2765.2423	3075.4799
3084.3582	3146.3171	3179.7663
3185.8275	3186.9982	3192.8398
3193.8640	3197.6570	3201.3609
3201.9247	3207.9284	3209.8140
3213.9801	3216.4026	3225.4620

TS5RR

Zero-point correction= 0.732397

Thermal correction to Energy= 0.777444

Thermal correction to Enthalpy= 0.778388

Thermal correction to Gibbs Free Energy= 0.650852

Sum of electronic and zero-point Energies= -5135.056222

Sum of electronic and thermal Energies= -5135.011175

Sum of electronic and thermal Enthalpies= -5135.010231

Sum of electronic and thermal Free Energies= -5135.137767

Cartesian coordinates

C	1.319907	0.134296	-1.404165
C	0.247823	-0.100898	-0.349599
C	-0.998177	-0.671017	-0.712997
O	-1.533650	-0.768560	-1.833403
C	0.885265	0.827184	-2.692731
C	0.778794	0.064659	-3.864923
C	0.646603	2.206506	-2.780983
C	0.427080	0.649882	-5.080761
H	0.970730	-1.003589	-3.819993
C	0.292556	2.797770	-3.996830
H	0.750832	2.832638	-1.902914
C	0.177941	2.023105	-5.151848
H	0.349935	0.034486	-5.973086
H	0.111241	3.868452	-4.037538
H	-0.095428	2.483528	-6.097137
C	-1.885255	-1.066983	0.449065
C	-3.621348	-1.243054	1.770171
C	-3.872186	0.447485	-0.026866
H	-3.135116	1.065925	-0.539305

N	-2.745580	-2.080278	2.262956
N	-1.663108	-1.960221	1.413911
N	-3.135585	-0.621168	0.651124
C	-4.920954	-0.743332	2.306064
H	-5.058780	-1.066895	3.338536
H	-5.762831	-1.105908	1.702198
C	-4.674228	1.308196	1.023789
O	-4.823662	0.681476	2.305253
C	-6.152382	0.555319	-0.751489
C	-4.929847	-0.084656	-0.970155
C	-4.780345	-1.058939	-1.956095
C	-5.895893	-1.400331	-2.724765
C	-7.127363	-0.767898	-2.508976
C	-7.263330	0.215376	-1.524619
C	-6.041056	1.582286	0.347978
H	-3.813554	-1.525118	-2.116075
H	-7.986553	-1.045121	-3.113264
H	-8.219894	0.703856	-1.360972
H	-6.845956	1.522102	1.086841
H	-6.057127	2.597744	-0.065162
C	-0.465427	-2.721428	1.645926
C	0.368402	-2.314408	2.695702
C	-0.192259	-3.821281	0.818757
C	1.525831	-3.068870	2.913185
C	0.983116	-4.530407	1.073816
C	1.850610	-4.169729	2.113668
H	2.194492	-2.777691	3.717456
H	1.226606	-5.384657	0.447270
C	-1.122341	-4.211750	-0.302926
H	-1.103449	-3.474522	-1.113705

H	-2.158906	-4.282847	0.044060
H	-0.834058	-5.178167	-0.722282
C	3.125821	-4.942356	2.337662
H	3.826141	-4.775476	1.511231
H	2.933895	-6.019712	2.386212
H	3.622265	-4.639662	3.263326
C	0.041943	-1.103805	3.532138
H	-0.815432	-1.301344	4.185898
H	-0.225996	-0.237593	2.912313
H	0.892417	-0.834112	4.163328
H	-4.121849	2.222314	1.239242
H	-5.807505	-2.159301	-3.496627
H	0.650207	-0.473321	0.588716
C	0.998089	3.477919	1.558475
C	2.289219	4.058176	1.601646
C	2.559710	5.208062	2.350508
C	1.517814	5.787506	3.069298
C	0.228699	5.225187	3.042557
C	-0.036256	4.081390	2.298758
C	0.942552	2.298716	0.706757
C	2.150834	2.001457	0.145355
H	3.556344	5.638433	2.369819
H	1.706105	6.681008	3.657455
H	-0.569353	5.690068	3.614363
H	-1.020686	3.628504	2.284493
S	3.421468	3.148315	0.614385
C	-0.392137	1.612482	0.459149
C	2.547744	0.851813	-0.746626
H	3.140233	1.259553	-1.572859
C	3.441258	-0.160502	-0.027111

C	4.306169	-1.008122	-0.737547
C	3.424276	-0.303462	1.367353
C	5.130034	-1.937520	-0.106072
C	4.241872	-1.224749	2.020548
H	2.758479	0.329309	1.944910
C	5.101334	-2.040571	1.285208
H	5.788815	-2.567429	-0.693310
H	4.205696	-1.302300	3.102192
H	5.747275	-2.756764	1.783150
Br	4.383453	-0.921488	-2.663114
O	-1.151507	1.389260	1.461092
H	-0.850556	1.986698	-0.479795
H	1.684372	-0.851992	-1.712327

Vibrational frequencies

-283.4858	9.4079	19.2156
25.6545	27.6328	29.8584
32.0883	35.7788	37.8800
42.3802	45.8803	51.2717
60.5272	65.0988	74.9400
86.3250	88.2786	91.9702
106.5622	120.7485	128.0095
135.3092	141.0306	144.7976
153.0668	156.2083	163.5298
174.7734	185.2968	200.3823
207.1371	213.3397	220.2333
233.2488	236.0781	242.2024
244.4395	251.6271	263.3783
265.5618	281.5478	287.0093
298.8602	309.7442	326.0804
333.4957	338.0983	360.0922

373.5855	383.6065	398.7768
404.7545	415.0900	416.6372
429.4599	441.2747	447.6072
450.2875	460.7833	484.1585
491.2664	498.6576	506.5846
508.2852	511.3516	517.4612
525.7201	530.5570	532.2099
548.5482	570.6739	577.6467
580.9422	585.2358	598.1879
603.5328	606.3754	616.2934
630.4822	639.1250	642.8892
667.8631	683.0076	704.5099
709.9164	712.2319	718.6019
724.9419	726.3806	733.7902
742.9427	747.5602	752.2364
764.2985	764.9353	773.3310
775.4394	785.3367	793.1235
800.4047	805.1984	824.7588
842.4630	849.9712	855.5960
861.3279	875.3833	877.2119
881.7416	888.7687	898.0559
906.1265	909.3571	916.1598
926.1976	943.1639	956.1669
960.7087	963.0051	972.8677
973.9249	976.2035	978.8158
981.2593	987.6791	996.4356
998.5970	1008.2935	1008.5061
1014.2096	1018.0071	1026.1106
1030.3054	1033.7904	1041.1621
1048.9735	1050.4393	1051.9074

1053.9668	1059.0278	1063.0733
1068.4582	1071.1187	1074.2218
1074.8006	1076.3620	1082.2978
1094.3402	1100.5299	1113.6152
1116.2193	1122.7139	1140.1439
1151.6931	1175.1743	1183.5489
1184.0098	1185.3383	1187.6355
1192.2766	1192.3852	1193.3972
1201.2860	1208.5747	1209.4191
1215.0304	1227.1503	1231.1601
1247.6303	1261.2129	1267.4155
1277.8012	1287.4606	1290.2199
1291.3285	1299.7795	1307.5093
1311.3091	1321.6818	1330.1188
1330.8646	1335.5899	1346.2512
1348.4010	1352.4496	1359.4985
1361.0494	1369.1554	1372.4925
1377.1761	1377.8364	1397.5593
1410.9717	1412.7620	1429.5519
1437.7334	1446.5272	1449.9544
1453.1023	1465.6850	1471.4298
1473.7541	1474.5145	1483.6362
1487.3478	1489.3798	1490.3725
1492.1093	1493.3362	1498.8436
1499.1892	1502.3321	1502.9987
1503.6354	1511.7804	1521.3892
1525.1707	1536.3047	1552.5781
1589.3199	1611.2894	1617.0303
1631.9993	1634.6776	1641.0653
1641.1996	1641.4304	1641.9492

1653.2506	1656.4943	1658.4329
1678.6113	2863.5657	3018.8436
3043.3030	3044.0252	3046.4506
3052.9823	3055.6831	3055.8690
3086.5952	3103.7945	3105.5393
3106.3682	3131.4660	3131.8159
3135.7211	3142.2840	3146.5079
3156.4244	3174.6263	3175.3511
3183.0818	3183.2410	3183.6101
3185.9497	3192.1998	3194.2687
3194.9129	3196.6901	3197.2021
3202.4866	3204.4380	3205.0391
3208.7590	3214.2695	3214.9924
3219.4893	3222.1979	3227.4305

TS5RS

Zero-point correction= 0.733414

Thermal correction to Energy= 0.777986

Thermal correction to Enthalpy= 0.778931

Thermal correction to Gibbs Free Energy= 0.654589

Sum of electronic and zero-point Energies= -5135.052034

Sum of electronic and thermal Energies= -5135.007461

Sum of electronic and thermal Enthalpies= -5135.006517

Sum of electronic and thermal Free Energies= -5135.130858

Cartesian coordinates

C	1.297857	-0.783093	-0.955164
C	0.082017	-0.288774	-0.184285
C	-1.193679	-0.889084	-0.316412
O	-1.677982	-1.555518	-1.249060
C	1.161707	-0.857717	-2.472241

C	0.907078	-2.106440	-3.057166
C	1.297603	0.249370	-3.323710
C	0.779235	-2.249432	-4.438715
H	0.798451	-2.976605	-2.416108
C	1.172444	0.112142	-4.708523
H	1.515659	1.226249	-2.909620
C	0.910991	-1.136973	-5.273256
H	0.579980	-3.229731	-4.862998
H	1.284566	0.986231	-5.344151
H	0.815084	-1.243729	-6.350112
C	-2.153816	-0.503472	0.790781
C	-3.943970	0.183026	1.847192
C	-4.086845	0.342322	-0.628288
H	-3.308763	0.519161	-1.370562
N	-3.101151	-0.133373	2.796890
N	-1.984076	-0.567492	2.116549
N	-3.401451	-0.042403	0.609878
C	-5.253737	0.895933	1.888962
H	-5.435179	1.303245	2.884295
H	-6.080115	0.226022	1.618947
C	-4.935522	1.653440	-0.395306
O	-5.125813	1.994184	0.984271
C	-6.330781	-0.097087	-1.344828
C	-5.095574	-0.692368	-1.077210
C	-4.896474	-2.063327	-1.235331
C	-5.973153	-2.846039	-1.658850
C	-7.216894	-2.258176	-1.924729
C	-7.402562	-0.881015	-1.774396
C	-6.278335	1.394032	-1.123956
H	-3.920658	-2.496107	-1.041207

H	-8.045869	-2.879507	-2.251710
H	-8.368028	-0.428402	-1.982761
H	-7.111241	1.776825	-0.526117
H	-6.295004	1.929720	-2.080500
C	-0.775149	-0.917176	2.818054
C	-0.018985	0.136380	3.362693
C	-0.359325	-2.253623	2.833568
C	1.208205	-0.197766	3.937962
C	0.882012	-2.528892	3.419124
C	1.678344	-1.518252	3.966693
H	1.822634	0.596029	4.354654
H	1.233189	-3.556930	3.439411
C	-1.183667	-3.348002	2.204516
H	-1.074530	-3.346457	1.113565
H	-2.249163	-3.232388	2.426112
H	-0.862259	-4.327702	2.565962
C	3.038694	-1.823152	4.540905
H	3.823755	-1.497307	3.849084
H	3.173750	-2.894569	4.714455
H	3.199550	-1.297724	5.487763
C	-0.483479	1.566100	3.261165
H	-1.387900	1.730822	3.856858
H	-0.727166	1.832441	2.222898
H	0.291713	2.246695	3.621165
H	-4.397630	2.507844	-0.805385
H	-5.844580	-3.916996	-1.785772
H	0.333702	-0.060640	0.844329
C	1.203020	3.611156	-0.163997
C	2.548910	3.996060	0.051170
C	2.912173	5.322917	0.305082

C	1.906197	6.283035	0.360650
C	0.561483	5.921862	0.159500
C	0.205093	4.604049	-0.099612
C	1.063811	2.187428	-0.428802
C	2.267542	1.533255	-0.421317
H	3.951619	5.596106	0.460063
H	2.164539	7.318512	0.562713
H	-0.209985	6.685140	0.209751
H	-0.828223	4.311781	-0.240840
S	3.627358	2.615487	-0.062140
C	-0.315489	1.576715	-0.674311
C	2.512516	0.039045	-0.417387
H	2.556779	-0.217582	0.648822
C	3.820388	-0.457247	-1.008180
C	4.457840	-1.595223	-0.485377
C	4.416846	0.137318	-2.130610
C	5.631360	-2.113327	-1.029037
C	5.590978	-0.364243	-2.690479
H	3.945684	1.008949	-2.569385
C	6.202138	-1.489924	-2.138620
H	6.093469	-2.991103	-0.591347
H	6.023572	0.123333	-3.558632
H	7.117501	-1.888765	-2.564989
Br	3.706413	-2.525255	1.036117
O	-1.304992	2.042826	-0.010278
H	-0.471428	1.340352	-1.745308
H	1.493094	-1.810701	-0.623392

Vibrational frequencies

-316.0001	14.8322	22.8764
25.9129	31.7342	37.8661

38.1018	43.3596	46.0185
52.7002	57.9226	62.9495
67.2495	76.9964	80.3826
83.2496	90.4425	105.0767
107.6740	124.5507	135.0718
141.0693	142.3456	150.1878
158.0663	166.2158	171.0586
180.9270	198.1919	209.3173
210.8489	215.1924	223.0305
231.8656	235.8419	241.9329
252.9821	264.3896	267.9774
276.8344	285.4328	295.2560
297.3147	310.3882	325.8104
336.5016	340.0764	349.1116
377.5656	386.5132	403.0917
404.4581	421.9162	427.4719
431.0118	438.2379	446.1703
447.1697	469.5318	489.6055
490.7331	493.8255	502.9630
505.8456	508.4520	516.8082
527.6065	529.8617	532.0806
544.7730	559.7528	580.5349
581.3922	591.2812	601.7469
605.4889	615.8953	616.5375
632.7373	641.7394	653.6645
664.0179	679.1826	702.5001
706.6345	711.6297	719.1738
722.2085	725.4145	733.9964
742.0231	745.3504	753.8187
760.7541	763.7265	774.5587

776.5270	788.7897	791.2151
795.4017	814.3988	824.0979
839.6798	842.5515	855.6446
865.4795	873.6334	875.1043
880.0105	887.0374	896.6572
905.2636	905.9358	926.2988
940.2918	944.9873	959.5593
961.9166	972.0836	974.8990
976.0146	976.7922	986.1101
986.5301	990.0811	997.8501
1002.9709	1003.8131	1009.9772
1013.6986	1015.8050	1027.0944
1030.9337	1040.3300	1041.6786
1048.6532	1049.3341	1051.4806
1052.7585	1060.8582	1063.2553
1067.9979	1072.0140	1074.0482
1077.7507	1080.8890	1086.3139
1095.1932	1104.3640	1112.8531
1116.5454	1121.7882	1136.8163
1153.4358	1173.0794	1183.3576
1184.2749	1185.4358	1189.8571
1193.3054	1194.5687	1198.9434
1204.6421	1211.7562	1215.0458
1228.8675	1234.5456	1239.5517
1247.3350	1272.2812	1277.1168
1287.9462	1292.0767	1293.4037
1295.3934	1299.7951	1309.2031
1311.7671	1321.9855	1327.0403
1333.7617	1335.2272	1341.9997
1347.4363	1354.4827	1361.4174

1361.7309	1366.9384	1369.3797
1383.6705	1386.8500	1400.7989
1412.0119	1419.2919	1426.1292
1437.6337	1443.8434	1450.2662
1452.3014	1467.7859	1469.8476
1473.8947	1477.2065	1488.9659
1489.6197	1490.7738	1491.4820
1491.9166	1494.7814	1498.2420
1499.5968	1501.0251	1504.3067
1507.1631	1512.9360	1521.5258
1525.7264	1536.5811	1537.8929
1567.6119	1605.1956	1617.7222
1630.7400	1635.1654	1640.3320
1640.6919	1641.0860	1643.1888
1652.1762	1656.7771	1658.2625
1688.0386	2893.6253	3013.2789
3026.3591	3033.5310	3043.9824
3045.7650	3049.2957	3056.0554
3091.4876	3103.9619	3107.8827
3108.1519	3127.4730	3134.4580
3136.6936	3139.3934	3145.3063
3156.6320	3175.5416	3182.8715
3183.1142	3184.1148	3185.1002
3187.7282	3192.2201	3192.3541
3195.2606	3195.9209	3202.5795
3202.7895	3204.0118	3207.5783
3208.1428	3213.9724	3219.8634
3221.9517	3226.1036	3232.7461

TS5SR

Zero-point correction= 0.732828

Thermal correction to Energy= 0.777528

Thermal correction to Enthalpy= 0.778472

Thermal correction to Gibbs Free Energy= 0.653550

Sum of electronic and zero-point Energies= -5135.063949

Sum of electronic and thermal Energies= -5135.019249

Sum of electronic and thermal Enthalpies= -5135.018305

Sum of electronic and thermal Free Energies= -5135.143227

Cartesian coordinates

C	1.146045	-0.085379	-1.465138
C	0.093057	0.008985	-0.378321
H	0.694158	0.295609	-2.388674
C	-1.126313	-0.684334	-0.602461
O	-1.580693	-1.083762	-1.690318
C	1.582979	-1.517443	-1.743377
C	1.669677	-1.985998	-3.059023
C	1.915640	-2.390556	-0.698339
C	2.088226	-3.289566	-3.329516
H	1.409280	-1.320612	-3.878494
C	2.339568	-3.692644	-0.963588
H	1.844719	-2.051055	0.328819
C	2.430641	-4.146963	-2.281661
H	2.146649	-3.635275	-4.358130
H	2.596430	-4.351012	-0.138035
H	2.757510	-5.162059	-2.489925
C	-2.086648	-0.726123	0.560719
C	-3.917176	-0.538932	1.746042
C	-4.097072	0.358914	-0.561191
H	-3.343642	0.812208	-1.204332
N	-3.042120	-1.058463	2.568486

N	-1.899221	-1.174358	1.804019
N	-3.371816	-0.336880	0.506625
C	-5.278168	0.024987	1.983942
H	-5.484057	0.088828	3.053061
H	-6.052415	-0.588203	1.505287
C	-5.032793	1.472521	0.051709
O	-5.242475	1.354918	1.465012
C	-6.308275	0.011908	-1.414723
C	-5.034688	-0.554801	-1.320483
C	-4.743165	-1.792820	-1.891981
C	-5.765095	-2.474005	-2.557739
C	-7.046692	-1.915599	-2.652180
C	-7.325248	-0.668282	-2.086207
C	-6.357459	1.362431	-0.744616
H	-3.739470	-2.198988	-1.824628
H	-7.832088	-2.457198	-3.171760
H	-8.319618	-0.237344	-2.162772
H	-7.212562	1.486025	-0.072893
H	-6.414372	2.164520	-1.489815
C	-0.680563	-1.663247	2.392965
C	0.022828	-0.786911	3.233015
C	-0.255595	-2.965865	2.100846
C	1.206805	-1.267129	3.799074
C	0.939676	-3.390102	2.688159
C	1.683544	-2.556569	3.532418
H	1.776401	-0.612070	4.451743
H	1.298696	-4.393428	2.475192
C	-1.027086	-3.856489	1.161643
H	-0.922741	-3.514428	0.125490
H	-2.095826	-3.864719	1.399988

H	-0.655244	-4.882371	1.209986
C	3.002027	-3.021452	4.095719
H	3.802678	-2.864803	3.362420
H	2.982715	-4.089084	4.335577
H	3.272217	-2.467782	4.999467
C	-0.462649	0.618470	3.480221
H	-1.380980	0.618120	4.078220
H	-0.696306	1.141638	2.542648
H	0.292682	1.194158	4.020763
H	-4.553866	2.444360	-0.064044
H	-5.563758	-3.441457	-3.008445
H	0.450170	0.020839	0.645064
C	0.543537	4.085000	-0.179865
C	1.799396	4.725253	-0.322442
C	1.964900	6.094325	-0.088701
C	0.852513	6.837348	0.296606
C	-0.403130	6.221312	0.446418
C	-0.563765	4.860303	0.214693
C	0.603013	2.663645	-0.488377
C	1.856894	2.258092	-0.840912
H	2.936018	6.565970	-0.205456
H	0.958870	7.901864	0.484431
H	-1.258351	6.817984	0.750827
H	-1.521341	4.369576	0.340989
S	3.037509	3.581925	-0.817809
C	-0.662793	1.815392	-0.475962
C	2.353708	0.872023	-1.170510
H	2.920826	0.930294	-2.104817
C	3.313696	0.361421	-0.095035
C	4.458838	-0.395845	-0.389017

C	3.073013	0.634454	1.260936
C	5.314634	-0.870654	0.605357
C	3.915803	0.171956	2.268761
H	2.209027	1.236858	1.521522
C	5.040837	-0.585961	1.942036
H	6.187275	-1.453698	0.333523
H	3.693886	0.405508	3.304436
H	5.708776	-0.949261	2.716884
Br	4.922173	-0.832514	-2.203193
O	-1.523008	2.025546	0.447543
H	-1.029783	1.671536	-1.518701

Vibrational frequencies

-276.4433	13.9148	20.3598
27.6573	32.1664	34.8795
40.1876	44.4177	48.5264
52.1045	52.6918	60.1094
71.3014	75.7116	79.4932
85.8639	91.1290	102.8972
109.8773	113.6906	117.0005
123.8049	138.0613	148.0455
156.1648	165.3221	177.1614
192.1845	196.1751	201.3978
207.1436	212.7083	215.3208
226.0912	231.0944	240.6733
245.0522	258.5655	272.5914
279.8245	290.8962	295.6053
300.8002	319.1966	332.1225
334.3431	337.5761	356.3512
377.6646	382.8498	398.9941
406.3877	415.6074	419.4686

429.5601	440.9660	445.7945
447.4842	469.6390	489.7926
493.6906	495.8480	503.6147
507.8507	511.4687	519.2129
530.9414	531.1125	535.0957
549.4517	557.5383	579.0917
581.4969	587.3660	600.8443
603.1662	608.5085	617.8885
626.8019	632.8515	643.3517
662.6254	687.2679	698.0559
709.3368	714.2621	715.4954
720.5650	727.4042	735.1719
747.6592	751.1526	755.7431
762.3982	764.1566	778.7852
783.8314	785.5382	792.8480
796.5676	801.7905	815.2560
833.6277	843.0962	862.7436
865.3276	875.3075	879.3019
880.8971	888.9281	902.6265
905.4851	911.9230	917.2472
929.6067	943.9297	959.8594
961.2271	965.5415	975.1817
976.3107	978.0337	984.8437
985.5181	991.9761	997.8684
1000.6965	1002.8829	1013.4094
1015.2101	1018.5544	1030.0652
1030.4223	1043.3191	1044.6259
1047.6005	1049.3323	1050.7873
1056.3354	1057.6159	1065.8438
1068.7412	1070.2648	1076.3835

1077.7665	1079.3175	1086.6676
1097.8817	1102.5840	1115.0920
1116.2663	1132.1979	1145.0856
1151.3825	1169.9579	1182.8182
1183.4078	1183.7803	1189.1667
1191.8326	1193.5991	1197.1709
1203.0070	1205.8410	1211.4056
1212.0399	1225.2676	1229.4511
1245.0342	1258.7394	1271.7087
1285.4543	1289.3972	1289.6616
1295.5810	1299.8688	1307.9219
1311.6817	1320.0661	1328.4913
1331.8120	1333.3857	1342.1136
1343.4441	1353.2732	1357.2040
1361.9765	1363.7556	1368.4272
1372.2492	1380.8596	1386.5854
1411.9186	1421.2841	1425.4535
1434.4079	1445.5779	1447.8093
1453.2205	1467.3635	1469.6097
1472.5016	1472.7266	1484.4520
1487.1820	1488.4779	1491.0848
1491.4558	1493.9691	1497.9107
1498.1780	1504.4254	1505.1855
1508.1547	1510.6764	1520.0844
1523.1518	1535.9050	1549.8426
1587.6282	1610.1763	1616.0912
1629.3906	1637.0918	1640.3928
1640.7648	1641.0964	1642.9366
1652.1340	1657.0645	1657.6819
1673.1406	2796.3402	3024.4681

3039.7672	3043.0076	3046.1433
3046.3184	3056.1224	3068.0191
3088.6499	3103.4849	3104.6023
3105.3577	3130.4042	3131.7808
3138.5110	3140.5136	3150.1284
3158.2402	3171.3709	3178.2858
3182.9197	3183.1076	3184.5714
3187.8831	3191.8767	3192.4808
3194.3376	3196.2550	3200.2122
3202.1404	3204.5156	3205.7855
3209.0892	3216.1569	3216.9386
3218.0612	3222.8087	3230.2802

TS5SS

Zero-point correction= 0.732588

Thermal correction to Energy= 0.777387

Thermal correction to Enthalpy= 0.778331

Thermal correction to Gibbs Free Energy= 0.651972

Sum of electronic and zero-point Energies= -5135.056657

Sum of electronic and thermal Energies= -5135.011858

Sum of electronic and thermal Enthalpies= -5135.010914

Sum of electronic and thermal Free Energies= -5135.137273

Cartesian coordinates

C	-1.197657	-1.266490	0.071694
C	0.035299	-0.390071	-0.045416
H	-1.045742	-1.931102	0.929004
C	1.273267	-1.084966	-0.164751
O	1.466569	-2.272893	0.148483
C	-1.420078	-2.145253	-1.155064
C	-1.646605	-3.518762	-1.018679

C	-1.429985	-1.588947	-2.441786
C	-1.875119	-4.321057	-2.139453
H	-1.647323	-3.960177	-0.025762
C	-1.655055	-2.385001	-3.564023
H	-1.268503	-0.520820	-2.563856
C	-1.878028	-3.756888	-3.416555
H	-2.047686	-5.386497	-2.013641
H	-1.661346	-1.935196	-4.553205
H	-2.054007	-4.379125	-4.289563
C	2.498711	-0.283428	-0.538867
C	3.936693	1.118383	-1.438025
C	1.656685	1.404496	-2.304009
H	0.811445	0.724944	-2.420147
N	4.654525	0.359985	-0.653298
N	3.746719	-0.509901	-0.096780
N	2.614674	0.756685	-1.398177
C	4.336071	2.142654	-2.447561
H	5.417281	2.132756	-2.590199
H	4.026910	3.145896	-2.129792
C	2.305191	1.650964	-3.713523
O	3.736221	1.757890	-3.686516
C	1.175499	3.649565	-2.950726
C	1.215924	2.784758	-1.851697
C	0.865249	3.209251	-0.571081
C	0.438904	4.532025	-0.411523
C	0.375371	5.400209	-1.507650
C	0.749305	4.966428	-2.784231
C	1.630084	2.950589	-4.208891
H	0.954426	2.546656	0.289800
H	0.045887	6.425568	-1.364686

H	0.718218	5.647694	-3.630093
H	2.330287	3.537170	-4.810538
H	0.774947	2.702191	-4.849754
C	4.238457	-1.514316	0.819250
C	4.514128	-2.793553	0.315934
C	4.501862	-1.133749	2.141749
C	5.025497	-3.734931	1.212288
C	5.010154	-2.117775	2.996691
C	5.267569	-3.420118	2.555321
H	5.241589	-4.736962	0.850956
H	5.215998	-1.853775	4.030694
C	4.265353	0.275611	2.614483
H	3.230783	0.589253	2.426672
H	4.918343	0.977012	2.081158
H	4.478005	0.363147	3.683119
C	5.779230	-4.470061	3.510055
H	4.944898	-5.017589	3.966305
H	6.359710	-4.024032	4.323221
H	6.408872	-5.204411	2.998387
C	4.258213	-3.142325	-1.125760
H	4.695790	-2.400164	-1.802528
H	3.180515	-3.174430	-1.314283
H	4.683484	-4.118341	-1.371484
H	2.104787	0.805251	-4.373761
H	0.161502	4.885808	0.577351
H	-0.089448	0.537769	-0.589815
C	-1.238753	2.269481	2.761352
C	-2.578060	2.731911	2.773433
C	-2.971096	3.855194	3.508221
C	-2.003656	4.537142	4.240371

C	-0.667383	4.098394	4.241012
C	-0.281130	2.978766	3.513227
C	-1.068933	1.080163	1.937257
C	-2.236796	0.677542	1.357547
H	-4.004541	4.188279	3.505234
H	-2.285885	5.414602	4.814857
H	0.074226	4.643116	4.818397
H	0.746943	2.639682	3.497834
S	-3.608335	1.716996	1.776527
C	0.290292	0.424369	1.756604
C	-2.471234	-0.414548	0.344453
C	-3.632681	-1.322570	0.733270
C	-4.715871	-1.611215	-0.104967
C	-3.613419	-1.950988	1.989160
C	-5.735252	-2.487247	0.275594
C	-4.617553	-2.827700	2.387912
H	-2.785147	-1.734356	2.658172
C	-5.683258	-3.098733	1.526069
H	-6.558619	-2.686692	-0.401086
H	-4.570478	-3.296457	3.365986
H	-6.475045	-3.779786	1.822789
Br	-4.865936	-0.803975	-1.846263
O	1.312473	1.189028	1.783125
H	0.356208	-0.568897	2.247732
H	-2.732126	0.086383	-0.593923

Vibrational frequencies

-282.6274	11.4995	18.8081
21.7982	25.2020	27.6291
34.6028	36.0519	38.7699
52.6761	54.7477	60.3644

71.0052 75.2851 76.6213

84.9101 91.3515 97.8867

105.4612 116.7671 125.3228

132.8721 143.1260 146.7918

160.6279 167.2660 183.1075

192.8864 204.0104 207.3487

212.6116 213.9743 216.1317

224.7425 226.4964 234.7183

249.4197 258.5171 266.3672

281.3599 287.8570 293.7551

305.1420 316.8667 330.6843

335.0745 339.0976 345.5565

362.3278 378.6470 394.4109

407.6472 414.8874 417.0091

423.1875 436.7450 441.1012

449.8209 471.8324 480.9167

489.2041 494.8562 497.9825

505.3140 514.7923 519.9446

526.1871 531.3239 537.2300

550.7627 555.7880 573.5311

579.5516 583.6009 595.3649

609.5067 614.0922 616.7716

624.9531 633.2333 646.8291

651.9260 682.8849 690.8707

706.4858 715.1781 716.5725

720.4442 731.6190 739.5524

742.3754 751.3705 757.3971

765.0702 770.7336 774.7120

783.7043 789.2512 796.1560

804.4829 813.8404 821.0609

832.1789	839.5977	861.3972
863.5756	871.8518	875.1824
879.4978	893.4972	895.2744
899.2597	916.2557	917.4459
930.1640	946.5123	958.4597
960.9398	964.1772	975.5283
977.6695	978.1595	989.0314
991.4211	996.7114	998.7389
1007.7031	1009.3974	1014.4970
1028.5184	1029.1502	1035.5475
1046.0474	1048.5755	1049.1011
1050.1515	1051.8879	1054.6464
1061.6260	1064.0103	1065.4963
1068.9253	1074.0798	1076.0664
1081.1004	1084.7935	1086.2243
1094.2809	1106.4394	1112.9338
1117.3345	1128.7469	1142.0450
1148.7419	1174.7181	1179.5019
1183.8636	1184.5523	1190.3728
1191.4045	1193.6424	1199.7805
1204.5029	1206.9206	1217.5187
1219.2317	1224.3184	1236.5697
1248.4296	1253.9796	1268.1929
1284.8443	1289.4691	1290.1517
1293.5666	1296.6029	1306.8000
1318.3514	1320.4351	1332.4360
1333.1997	1342.5377	1343.0546
1345.1689	1351.9170	1358.9627
1360.3563	1365.5755	1368.1201
1371.2137	1378.0578	1385.7545

1410.6287	1415.5316	1421.2550
1436.0458	1440.6774	1447.5367
1450.4314	1465.2910	1470.1443
1471.4801	1474.9355	1475.3267
1487.2519	1488.3585	1490.1736
1490.8408	1492.5146	1493.3743
1493.7896	1497.3408	1500.3869
1508.8981	1511.3333	1518.1855
1526.1760	1530.9813	1534.6527
1587.3290	1610.0999	1617.7741
1632.4571	1637.9567	1639.2891
1640.5821	1641.8670	1644.1999
1652.7185	1656.4265	1657.6672
1671.0894	2865.1102	3014.7475
3038.7564	3047.5985	3051.0299
3053.7076	3057.3720	3067.5665
3084.5503	3100.8536	3108.8408
3114.2686	3115.9058	3121.0734
3127.4673	3127.9436	3128.0516
3139.0499	3155.6655	3172.0207
3177.2319	3181.4050	3182.6525
3183.2868	3184.7976	3186.4340
3187.6246	3193.0089	3193.6129
3195.9546	3198.1722	3204.5004
3205.1181	3208.0597	3210.7019
3220.2890	3221.1113	3237.4540

M5RR

Zero-point correction= 0.734949

Thermal correction to Energy= 0.779431

Thermal correction to Enthalpy= 0.780375

Thermal correction to Gibbs Free Energy= 0.655396

Sum of electronic and zero-point Energies= -5135.080638

Sum of electronic and thermal Energies= -5135.036156

Sum of electronic and thermal Enthalpies= -5135.035212

Sum of electronic and thermal Free Energies= -5135.160191

Cartesian coordinates

C	-1.296065	1.237399	0.933298
C	-0.416340	0.154347	0.306768
C	0.798315	-0.431175	0.941105
O	1.143415	-0.451553	2.102186
C	-0.543511	2.544251	1.148638
C	0.310411	2.643286	2.259375
C	-0.623041	3.632283	0.268835
C	1.070396	3.791341	2.479524
H	0.385814	1.803808	2.943287
C	0.132256	4.787058	0.492912
H	-1.267185	3.586076	-0.602964
C	0.984157	4.869897	1.594856
H	1.729210	3.843050	3.341802
H	0.055254	5.619274	-0.201147
H	1.573260	5.766373	1.765506
C	1.607256	-1.102255	-0.228056
C	3.632104	-2.154202	-0.339427
C	3.758806	0.302902	-0.383161
H	3.036564	1.071920	-0.673084
N	2.804767	-3.144491	-0.364745
N	1.531653	-2.540756	-0.253291
N	3.025552	-0.928622	-0.153173
C	5.088106	-2.112421	-0.657272

H	5.437365	-3.086967	-1.001826
H	5.674736	-1.814455	0.222195
C	4.813061	0.155467	-1.540313
O	5.266257	-1.192499	-1.743850
C	5.839566	1.229676	0.368983
C	4.588441	0.777334	0.798628
C	4.234290	0.804489	2.145889
C	5.156450	1.305251	3.069993
C	6.408656	1.766257	2.645183
C	6.758913	1.729250	1.291535
C	5.975681	1.089002	-1.128984
H	3.270277	0.424847	2.467361
H	7.118108	2.147441	3.374442
H	7.736257	2.075405	0.965789
H	6.935295	0.670626	-1.446820
H	5.864659	2.063564	-1.621778
C	0.403379	-3.283597	0.199905
C	-0.697701	-3.454567	-0.663331
C	0.387547	-3.811516	1.510238
C	-1.835258	-4.105084	-0.168528
C	-0.767890	-4.460798	1.952355
C	-1.898175	-4.597776	1.137025
H	-2.689998	-4.235280	-0.827627
H	-0.791760	-4.856812	2.964912
C	1.588078	-3.688503	2.414264
H	1.977912	-2.667496	2.419168
H	2.400750	-4.340430	2.076379
H	1.331340	-3.966514	3.440106
C	-3.163500	-5.226629	1.665544
H	-3.806759	-4.466116	2.126584

H	-2.951350	-5.981134	2.429338
H	-3.741977	-5.699881	0.865986
C	-0.691367	-2.957076	-2.087720
H	0.320168	-2.923838	-2.496100
H	-1.087737	-1.939473	-2.159193
H	-1.313755	-3.600224	-2.717390
H	4.370799	0.448251	-2.495521
H	4.901923	1.330762	4.125832
H	-1.042874	-0.732757	0.120316
C	-0.951737	0.875214	-3.423083
C	-2.184017	1.300585	-3.977568
C	-2.369402	1.398538	-5.359780
C	-1.303279	1.065263	-6.191579
C	-0.073826	0.637818	-5.657205
C	0.109094	0.538123	-4.283426
C	-0.994944	0.842195	-1.981905
C	-2.195349	1.235902	-1.457716
H	-3.317032	1.726804	-5.775114
H	-1.426519	1.134704	-7.268206
H	0.739965	0.379378	-6.328049
H	1.048220	0.195629	-3.862261
S	-3.359176	1.663528	-2.714540
C	0.143871	0.566010	-1.052553
C	-2.567270	1.338520	0.008734
H	-3.019769	2.320076	0.180817
C	-3.590416	0.286879	0.435455
C	-4.395987	0.470920	1.570695
C	-3.723095	-0.933314	-0.242324
C	-5.296340	-0.495149	2.013279
C	-4.615119	-1.916558	0.186533

H	-3.112919	-1.111886	-1.121464
C	-5.405970	-1.697765	1.313574
H	-5.901727	-0.311158	2.893680
H	-4.687562	-2.850770	-0.360060
H	-6.106401	-2.454045	1.654016
Br	-4.260941	2.093532	2.601671
O	1.022536	-0.507970	-1.431374
H	0.740152	1.484970	-0.950282
H	-1.629809	0.887047	1.913125

Vibrational frequencies

15.4437	19.7886	21.5678
23.2569	28.8896	38.0491
41.3145	44.9376	48.5076
55.5621	60.9861	64.5264
76.0379	83.7999	89.8121
90.7877	97.3723	109.7246
121.0276	134.6180	141.8395
150.4624	153.0269	159.3612
174.9886	180.9045	184.8902
194.8773	198.5303	207.4346
215.2376	220.4403	231.4611
235.4589	248.2865	252.0825
259.0716	268.3675	279.0856
285.5148	292.8337	313.6566
326.5478	338.3591	342.1225
351.2795	364.2430	375.3293
383.8456	406.0531	414.0632
418.9972	421.4892	437.4189
438.7981	445.5974	462.0339
477.1952	490.9547	503.7444

505.3931	509.4933	512.6938
513.6424	525.8878	528.8519
531.9060	553.4054	568.8330
579.3494	587.1864	594.6121
596.2941	600.4382	608.2689
611.4652	624.9497	631.2129
640.2660	642.8357	669.7330
673.9323	682.3131	697.3480
715.3217	719.3688	724.5329
726.1201	733.8883	744.6735
746.8395	751.3573	760.8423
771.8991	775.2465	777.9548
785.8173	791.6992	805.2350
818.0294	829.9811	838.6661
860.0754	864.6923	869.4840
870.2028	881.2254	882.2487
889.8065	896.8686	898.7958
906.9108	922.2757	936.3206
938.3817	956.7755	959.5896
964.7781	968.8554	973.6193
976.9173	980.5836	984.4552
984.7884	998.4261	999.2910
1004.0340	1005.9116	1010.8889
1015.5279	1023.5601	1026.9774
1036.9604	1039.7016	1042.7281
1045.7634	1048.1655	1049.2736
1053.2639	1058.3077	1060.0921
1064.0043	1066.3662	1074.4966
1075.6739	1078.5939	1086.2628
1091.7056	1101.4055	1114.8245

1116.3164	1119.4472	1141.7233
1150.5372	1159.1333	1181.1106
1181.8330	1187.1243	1187.5078
1191.1227	1193.0514	1198.8905
1201.6194	1212.4099	1218.0113
1218.3639	1221.1186	1224.2262
1235.5438	1261.6376	1267.3285
1271.1696	1273.1255	1284.1842
1285.7445	1288.4066	1297.3064
1307.8526	1312.9359	1317.5844
1324.6333	1333.5887	1336.0686
1340.4475	1351.7868	1352.6396
1358.3566	1361.6287	1366.0808
1368.8535	1369.9126	1380.9918
1381.6648	1394.0864	1407.3793
1410.9649	1417.6770	1422.4450
1431.1477	1433.0442	1445.4772
1461.0345	1465.4162	1472.3139
1472.9035	1477.8757	1484.2624
1485.5930	1486.0517	1489.1532
1492.6907	1494.2946	1498.0034
1503.1434	1503.7120	1504.5226
1520.2629	1525.9355	1538.3185
1585.1775	1612.7067	1617.4025
1623.4900	1634.5193	1640.2962
1640.8382	1645.0802	1653.9654
1657.8944	1659.7014	1692.6889
1840.5023	2998.2415	3010.8405
3033.2989	3033.9398	3044.6036
3052.0580	3053.7650	3069.0077

3081.8037	3096.0199	3096.7612
3100.4994	3104.7463	3113.5481
3117.2881	3123.1963	3141.5110
3146.4967	3149.6400	3172.2116
3175.5616	3180.2571	3182.5151
3189.5909	3189.6781	3190.4408
3198.5868	3200.6184	3201.3071
3202.7989	3206.4084	3207.4304
3210.5515	3212.1808	3218.5262
3219.6059	3220.1719	3225.2441

M5RS

Zero-point correction= 0.735327

Thermal correction to Energy= 0.779708

Thermal correction to Enthalpy= 0.780653

Thermal correction to Gibbs Free Energy= 0.656097

Sum of electronic and zero-point Energies= -5135.061078

Sum of electronic and thermal Energies= -5135.016697

Sum of electronic and thermal Enthalpies= -5135.015753

Sum of electronic and thermal Free Energies= -5135.140309

Cartesian coordinates

C	-1.556173	-0.071123	0.385354
C	-0.262390	-0.091063	-0.444603
H	-1.912125	-1.103848	0.430541
C	1.137428	-0.066858	0.287523
O	1.312777	-0.168689	1.550657
C	-1.530948	0.435026	1.819400
C	-2.220844	-0.306830	2.787735
C	-0.940765	1.646897	2.213481
C	-2.335777	0.143515	4.105582

H	-2.683328	-1.248416	2.502044
C	-1.060263	2.104620	3.524913
H	-0.355935	2.215489	1.502958
C	-1.761688	1.358681	4.478039
H	-2.877571	-0.453424	4.834349
H	-0.592485	3.044108	3.807192
H	-1.849966	1.718252	5.499596
C	2.147189	-1.028799	-0.402504
C	4.028289	-2.001831	-1.010221
C	4.248963	0.430877	-0.546078
H	3.548450	1.253909	-0.692297
N	3.152901	-2.967854	-1.002086
N	1.979264	-2.345767	-0.605878
N	3.455253	-0.804464	-0.651490
C	5.447091	-1.966625	-1.472577
H	5.673710	-2.844384	-2.079491
H	6.140515	-1.936911	-0.621750
C	5.393707	0.441069	-1.635295
O	5.567165	-0.813209	-2.306098
C	6.337503	0.787888	0.581388
C	4.979198	0.528310	0.777364
C	4.434102	0.397006	2.055201
C	5.289661	0.526783	3.152335
C	6.654216	0.786181	2.966851
C	7.186469	0.921004	1.681377
C	6.672675	0.896300	-0.884333
H	3.370009	0.198384	2.171960
H	7.305891	0.882493	3.830837
H	8.245346	1.120153	1.540496
H	7.523733	0.274318	-1.180593

H	6.921077	1.928605	-1.156340
C	0.771255	-3.119236	-0.466777
C	0.024529	-3.396668	-1.623374
C	0.396119	-3.561940	0.809098
C	-1.172969	-4.097196	-1.464744
C	-0.816349	-4.253906	0.912715
C	-1.615468	-4.520061	-0.203798
H	-1.773898	-4.314049	-2.343958
H	-1.138080	-4.596786	1.892557
C	1.257072	-3.296142	2.014405
H	1.288798	-2.219681	2.217182
H	2.287256	-3.627641	1.840366
H	0.869606	-3.820567	2.891154
C	-2.948057	-5.207329	-0.050086
H	-3.745008	-4.457555	0.016096
H	-2.986209	-5.819105	0.855722
H	-3.173902	-5.845098	-0.910558
C	0.488100	-2.924001	-2.977472
H	1.483953	-3.312523	-3.214498
H	0.555329	-1.830121	-3.013370
H	-0.203367	-3.244877	-3.759781
H	5.130295	1.131157	-2.437455
H	4.892796	0.426590	4.158578
H	-0.367378	-0.904809	-1.159602
C	-0.529756	3.723174	-1.335669
C	-1.701343	4.518192	-1.306057
C	-1.662225	5.892721	-1.559074
C	-0.429580	6.474716	-1.845495
C	0.745600	5.700733	-1.873960
C	0.704469	4.335009	-1.620008

C	-0.808363	2.340090	-1.041840
C	-2.122897	2.093337	-0.766767
H	-2.566778	6.492530	-1.532147
H	-0.376761	7.540956	-2.044739
H	1.695570	6.180205	-2.091531
H	1.608910	3.734519	-1.623029
S	-3.116663	3.547979	-0.905884
C	0.170479	1.212690	-1.126905
O	1.369430	1.334562	-0.322345
H	0.438874	1.064133	-2.184240
C	-2.632400	0.699020	-0.483243
H	-2.642797	0.183860	-1.450251
C	-4.014423	0.526714	0.108789
C	-4.788369	-0.604503	-0.200716
C	-4.538485	1.395861	1.078410
C	-6.035840	-0.841908	0.372377
C	-5.786094	1.180688	1.662386
H	-3.940999	2.240937	1.399473
C	-6.542076	0.065341	1.303533
H	-6.601055	-1.726034	0.099387
H	-6.156838	1.878463	2.406693
H	-7.514457	-0.113184	1.752270
Br	-4.113283	-1.945456	-1.418319

Vibrational frequencies

14.0419	18.8907	22.4497
28.7350	33.2582	38.8186
41.7206	47.2086	52.3065
53.3970	57.9210	68.5427
69.4502	80.7015	84.0431
98.9963	106.5206	117.4101

127.5514	133.7628	138.4115
148.4186	151.5527	158.8889
166.2203	180.9299	184.1182
189.9415	202.5340	207.6416
210.4212	218.5704	221.5318
233.0259	244.7442	248.3035
261.3018	274.0580	292.1275
295.8831	305.4157	313.5849
321.7944	326.4156	336.9324
353.1778	372.9279	385.9248
398.3712	412.9721	417.3114
422.4322	425.9636	440.6033
446.8900	449.2576	467.9366
473.8668	486.3375	494.9863
505.2426	509.9247	515.8789
516.6040	533.8457	533.9852
537.4924	544.0334	566.7178
579.9615	583.2482	588.0614
595.5056	599.6077	608.7725
617.7526	626.3735	630.8062
646.7692	666.0939	676.8395
688.8055	703.1640	705.7654
713.3794	715.3894	718.4997
723.1078	729.1309	741.8444
750.7688	752.8701	754.6692
767.8813	770.0566	771.0021
779.7140	789.5686	792.6533
813.4878	820.3510	825.3127
843.2617	853.4461	869.8534
871.9011	877.2851	879.3381

891.5966	904.4405	908.0643
908.5579	919.8933	924.5911
933.7388	951.8604	954.3002
961.3095	963.2562	969.4212
974.2176	977.7983	981.8330
982.5041	988.0327	992.7247
993.3228	1005.2036	1015.9183
1017.7422	1022.7677	1026.9129
1032.9624	1043.0009	1045.5552
1045.7924	1049.7927	1054.3153
1058.3671	1060.2207	1066.2597
1070.9916	1072.3287	1073.7129
1079.6979	1081.6622	1088.2464
1094.4697	1098.7884	1115.5413
1116.2652	1138.4843	1152.7240
1155.3510	1181.1330	1182.3025
1184.8157	1186.3024	1191.1720
1196.0606	1196.4007	1202.9812
1204.2612	1220.8750	1221.3143
1229.2036	1233.7222	1245.8041
1253.2394	1266.9560	1271.3357
1282.3611	1290.2073	1293.1262
1296.4857	1302.9585	1305.0147
1315.3436	1315.8836	1322.9686
1328.7411	1332.6558	1336.0860
1343.3289	1346.0763	1356.7012
1363.9159	1365.7820	1368.9115
1378.3346	1381.5034	1388.6194
1400.1987	1407.6071	1419.0508
1421.6541	1427.8261	1430.4479

1435.7526	1440.7885	1450.7363
1468.7966	1470.6325	1473.2272
1476.0142	1478.0818	1484.5722
1485.8575	1487.9602	1494.7833
1496.0668	1499.1070	1499.8246
1502.6200	1506.4434	1511.0252
1511.0427	1528.1661	1531.3481
1538.7364	1583.8337	1613.7117
1617.6946	1634.1363	1637.2313
1639.9591	1644.0788	1644.2078
1644.3940	1653.3504	1656.1889
1657.4929	2988.4559	3030.8530
3042.1310	3044.4765	3045.6576
3048.0753	3056.3579	3078.4806
3097.7060	3098.7442	3102.2089
3110.2632	3125.3168	3128.4816
3132.2151	3135.4668	3142.0185
3151.8801	3152.1364	3153.8623
3170.5571	3177.7751	3180.8500
3182.6252	3185.6517	3186.3181
3187.8289	3191.7333	3194.4232
3196.1958	3200.7466	3203.4652
3205.5731	3207.6667	3212.1028
3219.4893	3224.6814	3243.3357

M5SR

Zero-point correction= 0.735714

Thermal correction to Energy= 0.779954

Thermal correction to Enthalpy= 0.780898

Thermal correction to Gibbs Free Energy= 0.657227

Sum of electronic and zero-point Energies= -5135.070110

Sum of electronic and thermal Energies= -5135.025870

Sum of electronic and thermal Enthalpies= -5135.024926

Sum of electronic and thermal Free Energies= -5135.148598

Cartesian coordinates

C	-0.896090	0.892108	-0.945278
C	-0.314612	-0.283545	-0.155352
H	-0.571489	0.753591	-1.979968
C	1.025279	-0.832541	-0.810107
O	1.486853	-0.291915	-1.866874
C	-0.365931	2.237909	-0.487676
C	0.099737	3.155162	-1.439625
C	-0.356438	2.621489	0.861844
C	0.551933	4.420067	-1.061817
H	0.106546	2.871427	-2.488542
C	0.093645	3.885472	1.245189
H	-0.720145	1.936408	1.620059
C	0.547771	4.791708	0.285062
H	0.907772	5.114108	-1.818330
H	0.086194	4.161912	2.296103
H	0.897626	5.776249	0.582891
C	2.165180	-1.178583	0.208840
C	4.185396	-1.522242	1.025795
C	4.190053	-0.670092	-1.311536
H	3.522975	-0.901107	-2.138392
N	3.382766	-1.812914	2.011041
N	2.124858	-1.588472	1.488933
N	3.487445	-1.131546	-0.089078
C	5.667341	-1.663078	0.926326
H	6.033687	-2.351511	1.689391

H	6.164910	-0.692835	1.061459
C	5.597981	-1.377402	-1.447090
O	5.936527	-2.232816	-0.351080
C	5.871243	1.045081	-1.412433
C	4.505172	0.808828	-1.240872
C	3.605564	1.858415	-1.047202
C	4.102794	3.162154	-1.001496
C	5.473762	3.406267	-1.159418
C	6.364581	2.351182	-1.373369
C	6.630495	-0.234570	-1.650484
H	2.544267	1.653402	-0.964707
H	5.846965	4.425987	-1.121652
H	7.426036	2.543475	-1.504868
H	7.476451	-0.365216	-0.966808
H	7.038471	-0.268924	-2.666594
C	0.998417	-1.761009	2.369730
C	0.348060	-3.002404	2.406283
C	0.643294	-0.682605	3.192303
C	-0.750507	-3.119814	3.263117
C	-0.467468	-0.849543	4.024652
C	-1.178987	-2.054470	4.065680
H	-1.285729	-4.065087	3.302207
H	-0.780784	-0.020336	4.652759
C	1.436509	0.598289	3.178571
H	1.554907	0.993181	2.165275
H	2.443426	0.430552	3.577594
H	0.951025	1.365167	3.785996
C	-2.376181	-2.218788	4.968746
H	-2.681421	-1.266592	5.410650
H	-2.155152	-2.912557	5.788812

H	-3.229740	-2.633211	4.421602
C	0.816109	-4.148994	1.549421
H	1.853084	-4.413285	1.786861
H	0.782620	-3.871875	0.490639
H	0.193005	-5.032517	1.706393
H	5.573822	-2.049929	-2.304841
H	3.416207	3.989490	-0.849513
H	-0.253791	-0.052002	0.903877
C	-2.694486	-2.821880	-1.973421
C	-3.897493	-2.512141	-2.655187
C	-4.622489	-3.489697	-3.343035
C	-4.132815	-4.794106	-3.345534
C	-2.938158	-5.118469	-2.676836
C	-2.217191	-4.144057	-1.996353
C	-2.116579	-1.663488	-1.334206
C	-2.839967	-0.526568	-1.527671
H	-5.542381	-3.241069	-3.863517
H	-4.680796	-5.568217	-3.874624
H	-2.574237	-6.141530	-2.698190
H	-1.285287	-4.382648	-1.493436
S	-4.290691	-0.799318	-2.497593
C	-0.922131	-1.667208	-0.429461
O	0.288567	-2.202548	-1.005564
H	-1.180742	-2.215396	0.485699
C	-2.468751	0.833109	-0.998728
H	-2.783696	1.587098	-1.725126
C	-3.136116	1.167109	0.333190
C	-3.558722	2.463995	0.665734
C	-3.290463	0.185207	1.324833
C	-4.094891	2.776673	1.915724

C	-3.818108	0.476675	2.580900
H	-2.988465	-0.831336	1.102459
C	-4.221839	1.778451	2.879998
H	-4.404704	3.793188	2.130504
H	-3.914913	-0.312491	3.319603
H	-4.636447	2.021630	3.853603
Br	-3.389243	3.915495	-0.585385

Vibrational frequencies

15.4755	23.7532	25.0137
27.5703	32.4002	43.7093
44.7441	48.8189	54.4804
57.5174	61.3128	66.8395
70.6219	84.7707	87.2796
94.6652	97.5829	109.2513
118.7501	129.5151	139.0645
150.7119	152.4434	170.5779
171.6694	185.5369	190.1242
195.9312	200.7027	207.2829
210.5557	217.4594	226.3038
238.3739	240.9477	254.6806
271.1786	281.0677	285.7874
298.9762	308.2333	319.5456
331.1015	337.4865	347.7245
364.4087	379.9519	382.5503
401.1060	408.1774	415.8700
421.8451	428.7802	439.7740
444.3263	451.5333	452.9444
473.1780	491.4472	502.2266
503.9496	512.9957	517.7493
519.9916	528.4683	529.1481

534.9518	549.7001	561.2623
580.1835	582.7113	597.6725
599.1958	601.4603	612.0184
619.8876	626.7040	631.1491
635.8435	654.6012	663.7788
679.0447	688.3179	696.0079
705.5294	716.3816	717.7033
721.9491	733.7578	744.8651
749.0012	755.4363	759.9172
765.1051	771.3342	772.8193
786.9938	794.6689	799.5896
805.2839	823.8414	840.7218
851.1109	863.8469	868.8481
875.4363	875.8842	876.1728
892.7656	902.2741	904.2173
904.6559	925.0809	930.5579
933.7744	951.3689	952.3352
959.5075	971.7853	974.7671
977.1735	981.5655	985.4852
991.2049	992.1300	994.7320
1001.2130	1005.6788	1006.5206
1014.3461	1027.6534	1032.6726
1037.3858	1037.7764	1044.4889
1045.6600	1049.1269	1053.9022
1057.6077	1060.8857	1063.8843
1066.6096	1069.3524	1072.8027
1076.2771	1079.3755	1082.2687
1089.9405	1105.0852	1110.3381
1119.4547	1143.9992	1150.4089
1156.0463	1178.7250	1183.9042

1184.5873	1186.2175	1193.0651
1194.0095	1194.9671	1197.3766
1198.1739	1211.9040	1214.7896
1216.7315	1220.6616	1226.7806
1241.8691	1253.0044	1273.0701
1277.6132	1283.0189	1291.9378
1293.7428	1295.7951	1303.6227
1310.3756	1312.4082	1319.4086
1322.6241	1326.5040	1333.6772
1341.7610	1345.4017	1361.3268
1363.5794	1364.9565	1368.5727
1375.8154	1376.7733	1383.7150
1407.0202	1409.6434	1416.5525
1419.6379	1421.7955	1425.0791
1427.5977	1446.9428	1447.8628
1466.7020	1473.0590	1474.1012
1474.4666	1476.9007	1477.2697
1480.3708	1485.9013	1491.6870
1495.9132	1496.7021	1499.8542
1501.8395	1502.5524	1509.0064
1512.0309	1522.0383	1532.2264
1537.2327	1595.7847	1616.7179
1626.1762	1636.0932	1638.2011
1639.3132	1642.8648	1644.2101
1645.2169	1653.1987	1656.2044
1657.2438	3030.6333	3040.1134
3040.9879	3044.3061	3047.4955
3057.4690	3079.7082	3087.4551
3094.5593	3099.1494	3106.2883
3109.1748	3128.8220	3128.8238

3138.1597	3142.1080	3151.2447
3161.8562	3175.1857	3178.5589
3180.6560	3181.8920	3181.9690
3185.7709	3187.7658	3191.0446
3194.3222	3195.5172	3196.3607
3201.3896	3204.8875	3206.3002
3209.0437	3211.9124	3212.4332
3222.0135	3225.7302	3229.5622

M5SS

Zero-point correction= 0.734897

Thermal correction to Energy= 0.778515

Thermal correction to Enthalpy= 0.779459

Thermal correction to Gibbs Free Energy= 0.657377

Sum of electronic and zero-point Energies= -5135.067717

Sum of electronic and thermal Energies= -5135.024098

Sum of electronic and thermal Enthalpies= -5135.023154

Sum of electronic and thermal Free Energies= -5135.145236

Cartesian coordinates

C	-1.067588	0.718241	-0.383691
C	-0.212900	-0.417309	0.190115
H	-0.782568	0.815018	-1.434627
C	1.112505	-0.662794	-0.653063
O	1.319566	0.014462	-1.712814
C	-0.780300	2.041164	0.302596
C	-0.193857	3.094220	-0.412247
C	-1.083527	2.243826	1.657523
C	0.086487	4.315382	0.206910
H	0.050067	2.950619	-1.460560
C	-0.811122	3.463245	2.278467

H	-1.538732	1.443426	2.232413
C	-0.221230	4.503986	1.555993
H	0.540066	5.118392	-0.367580
H	-1.058742	3.600146	3.327496
H	-0.006641	5.452578	2.039911
C	2.425386	-0.859874	0.170309
C	4.577203	-0.980362	0.641025
C	4.107158	-0.106705	-1.634691
H	3.334558	-0.371513	-2.352662
N	3.982896	-1.362023	1.737045
N	2.638774	-1.274662	1.430385
N	3.667373	-0.666486	-0.336574
C	6.028335	-0.948770	0.292461
H	6.594319	-1.593479	0.966657
H	6.427502	0.072193	0.366044
C	5.527963	-0.668669	-2.034450
O	6.143144	-1.477081	-1.025574
C	5.571469	1.768121	-1.964796
C	4.295442	1.391334	-1.541584
C	3.366285	2.333503	-1.099801
C	3.742263	3.677466	-1.071638
C	5.022291	4.064918	-1.491538
C	5.941608	3.114854	-1.945081
C	6.381683	0.575738	-2.405842
H	2.372099	2.014677	-0.807756
H	5.302681	5.114292	-1.465361
H	6.932611	3.419228	-2.270827
H	7.361468	0.519341	-1.919412
H	6.565390	0.599241	-3.485775
C	1.690772	-1.595011	2.465564

C	1.228267	-2.914031	2.571432
C	1.308663	-0.571774	3.343623
C	0.293490	-3.181115	3.575634
C	0.368494	-0.890986	4.328099
C	-0.155428	-2.183379	4.451303
H	-0.094520	-4.191602	3.675050
H	0.039267	-0.111765	5.010006
C	1.866392	0.820443	3.200753
H	1.600013	1.255398	2.232026
H	2.959894	0.815947	3.264732
H	1.477672	1.478510	3.980578
C	-1.176860	-2.511232	5.511732
H	-1.475783	-1.621374	6.072249
H	-0.781223	-3.243293	6.225526
H	-2.076233	-2.951995	5.067354
C	1.717556	-3.983713	1.630946
H	2.805886	-4.095198	1.699084
H	1.481049	-3.718273	0.595085
H	1.258701	-4.947121	1.864778
H	5.420017	-1.346517	-2.881343
H	3.034673	4.424732	-0.723833
H	-0.064543	-0.277551	1.257408
C	-2.255530	-3.163807	-1.720022
C	-3.539148	-3.015834	-2.301417
C	-4.129363	-4.041304	-3.046392
C	-3.421618	-5.230208	-3.208979
C	-2.143080	-5.391851	-2.643853
C	-1.556516	-4.369658	-1.906780
C	-1.847612	-1.983212	-0.996967
C	-2.763714	-0.976901	-1.047331

H	-5.113294	-3.916011	-3.488374
H	-3.862991	-6.039285	-3.783542
H	-1.607397	-6.325174	-2.791595
H	-0.562474	-4.478767	-1.485051
S	-4.210814	-1.421583	-1.961640
C	-0.610246	-1.857796	-0.162505
O	0.622209	-2.141155	-0.860472
H	-0.709730	-2.507907	0.717705
C	-2.588678	0.352371	-0.352588
H	-2.887114	0.217921	0.691371
C	-3.421404	1.477346	-0.942970
C	-4.321691	2.252616	-0.200670
C	-3.261965	1.816551	-2.297602
C	-5.031824	3.314152	-0.764899
C	-3.960939	2.869063	-2.880991
H	-2.569375	1.232616	-2.896098
C	-4.849653	3.622496	-2.111217
H	-5.718980	3.890863	-0.156082
H	-3.811347	3.101242	-3.930862
H	-5.401267	4.447520	-2.551489
Br	-4.636803	1.900062	1.669234

Vibrational frequencies

-3.2709	18.3291	20.6261
23.3426	31.1318	31.9865
40.0914	47.5369	50.9073
53.2552	61.3403	68.8284
71.4961	78.0722	82.0288
91.2679	96.0214	107.8144
115.2146	127.4902	134.0030
140.9518	156.3143	170.5524

174.9077	177.0457	181.8923
194.4371	199.9550	200.3889
207.7468	215.4368	225.0532
236.9776	243.6847	251.6360
264.6413	277.1211	288.8159
291.5659	307.4177	317.1103
325.1244	333.7635	347.5242
356.8007	372.2215	382.4494
404.3236	409.6659	422.3167
424.0037	431.6810	434.7970
441.4838	450.7605	453.0483
476.8402	489.4161	500.2813
501.6586	507.1554	511.4106
517.8795	528.3874	532.0477
533.2698	550.6684	555.4534
573.6421	580.9773	583.7040
593.1188	598.3537	611.5125
618.2400	620.5175	626.5947
632.9207	654.8481	661.2663
676.5661	687.0034	702.0021
711.7544	715.8628	717.7462
719.9271	732.7519	737.9005
746.4396	752.7870	754.5780
762.2231	770.4272	772.8322
775.3687	787.8687	797.9397
819.3141	824.8456	840.5255
849.1266	863.3881	869.9627
870.1245	875.8525	877.7725
890.1332	898.6766	905.8423
906.2120	921.2359	931.3326

944.1496	947.2818	950.0465
960.6801	971.4183	973.8548
976.8568	978.9685	982.3412
987.4902	991.0946	998.1376
1005.0619	1005.8840	1015.1764
1016.3861	1024.7419	1033.9392
1035.2537	1038.4269	1045.4939
1048.2286	1050.9440	1054.9907
1056.4947	1062.4041	1064.9644
1067.6261	1072.5634	1073.0998
1076.0658	1079.3629	1088.3873
1095.0822	1103.3174	1110.1400
1118.4008	1137.7120	1150.9973
1154.5439	1180.6231	1183.6880
1184.4273	1185.9134	1191.3074
1192.9954	1195.2827	1197.1672
1207.5892	1208.9372	1211.1487
1219.7225	1223.2277	1231.4975
1242.5847	1250.4036	1271.4170
1276.7400	1282.2162	1287.1733
1288.9975	1289.2739	1298.0238
1298.9847	1309.3923	1319.6778
1327.6375	1333.9645	1334.8280
1342.5378	1343.7545	1356.1441
1361.0844	1362.9390	1368.7810
1371.1492	1372.0580	1380.6388
1404.2338	1408.3274	1411.2433
1419.5460	1421.7669	1426.7267
1428.2379	1447.1722	1449.1391
1466.8081	1471.0239	1472.3576

1474.8131	1479.1591	1480.1739
1481.2985	1485.7815	1492.7393
1493.6158	1496.3361	1496.9551
1501.8855	1503.4302	1510.1155
1512.7291	1523.8068	1530.5423
1535.1162	1592.5432	1616.3017
1621.2942	1634.7851	1638.9727
1640.0270	1643.1509	1644.3573
1645.3039	1652.7481	1655.3390
1657.3086	3016.7528	3038.4679
3039.2626	3041.8223	3049.8317
3056.6616	3072.6023	3090.6392
3095.2026	3101.0691	3103.4477
3110.5442	3128.6875	3130.5127
3137.4637	3144.4513	3147.8537
3160.1502	3166.3104	3177.2009
3181.5845	3182.6709	3184.0756
3185.9791	3188.2171	3191.1778
3191.9463	3194.5881	3195.2058
3199.9164	3200.1502	3204.1073
3204.5522	3207.0464	3211.4820
3211.6616	3221.3751	3227.6061

TS6RR

Zero-point correction= 0.735652

Thermal correction to Energy= 0.779407

Thermal correction to Enthalpy= 0.780352

Thermal correction to Gibbs Free Energy= 0.658470

Sum of electronic and zero-point Energies= -5135.058489

Sum of electronic and thermal Energies= -5135.014733

Sum of electronic and thermal Enthalpies= -5135.013789

Sum of electronic and thermal Free Energies= -5135.135671

Cartesian coordinates

C	-0.462585	1.779958	-0.712415
C	0.010760	0.373380	-0.284800
C	0.555943	-0.604258	-1.363900
O	1.108032	-0.385785	-2.445319
C	-0.884897	2.060261	-2.152525
C	-0.654853	3.356552	-2.641394
C	-1.551459	1.151484	-2.987303
C	-1.071062	3.738499	-3.917286
H	-0.163539	4.081975	-1.999840
C	-1.969561	1.530847	-4.264407
H	-1.725838	0.136653	-2.655847
C	-1.734015	2.823484	-4.737100
H	-0.876971	4.748929	-4.266883
H	-2.479827	0.806532	-4.893707
H	-2.060538	3.112935	-5.732075
C	1.785926	-1.771223	-0.426388
C	3.635275	-3.014781	-0.404181
C	3.938315	-0.685094	-1.309990
H	3.587564	-0.559554	-2.333634
N	2.713482	-3.799036	0.080102
N	1.575287	-3.004167	0.057379
N	3.122425	-1.774408	-0.707359
C	5.078252	-3.362642	-0.605943
H	5.156309	-4.354766	-1.056912
H	5.591246	-3.396140	0.365143
C	5.438572	-1.083133	-1.200542
O	5.700805	-2.447268	-1.495808

C	4.998680	0.626756	0.390291
C	3.908057	0.584333	-0.491005
C	2.997779	1.633921	-0.562681
C	3.141237	2.708206	0.321698
C	4.200614	2.732588	1.235687
C	5.147633	1.702801	1.263367
C	5.895164	-0.569972	0.192675
H	2.206050	1.602904	-1.300686
H	4.298443	3.570886	1.919815
H	5.988829	1.746389	1.949674
H	5.725566	-1.319362	0.974702
H	6.960033	-0.322721	0.206252
C	0.360647	-3.570251	0.578101
C	-0.412699	-4.386365	-0.258541
C	0.021472	-3.313819	1.913536
C	-1.578649	-4.938369	0.278191
C	-1.162412	-3.879540	2.400974
C	-1.976280	-4.685279	1.597771
H	-2.200623	-5.567159	-0.354113
H	-1.452530	-3.683713	3.430024
C	0.883555	-2.433822	2.783626
H	0.857553	-1.392538	2.442874
H	1.930500	-2.754011	2.762648
H	0.538921	-2.455308	3.820266
C	-3.281533	-5.230623	2.119828
H	-3.276439	-5.316873	3.210335
H	-3.503294	-6.214851	1.695759
H	-4.108582	-4.563842	1.844651
C	-0.019545	-4.614228	-1.693502
H	1.014688	-4.963257	-1.777090

H	-0.098862	-3.673786	-2.249087
H	-0.672219	-5.352794	-2.165474
H	5.968293	-0.519245	-1.972179
H	2.421622	3.520357	0.316291
H	0.670454	0.486723	0.573802
C	-3.708559	-0.909963	-0.232251
C	-4.863690	-0.105428	-0.069366
C	-6.150320	-0.646928	-0.150568
C	-6.276355	-2.011333	-0.401435
C	-5.139484	-2.822687	-0.574717
C	-3.861488	-2.281857	-0.496006
C	-2.494161	-0.142865	-0.100584
C	-2.715667	1.180958	0.138934
H	-7.029159	-0.022549	-0.022382
H	-7.266875	-2.451437	-0.467832
H	-5.262459	-3.882499	-0.777623
H	-2.982208	-2.900299	-0.635812
S	-4.427392	1.576934	0.233617
C	-1.098778	-0.672077	-0.091222
O	-0.669012	-1.411057	-1.278566
H	-0.954773	-1.295577	0.795505
C	-1.624300	2.205884	0.269158
H	-1.994595	3.178263	-0.069341
C	-1.080263	2.381473	1.685944
C	-0.308483	3.497879	2.044007
C	-1.254132	1.400337	2.673952
C	0.277547	3.636319	3.300846
C	-0.677562	1.516669	3.938210
H	-1.852550	0.526677	2.439341
C	0.093924	2.634858	4.253860

H	0.867707	4.516138	3.531173
H	-0.832004	0.732075	4.672525
H	0.550277	2.736500	5.233537
Br	-0.005785	4.932541	0.787396
H	0.364217	2.459134	-0.507482

Vibrational frequencies

-195.6968	14.7621	23.4425
30.7081	34.9173	39.2802
44.0787	48.6737	54.1082
58.7674	60.3035	63.9225
70.9015	75.9177	78.9328
83.2277	97.2844	107.4694
113.7528	128.7519	134.9098
137.6943	151.6135	156.5096
168.6667	178.2626	182.7065
190.9031	196.9111	205.8073
210.7598	220.6100	230.6796
232.0752	242.5459	243.7959
254.7967	265.7343	271.1238
289.9351	299.9432	306.9810
313.5513	324.6260	336.6715
343.2083	359.4950	376.4349
387.3387	393.2403	410.2022
417.2419	423.8597	431.6637
442.3126	465.0200	468.1208
475.1097	490.0660	504.6238
513.6904	515.8768	519.6004
523.4003	530.4764	532.8102
543.0469	549.0864	554.5219
570.1826	581.9268	587.7524

593.3921	604.8114	606.9365
620.6343	630.5536	632.8699
636.4394	647.9197	658.5995
663.7327	683.8838	693.0266
703.3201	712.8753	719.7921
734.1844	736.7512	738.6100
743.6492	753.8418	761.3259
764.3583	771.4351	773.9098
784.3654	789.2871	794.4415
804.5355	824.9086	843.9389
855.2787	867.9376	873.9092
875.9151	885.6526	887.0927
889.6120	898.0227	904.2621
918.5494	926.9691	938.1990
951.6236	955.1450	960.5045
965.1395	971.3142	973.8367
979.6914	983.7713	987.2690
989.7872	993.8300	994.5027
1005.4878	1012.7921	1013.9428
1017.2731	1019.0888	1025.6023
1041.6160	1043.9518	1045.1587
1045.6953	1050.4576	1051.8329
1055.6040	1061.1906	1062.7117
1068.5029	1069.5165	1071.4081
1074.2264	1076.4071	1078.3187
1082.7409	1117.5128	1123.6582
1136.3670	1137.9180	1143.1604
1150.8910	1159.2152	1182.0515
1183.6200	1188.0539	1190.5021
1193.0848	1193.7122	1201.4739

1209.5992	1218.1645	1219.4274
1221.0904	1229.9795	1235.1898
1250.6555	1265.7054	1266.7597
1274.5952	1276.5964	1288.3948
1292.9870	1294.0247	1296.6163
1301.0290	1315.5446	1317.9192
1330.7731	1334.7585	1337.1449
1341.8612	1343.2603	1347.6741
1350.5722	1360.4753	1363.9485
1374.7894	1376.7273	1388.1757
1394.8473	1410.0810	1414.7505
1417.7093	1418.1846	1421.7970
1423.9082	1435.1365	1447.1626
1449.6880	1473.2715	1474.3761
1482.7232	1483.8885	1484.8110
1488.4886	1492.0312	1492.5256
1494.2684	1494.9795	1502.5427
1505.4360	1508.6239	1509.3830
1519.3641	1535.1124	1541.7204
1592.5241	1615.8017	1620.6109
1628.3831	1635.9896	1639.7422
1640.1961	1641.9977	1645.4707
1654.7028	1657.5913	1663.5647
1674.0992	3028.5418	3037.4032
3045.9532	3050.2208	3061.6485
3074.8225	3092.2938	3100.7098
3105.4516	3106.5987	3117.6877
3118.3516	3122.7057	3127.5870
3128.1435	3136.9096	3137.4408
3144.7557	3148.5159	3177.2851

3178.1744	3182.4540	3183.5131
3185.5411	3186.9305	3194.3616
3196.9765	3197.8146	3198.2902
3205.1984	3206.7876	3209.1973
3214.8865	3216.1408	3221.4568
3222.8313	3237.1164	3243.0315

TS6RS

Zero-point correction= 0.734157

Thermal correction to Energy= 0.778363

Thermal correction to Enthalpy= 0.779307

Thermal correction to Gibbs Free Energy= 0.654932

Sum of electronic and zero-point Energies= -5135.052153

Sum of electronic and thermal Energies= -5135.007947

Sum of electronic and thermal Enthalpies= -5135.007003

Sum of electronic and thermal Free Energies= -5135.131378

Cartesian coordinates

C	-1.667510	-0.063565	0.512652
C	-0.308940	-0.107768	-0.214354
H	-2.008635	-1.099242	0.585837
C	0.986974	0.064280	0.614308
O	1.265618	-0.198052	1.782641
C	-1.740260	0.510990	1.918649
C	-2.495903	-0.185523	2.873156
C	-1.161118	1.732196	2.298221
C	-2.682858	0.318743	4.161422
H	-2.954224	-1.131854	2.597375
C	-1.348178	2.241022	3.584064
H	-0.539677	2.277510	1.599937
C	-2.112982	1.540874	4.520755

H	-3.274805	-0.242113	4.879498
H	-0.887330	3.186830	3.855655
H	-2.255471	1.940470	5.520931
C	2.260331	-1.082872	-0.449156
C	4.237447	-2.028813	-0.863636
C	4.303277	0.431127	-0.591346
H	3.569812	1.211573	-0.802437
N	3.406546	-3.033455	-0.843502
N	2.184901	-2.418371	-0.569331
N	3.582279	-0.842160	-0.629850
C	5.678844	-1.943096	-1.241169
H	6.002076	-2.851759	-1.751189
H	6.312443	-1.787464	-0.357775
C	5.471129	0.437297	-1.653837
O	5.786987	-0.862052	-2.172712
C	6.332651	1.045628	0.536197
C	4.999801	0.675245	0.733235
C	4.450350	0.582078	2.012122
C	5.271331	0.864079	3.107449
C	6.609259	1.234437	2.919348
C	7.147542	1.330564	1.632923
C	6.676472	1.092026	-0.931678
H	3.408246	0.302144	2.146212
H	7.234586	1.448896	3.781560
H	8.186166	1.616178	1.489475
H	7.599600	0.558668	-1.180023
H	6.801820	2.127097	-1.271317
C	0.987481	-3.207758	-0.468608
C	0.218654	-3.407814	-1.625154
C	0.614678	-3.712839	0.785187

C	-0.984159	-4.108330	-1.492674
C	-0.596101	-4.409273	0.865327
C	-1.411527	-4.605952	-0.255273
H	-1.599057	-4.266231	-2.374947
H	-0.911032	-4.802050	1.828769
C	1.473767	-3.480452	2.000189
H	1.463920	-2.417889	2.265544
H	2.514983	-3.761872	1.809940
H	1.109220	-4.060225	2.851833
C	-2.742661	-5.302417	-0.122821
H	-2.732116	-6.043212	0.682229
H	-3.027355	-5.805639	-1.052125
H	-3.529015	-4.573180	0.105038
C	0.662625	-2.850129	-2.953416
H	1.686094	-3.157761	-3.192057
H	0.653876	-1.753584	-2.943011
H	0.003777	-3.185087	-3.758076
H	5.170761	1.005764	-2.535115
H	4.867396	0.796506	4.113560
H	-0.315887	-0.979175	-0.862403
C	-0.573812	3.637143	-1.393803
C	-1.759661	4.401738	-1.509308
C	-1.730811	5.752927	-1.866960
C	-0.492927	6.341769	-2.113249
C	0.696279	5.597668	-2.000511
C	0.664862	4.255411	-1.641815
C	-0.848025	2.274650	-1.010830
C	-2.175098	2.016810	-0.813748
H	-2.647261	6.328979	-1.950055
H	-0.447106	7.390276	-2.392053

H	1.649418	6.082156	-2.191011
H	1.581249	3.682370	-1.538307
S	-3.181350	3.429301	-1.138518
C	0.155330	1.175569	-0.925649
O	1.235881	1.370678	0.050146
H	0.595379	0.983155	-1.912058
C	-2.684474	0.635698	-0.473426
H	-2.621387	0.060388	-1.403978
C	-4.103771	0.483806	0.030304
C	-4.849151	-0.669316	-0.267415
C	-4.697304	1.405205	0.907417
C	-6.134974	-0.879713	0.226253
C	-5.983494	1.216534	1.410786
H	-4.126187	2.271699	1.219629
C	-6.709225	0.077805	1.062729
H	-6.677862	-1.781368	-0.034206
H	-6.409391	1.954018	2.083821
H	-7.712104	-0.079384	1.447672
Br	-4.079492	-2.077350	-1.346430

Vibrational frequencies

-212.3022	16.2229	18.2830
24.0270	26.3500	34.3344
41.4279	43.6980	46.9424
48.7538	51.6209	56.1498
65.1223	67.5277	76.1966
80.3337	94.5618	102.2854
119.2935	121.0610	133.4592
143.4577	152.1596	159.2227
166.3085	174.0717	179.9350
186.6036	188.9997	198.8009

207.6536	211.9692	215.5058
220.8538	222.3415	240.3118
248.4264	266.0124	272.7784
278.7914	294.0745	307.9312
314.8529	325.4675	331.9929
342.3474	359.0891	372.7014
386.1328	399.9344	414.2736
418.8339	420.3288	428.6579
441.7230	443.6114	469.4683
479.3612	490.2796	492.0807
497.5416	505.7465	515.1951
515.6747	527.8014	532.1684
533.3927	540.8154	565.0952
570.4933	579.0360	582.8496
598.3510	599.4022	605.4975
615.4121	615.8461	630.9173
641.4508	649.1287	667.3973
691.2069	700.6034	702.6052
709.9997	718.7638	720.2212
722.1425	729.7014	735.6370
748.2656	750.6590	753.2057
764.5903	766.0429	772.2379
778.6583	787.0253	791.7542
815.5550	819.7124	823.7137
840.5146	859.2947	865.1269
871.3786	873.3610	882.6576
889.8785	898.7898	908.0020
910.2360	914.1139	929.0360
937.2499	945.8281	951.6393
961.7330	967.2821	969.8046

974.1248	976.3916	979.5442
979.6651	983.0648	991.8062
991.9194	999.5075	1006.3364
1013.8277	1016.1332	1025.8146
1029.0275	1030.2760	1042.1502
1043.7984	1047.6532	1047.8415
1051.6638	1055.0123	1061.8355
1066.3920	1070.9477	1072.6834
1073.6671	1078.0427	1080.9710
1092.1765	1094.6156	1115.9172
1117.4047	1139.3915	1151.8127
1155.6745	1179.9880	1182.7096
1185.8765	1186.5314	1191.7014
1194.3602	1194.6870	1200.0713
1203.5063	1223.0098	1224.3074
1228.1298	1228.3750	1243.5757
1249.5051	1265.1134	1268.0218
1272.3494	1276.9557	1287.2335
1290.5989	1297.4461	1301.9331
1307.5562	1313.2922	1321.2242
1322.9217	1331.5566	1333.9806
1341.0164	1341.3711	1343.0852
1361.9245	1365.6614	1368.4735
1375.6556	1377.5998	1386.6466
1406.7876	1409.4194	1417.1966
1422.0323	1422.2197	1427.7557
1430.7144	1438.4232	1451.0128
1451.9448	1467.0503	1473.7247
1474.9775	1482.7351	1485.0405
1488.2747	1491.1635	1494.0330

1497.0948	1497.8118	1498.6191
1503.8762	1510.3359	1510.6365
1526.4871	1532.5052	1540.4634
1584.6785	1614.2042	1617.5847
1634.8672	1637.5271	1638.1262
1640.1778	1643.9721	1645.1497
1653.9018	1657.7550	1658.1483
1696.7300	3037.6749	3042.5475
3043.6858	3044.2969	3044.6664
3044.8901	3051.8488	3088.2165
3098.8335	3103.6557	3105.9988
3113.0619	3118.5158	3126.8620
3127.1063	3135.5678	3138.6137
3147.8067	3173.9853	3174.7851
3179.3942	3181.0103	3181.4182
3182.2634	3182.4737	3188.0866
3190.7687	3192.3944	3194.9398
3197.9921	3202.5406	3204.8740
3207.3255	3208.1223	3213.7944
3220.6937	3225.0504	3239.1797

TS6SR

Zero-point correction= 0.733854

Thermal correction to Energy= 0.778223

Thermal correction to Enthalpy= 0.779167

Thermal correction to Gibbs Free Energy= 0.654530

Sum of electronic and zero-point Energies= -5135.060849

Sum of electronic and thermal Energies= -5135.016480

Sum of electronic and thermal Enthalpies= -5135.015535

Sum of electronic and thermal Free Energies= -5135.140173

Cartesian coordinates

C	0.865479	1.347742	-1.248904
C	0.021029	0.278944	-0.542651
H	0.357732	1.608797	-2.182737
C	-0.689585	-0.669602	-1.536597
O	-0.327104	-1.169708	-2.601573
C	2.255963	0.860180	-1.609208
C	2.773828	1.133904	-2.881960
C	3.065678	0.168828	-0.696605
C	4.063750	0.737216	-3.234387
H	2.157234	1.666127	-3.601994
C	4.357324	-0.229341	-1.044266
H	2.699553	-0.052394	0.298889
C	4.862982	0.055034	-2.313817
H	4.443859	0.959902	-4.227704
H	4.965509	-0.761880	-0.318111
H	5.868111	-0.255149	-2.585644
C	-1.032432	-2.232007	-0.356186
C	-0.702984	-4.380245	0.140667
C	1.330900	-3.138587	-0.506843
H	1.499965	-2.295259	-1.180485
N	-1.984935	-4.209670	0.314791
N	-2.159906	-2.857396	0.005858
N	-0.103591	-3.213499	-0.264057
C	0.166694	-5.593504	0.195710
H	-0.431646	-6.505721	0.173885
H	0.772812	-5.593099	1.111899
C	1.854855	-4.464430	-1.165924
O	0.978948	-5.588558	-0.981538
C	3.239673	-3.876878	0.737785

C	2.143494	-3.010685	0.766863
C	1.919426	-2.164037	1.850903
C	2.830448	-2.174196	2.910533
C	3.938906	-3.029598	2.880504
C	4.147118	-3.889863	1.797698
C	3.251492	-4.688176	-0.535265
H	1.051126	-1.513391	1.877996
H	4.639514	-3.030706	3.710668
H	5.000775	-4.561806	1.784908
H	3.433824	-5.755116	-0.375374
H	4.028451	-4.322309	-1.217709
C	-3.460571	-2.257156	0.101446
C	-4.225132	-2.123427	-1.065912
C	-3.892379	-1.793810	1.350826
C	-5.464851	-1.488502	-0.954097
C	-5.140996	-1.165085	1.412235
C	-5.936510	-1.002078	0.272490
H	-6.071422	-1.360461	-1.847091
H	-5.493117	-0.786329	2.368206
C	-3.024426	-1.944363	2.574463
H	-2.082592	-1.395429	2.460041
H	-2.762027	-2.993089	2.749590
H	-3.532467	-1.563454	3.463564
C	-7.279672	-0.318662	0.357104
H	-8.095166	-1.052480	0.340656
H	-7.436336	0.353828	-0.492533
H	-7.377057	0.261529	1.279060
C	-3.703911	-2.616092	-2.390257
H	-3.364976	-3.655606	-2.321820
H	-2.846034	-2.017001	-2.715213

H	-4.477997	-2.557084	-3.159617
H	1.913392	-4.347746	-2.249174
H	2.677004	-1.514861	3.759490
H	0.565386	-0.195551	0.268778
C	-2.912115	2.860559	-0.024608
C	-2.783473	4.266723	0.082018
C	-3.898947	5.092246	0.251736
C	-5.156344	4.494775	0.313091
C	-5.301251	3.099501	0.203092
C	-4.191201	2.280630	0.032924
C	-1.633706	2.211263	-0.187940
C	-0.583494	3.079539	-0.222506
H	-3.790996	6.169485	0.332638
H	-6.035828	5.118121	0.444651
H	-6.292170	2.657654	0.248365
H	-4.302074	1.205762	-0.065061
S	-1.091212	4.757700	-0.033578
C	-1.408442	0.740096	-0.217234
O	-1.928237	0.050303	-1.402022
H	-1.821549	0.267401	0.682841
C	0.859043	2.685647	-0.412789
H	1.348243	3.443617	-1.030567
C	1.632118	2.572464	0.898207
C	2.990586	2.908611	1.009681
C	1.019261	2.044787	2.046430
C	3.710359	2.717382	2.189831
C	1.721556	1.840773	3.232607
H	-0.034896	1.793055	2.003912
C	3.074718	2.174495	3.304903
H	4.759526	2.987494	2.230753

H	1.211568	1.425389	4.096439
H	3.635613	2.021621	4.221807
Br	3.959518	3.635557	-0.483165

Vibrational frequencies

-209.7415	13.7391	19.9597
31.8208	32.1109	35.1022
37.4786	42.7630	46.9016
51.4981	55.5522	56.0340
62.4835	75.1069	77.0632
84.6129	96.2341	101.8844
102.5646	104.9553	119.0498
133.0017	141.1282	147.4448
150.0747	157.2207	164.8472
176.2022	183.8518	192.9518
206.2783	209.6467	216.0624
229.5708	231.8990	238.2801
245.2976	270.0377	278.1819
282.4824	286.6685	300.2392
320.5592	327.1041	339.7817
350.1818	361.2941	370.3677
389.2739	397.9987	413.6720
417.9859	421.0066	429.0158
439.0768	442.2207	461.0840
482.5698	486.8716	492.5569
499.4166	505.0732	513.6329
519.1688	525.1996	532.0039
533.5539	550.9103	554.4542
558.9651	582.1085	590.0359
599.6559	604.9273	611.9663
614.8801	626.7821	629.1628

633.4115 646.2403 667.7737

681.9979 690.4382 707.3879

711.6135 716.1035 722.0358

725.8289 734.9484 744.1300

751.5368 755.7266 757.4013

761.7640 768.8127 772.4183

786.4644 788.9400 792.0303

803.9335 820.5875 832.9436

840.2444 865.8700 867.2249

874.8238 875.6677 883.7078

894.4729 898.8671 902.1476

902.9426 921.9552 929.0868

942.5573 953.4702 960.5766

962.0213 968.7797 970.1996

975.0518 977.7170 979.9953

982.9619 990.1136 992.4831

994.1831 995.4239 1002.8917

1006.6232 1014.6168 1028.5570

1031.1595 1037.0993 1038.8443

1040.8199 1046.9130 1047.7368

1051.8868 1053.0063 1058.1462

1065.5482 1069.3458 1071.1842

1074.2286 1074.6119 1078.8855

1082.7563 1094.8987 1109.9442

1116.1604 1142.7116 1145.0241

1152.2640 1183.1791 1183.5881

1184.0411 1187.5862 1188.5746

1192.9809 1194.1431 1199.0421

1200.8246 1214.1029 1216.1438

1223.0363 1223.7636 1235.1753

1248.0929	1250.0420	1267.4282
1271.0829	1277.6153	1290.2583
1293.0627	1297.9990	1299.2008
1299.9340	1311.4905	1319.9816
1321.2250	1323.1932	1331.1758
1339.8138	1340.6579	1343.2973
1361.4874	1364.2891	1365.2319
1369.1387	1377.6118	1382.1524
1408.5035	1413.3285	1417.0779
1419.6306	1422.2128	1424.1781
1430.5713	1446.7117	1447.5469
1459.6873	1463.3373	1473.4371
1474.1116	1481.2785	1482.3033
1487.2443	1491.5233	1493.8942
1494.9376	1496.5369	1497.4380
1502.9758	1507.0656	1508.6982
1518.2717	1535.4316	1538.7089
1595.4603	1616.3701	1624.7747
1637.7055	1637.9312	1640.2013
1640.8789	1642.3067	1645.1738
1654.9794	1657.7946	1658.4892
1698.1678	3035.5095	3038.2606
3041.7688	3045.0961	3045.8578
3050.2724	3068.9031	3085.1733
3098.6758	3103.7230	3105.2365
3109.3973	3111.0521	3122.5816
3127.6656	3134.6054	3138.6118
3144.1324	3173.8426	3180.4741
3181.1721	3182.8345	3184.0104
3184.5436	3188.8640	3190.7255

3193.6511	3193.9510	3199.6454
3202.7612	3203.3661	3206.7076
3208.4953	3212.5932	3215.2286
3217.2200	3221.0466	3222.6705

TS6SS

Zero-point correction= 0.733653

Thermal correction to Energy= 0.778187

Thermal correction to Enthalpy= 0.779131

Thermal correction to Gibbs Free Energy= 0.652592

Sum of electronic and zero-point Energies= -5135.057506

Sum of electronic and thermal Energies= -5135.012972

Sum of electronic and thermal Enthalpies= -5135.012028

Sum of electronic and thermal Free Energies= -5135.138567

Cartesian coordinates

C	-1.075923	0.878408	-0.550525
C	-0.184904	-0.305486	-0.145106
H	-0.971112	1.014777	-1.630423
C	0.939777	-0.604874	-1.172536
O	1.386014	0.111878	-2.065313
C	-0.644464	2.167478	0.126054
C	-0.262179	3.274706	-0.641225
C	-0.635196	2.287246	1.524111
C	0.116789	4.473327	-0.031226
H	-0.261699	3.195842	-1.724594
C	-0.254425	3.480719	2.137392
H	-0.932164	1.443620	2.139796
C	0.122443	4.580001	1.361328
H	0.407703	5.321098	-0.645017
H	-0.255829	3.553061	3.221334

H	0.417185	5.510588	1.837851
C	2.556825	-1.076101	0.003386
C	4.702110	-1.256277	0.590739
C	4.308210	-0.053514	-1.550369
H	3.598453	-0.253788	-2.351560
N	4.059422	-1.815521	1.576485
N	2.727682	-1.681485	1.188899
N	3.834202	-0.804500	-0.375700
C	6.166638	-1.132562	0.333605
H	6.725057	-1.864564	0.919496
H	6.525467	-0.127505	0.596578
C	5.775790	-0.490087	-1.947097
O	6.372794	-1.428749	-1.046753
C	5.697235	1.911430	-1.535873
C	4.415173	1.429844	-1.262607
C	3.410023	2.274311	-0.789166
C	3.715228	3.619162	-0.569853
C	5.002774	4.106585	-0.831521
C	5.998895	3.258142	-1.321595
C	6.596047	0.824117	-2.065140
H	2.409609	1.891632	-0.620099
H	5.227694	5.154913	-0.655497
H	6.994954	3.639670	-1.529397
H	7.533938	0.734189	-1.506128
H	6.868680	1.009118	-3.110197
C	1.697549	-2.143156	2.074225
C	1.161166	-3.422527	1.880960
C	1.262369	-1.280659	3.092659
C	0.133260	-3.827715	2.740377
C	0.229914	-1.728136	3.920932

C	-0.346221	-2.995665	3.758599
H	-0.306536	-4.812065	2.603165
H	-0.133827	-1.072400	4.708133
C	1.876146	0.086144	3.259239
H	1.761190	0.688194	2.351571
H	2.950641	0.013589	3.459102
H	1.407467	0.626762	4.084836
C	-1.444661	-3.459894	4.683015
H	-2.123699	-2.640263	4.938771
H	-1.027692	-3.839792	5.624118
H	-2.032338	-4.265750	4.234201
C	1.648210	-4.302339	0.758039
H	2.727796	-4.474944	0.829492
H	1.460058	-3.828387	-0.211865
H	1.142906	-5.271024	0.775125
H	5.745969	-1.024171	-2.897212
H	2.945315	4.288877	-0.199108
H	0.145976	-0.214955	0.885536
C	-2.625911	-2.953633	-1.714838
C	-3.986158	-2.753431	-2.054023
C	-4.740563	-3.752408	-2.676718
C	-4.120845	-4.968504	-2.955483
C	-2.770659	-5.184592	-2.623699
C	-2.020863	-4.187975	-2.010094
C	-2.048123	-1.789299	-1.088103
C	-2.921571	-0.750580	-0.962836
H	-5.781926	-3.587425	-2.935932
H	-4.689360	-5.758267	-3.437528
H	-2.309353	-6.140250	-2.854559
H	-0.975141	-4.345546	-1.764040

S	-4.523687	-1.137019	-1.598139
C	-0.682989	-1.719152	-0.492450
O	0.411815	-1.920747	-1.449760
H	-0.593397	-2.436670	0.327011
C	-2.585454	0.557644	-0.286493
H	-2.714194	0.408093	0.789948
C	-3.455371	1.727208	-0.713818
C	-4.151620	2.545224	0.185531
C	-3.530758	2.071799	-2.074181
C	-4.886744	3.654750	-0.235133
C	-4.260595	3.171794	-2.515286
H	-2.997682	1.456001	-2.792605
C	-4.940092	3.968374	-1.591574
H	-5.409937	4.265008	0.492218
H	-4.296099	3.407643	-3.574291
H	-5.511531	4.831351	-1.919300
Br	-4.135581	2.184241	2.078525

Vibrational frequencies

-207.4458	10.6684	14.9495
16.8522	26.8106	31.2187
34.0967	39.4206	50.1364
51.0980	54.6023	58.8990
63.6862	75.5034	76.6773
77.7441	81.7730	85.3608
103.8096	114.2506	116.8152
124.6592	139.8879	144.6860
148.9549	163.4597	170.6368
179.4785	191.0637	197.9977
205.1046	209.2547	216.4916
218.8406	230.2176	246.1841

247.1737	264.3371	275.4171
285.7036	289.6333	297.9732
316.8416	323.1726	332.6214
355.8032	359.7139	369.4272
387.4336	395.9357	418.1942
420.2192	429.8585	435.9406
438.4410	444.5179	464.9449
479.3029	486.5028	496.6039
502.2202	504.2373	509.8842
513.8068	526.6164	531.6883
534.5387	542.9676	551.5274
568.3427	580.8196	581.8400
596.9591	599.1681	604.5354
611.9609	615.6892	623.6621
633.3210	642.7991	653.9278
680.0175	695.0412	697.1037
706.6033	710.9814	714.6107
717.6039	732.0674	736.6642
743.5200	752.2237	757.5167
761.8161	764.4475	773.9866
780.2881	789.0536	791.6614
820.1461	821.3211	840.1908
845.4402	862.7014	865.7977
874.6492	875.3405	876.1614
896.5092	897.6946	903.2238
909.3196	920.7684	922.2888
945.0941	946.4837	953.0490
960.2789	967.7887	970.3156
975.6453	978.3838	978.8323
979.8334	992.7976	995.5684

996.8263	999.1737	1010.8326
1015.0675	1022.4853	1027.4802
1035.7638	1039.0879	1042.1517
1043.9188	1045.4586	1046.8642
1052.0561	1053.9694	1057.2042
1065.9834	1070.2325	1072.6713
1072.7785	1075.0898	1080.7306
1094.0006	1101.6355	1111.5553
1118.1647	1139.5018	1151.2385
1152.8011	1179.6648	1183.0666
1183.4741	1185.3178	1189.8010
1192.7499	1194.7296	1198.5360
1203.8238	1211.3059	1218.7786
1223.8530	1225.3510	1232.4020
1243.0511	1255.1183	1267.3781
1271.4999	1275.3221	1288.8846
1289.6059	1290.3785	1292.0039
1303.7707	1306.6578	1318.2469
1322.4037	1329.5338	1339.0753
1342.8161	1342.8252	1355.2421
1361.5834	1363.2078	1367.7379
1374.5946	1376.8877	1381.6265
1390.7106	1408.3519	1411.4865
1418.8813	1421.3199	1425.0010
1428.1287	1438.8633	1445.4724
1452.9006	1473.4008	1473.9530
1474.2984	1479.4585	1482.0958
1485.4693	1487.7809	1491.2977
1492.7666	1493.9575	1497.2197
1502.3884	1506.4975	1514.9376

1521.3010	1534.3183	1536.0447
1592.6396	1617.2528	1621.7967
1635.7950	1637.7176	1640.3952
1641.0834	1645.0111	1646.0281
1654.5984	1656.4604	1656.8321
1693.7392	3030.7566	3039.3639
3041.3242	3048.3738	3055.1821
3068.8030	3088.1783	3092.8163
3100.9938	3101.9966	3103.7976
3108.5842	3126.5925	3128.7860
3135.9139	3137.9160	3142.4682
3149.0411	3178.1697	3179.0667
3179.4658	3180.5060	3183.2814
3184.9537	3186.3529	3192.1186
3192.2347	3194.3757	3195.1142
3199.4155	3200.3985	3203.9807
3206.2059	3207.5575	3211.5829
3213.5797	3219.7494	3224.3605

M6RR

Zero-point correction= 0.352656

Thermal correction to Energy= 0.375279

Thermal correction to Enthalpy= 0.376224

Thermal correction to Gibbs Free Energy= 0.299071

Sum of electronic and zero-point Energies= -4083.008590

Sum of electronic and thermal Energies= -4082.985967

Sum of electronic and thermal Enthalpies= -4082.985023

Sum of electronic and thermal Free Energies= -4083.062175

Cartesian coordinates

C	-0.810811	0.862046	0.743860

C	0.017770	0.575272	2.026403
H	-1.857263	0.877432	1.051762
C	0.861531	1.707980	2.606615
O	0.680179	2.779682	3.113405
C	-0.550684	2.187195	0.035781
C	-1.657109	2.958542	-0.349494
C	0.730804	2.647004	-0.306127
C	-1.494481	4.152841	-1.052927
H	-2.657104	2.611719	-0.105652
C	0.895812	3.842547	-1.007666
H	1.610969	2.082115	-0.023148
C	-0.214515	4.600079	-1.385668
H	-2.368004	4.732657	-1.337545
H	1.897564	4.180244	-1.257601
H	-0.083002	5.529759	-1.931730
H	-0.616690	0.109311	2.782462
C	3.088965	-0.833536	0.016484
C	3.080610	-1.216222	-1.347422
C	4.255358	-1.569435	-2.017341
C	5.451900	-1.538161	-1.305768
C	5.478557	-1.159756	0.049081
C	4.309935	-0.806763	0.712988
C	1.763518	-0.506408	0.485129
C	0.800466	-0.627329	-0.473178
H	4.237248	-1.858589	-3.063417
H	6.376742	-1.806689	-1.807382
H	6.425385	-1.140613	0.580233
H	4.331043	-0.503712	1.755333
S	1.447950	-1.165798	-2.013210
C	1.383692	-0.130083	1.868753

O	2.067435	1.090429	2.395686
H	1.557098	-0.940519	2.580999
C	-0.659538	-0.336016	-0.268535
H	-1.081801	0.011094	-1.215712
C	-1.477607	-1.547047	0.178354
C	-2.869773	-1.592406	-0.002552
C	-0.890017	-2.648478	0.816776
C	-3.646197	-2.665009	0.431177
C	-1.648329	-3.732204	1.258821
H	0.184935	-2.657843	0.960665
C	-3.029408	-3.741885	1.068107
H	-4.718176	-2.660455	0.269593
H	-1.156985	-4.567158	1.748559
H	-3.630483	-4.580344	1.406013
Br	-3.789208	-0.143518	-0.884135

Vibrational frequencies

23.4442	37.8233	39.0852
56.1115	58.4912	70.0837
82.5667	107.9362	122.4949
134.9986	149.0201	154.8958
164.2596	213.3220	217.3607
232.3499	256.9750	287.6875
315.3210	319.3323	361.6759
384.2929	390.1934	419.1868
423.2282	440.4737	455.5576
483.8756	505.2699	518.4425
536.3408	542.2052	570.2333
602.8871	604.1069	630.9688
646.1332	655.8664	675.7096
692.3500	715.9587	721.1807

731.2639	741.2341	746.4754
758.8864	772.0817	773.7556
783.0844	804.2326	812.2132
854.8177	862.6342	876.2038
887.3021	894.9158	908.6262
933.0816	954.8575	956.5507
972.4523	978.9227	982.1745
990.9703	996.3720	1009.0921
1012.2139	1015.9384	1026.9155
1044.8081	1052.1605	1061.3378
1076.4320	1078.8549	1117.2931
1126.7911	1139.7605	1146.2781
1153.9727	1184.9795	1188.0483
1192.8657	1195.4129	1205.8037
1215.3948	1219.0815	1227.6669
1247.9885	1275.0978	1286.9273
1294.0926	1300.1385	1316.3637
1329.5424	1347.5687	1350.4623
1364.2305	1369.4612	1393.0932
1404.3463	1428.6735	1473.5191
1475.1432	1494.9901	1504.2665
1505.9578	1539.7187	1595.8412
1617.7823	1624.1194	1636.5474
1642.1014	1646.6049	1658.0182
1905.7588	3080.7526	3104.6492
3108.6628	3126.8784	3182.4085
3190.2700	3190.8122	3196.1963
3198.9067	3199.5592	3206.7744
3208.7969	3208.8136	3215.6575
3215.7250	3224.0316	3226.9816

M6RS

Zero-point correction= 0.352126

Thermal correction to Energy= 0.374049

Thermal correction to Enthalpy= 0.374993

Thermal correction to Gibbs Free Energy= 0.299909

Sum of electronic and zero-point Energies= -4083.000464

Sum of electronic and thermal Energies= -4082.978541

Sum of electronic and thermal Enthalpies= -4082.977596

Sum of electronic and thermal Free Energies= -4083.052680

Cartesian coordinates

C	-0.112903	1.558572	-1.143267
C	-1.166277	1.007391	-2.156275
H	0.555685	2.206761	-1.714455
C	-2.600805	1.513773	-2.033769
O	-3.185800	2.553835	-2.155911
C	-0.725198	2.426572	-0.048865
C	-0.422332	3.796478	-0.044056
C	-1.591601	1.936553	0.941995
C	-0.946382	4.650536	0.927184
H	0.242407	4.195598	-0.805692
C	-2.113287	2.788382	1.917076
H	-1.866208	0.889818	0.959763
C	-1.791950	4.147083	1.917308
H	-0.692018	5.706497	0.909876
H	-2.776606	2.385192	2.676984
H	-2.200184	4.806790	2.677468
H	-0.784982	1.091090	-3.175932
C	-2.030632	-2.099025	0.090762
C	-1.268305	-2.543429	1.200123

C	-1.739942	-3.538809	2.061181
C	-2.992558	-4.090603	1.806174
C	-3.764697	-3.656764	0.712554
C	-3.295931	-2.667045	-0.142601
C	-1.341227	-1.067128	-0.642963
C	-0.127279	-0.740185	-0.114614
H	-1.147873	-3.871521	2.908040
H	-3.378214	-4.863656	2.463971
H	-4.740487	-4.100242	0.538219
H	-3.895635	-2.323537	-0.979920
S	0.267150	-1.683404	1.310277
C	-1.812671	-0.370211	-1.865507
O	-3.143095	0.296364	-1.720428
H	-1.865576	-1.031910	-2.734074
C	0.761538	0.333019	-0.701903
H	1.123594	-0.072850	-1.653506
C	2.009812	0.604559	0.127255
C	3.174410	-0.162044	-0.064163
C	2.063330	1.573389	1.142049
C	4.339511	0.043585	0.672550
C	3.219286	1.794607	1.889553
H	1.183078	2.163770	1.352876
C	4.364199	1.036346	1.650737
H	5.214798	-0.567707	0.484999
H	3.218430	2.559016	2.660484
H	5.270828	1.202218	2.224452
Br	3.210488	-1.597031	-1.352524

Vibrational frequencies

-10.8427	28.9543	40.1002
51.5115	51.7609	58.4750

75.3066	95.8353	119.7140
127.4179	142.2428	154.3571
196.6231	214.5745	218.0909
222.2367	258.4827	276.6112
301.9826	325.4533	339.5853
374.6148	404.7160	416.8480
418.3027	435.9636	449.8566
486.4970	500.1847	506.5014
525.8086	549.7743	569.7942
581.6393	597.2198	630.0360
651.5300	658.3667	672.6191
689.4950	712.9521	719.1386
731.0592	737.6381	742.5046
754.2997	767.7346	776.8112
788.5987	796.9157	816.1072
825.3108	861.4878	872.2212
887.7603	893.4026	901.8119
935.5419	950.2688	952.9286
971.2870	974.8257	981.9590
991.9421	1005.4234	1007.8652
1013.7549	1014.8945	1028.2643
1048.1349	1057.7080	1068.7388
1080.9957	1086.4618	1114.4163
1120.2431	1144.8615	1148.3537
1154.9441	1180.3068	1187.4818
1191.1657	1195.0152	1200.4976
1217.7986	1227.0373	1229.9716
1245.8337	1263.0870	1285.2716
1299.7220	1304.3833	1318.1706
1337.1466	1338.3745	1349.3620

1362.9071	1367.0688	1384.8278
1419.6822	1426.6554	1473.5023
1474.2003	1495.2898	1504.8356
1507.8609	1537.3818	1590.0234
1616.7192	1618.4337	1634.8062
1643.5264	1646.6003	1656.9312
1905.0379	3049.0188	3092.4243
3099.6391	3123.3855	3178.6914
3186.6874	3187.6644	3196.2850
3196.7370	3198.3614	3205.4284
3207.8529	3212.0029	3212.7217
3225.7692	3236.1173	3260.9324

M6SR

Zero-point correction= 0.351900

Thermal correction to Energy= 0.374804

Thermal correction to Enthalpy= 0.375748

Thermal correction to Gibbs Free Energy= 0.297285

Sum of electronic and zero-point Energies= -4083.010488

Sum of electronic and thermal Energies= -4082.987584

Sum of electronic and thermal Enthalpies= -4082.986640

Sum of electronic and thermal Free Energies= -4083.065103

Cartesian coordinates

C	-0.435787	1.250780	-0.293263
C	0.296812	1.900225	0.901313
H	-0.006725	1.675524	-1.206683
C	0.845124	3.284396	0.572914
O	0.408876	4.372903	0.316038
C	-1.925424	1.536511	-0.319776
C	-2.522868	1.922290	-1.526776

C	-2.743011	1.355352	0.804617
C	-3.901972	2.109489	-1.616660
H	-1.900857	2.066549	-2.406644
C	-4.123422	1.535012	0.716294
H	-2.308675	1.047222	1.750329
C	-4.708606	1.909347	-0.494810
H	-4.345615	2.407529	-2.562479
H	-4.742193	1.378118	1.595351
H	-5.783852	2.048703	-0.562083
H	-0.273344	1.849219	1.828533
C	3.667304	0.080812	-0.028864
C	3.797674	-1.088612	-0.816495
C	5.049614	-1.620938	-1.137084
C	6.183100	-0.970794	-0.655003
C	6.071808	0.191576	0.129423
C	4.825862	0.721479	0.442888
C	2.283429	0.440378	0.172717
C	1.406224	-0.409670	-0.435231
H	5.138207	-2.517366	-1.742755
H	7.165650	-1.367892	-0.891524
H	6.970991	0.680989	0.491189
H	4.738939	1.625591	1.037876
S	2.217049	-1.717750	-1.285993
C	1.787498	1.531517	1.048917
O	2.163134	2.914812	0.618546
H	2.121279	1.408014	2.082452
C	-0.093902	-0.283010	-0.398117
H	-0.491725	-0.609352	-1.362336
C	-0.741451	-1.139531	0.685992
C	-1.980230	-1.776527	0.504916

C	-0.137600	-1.281911	1.945153
C	-2.594068	-2.508820	1.521447
C	-0.737859	-2.003883	2.974761
H	0.829654	-0.822247	2.117394
C	-1.971666	-2.619671	2.763527
H	-3.551427	-2.984739	1.341328
H	-0.239484	-2.087569	3.935529
H	-2.450451	-3.187947	3.554983
Br	-2.928536	-1.652082	-1.162230

Vibrational frequencies

20.9404	34.4509	38.5875
45.5741	49.8773	62.7452
69.8224	91.7980	115.8346
136.2495	144.8755	146.6144
170.3677	186.9019	209.4924
227.9109	263.4825	282.4778
307.2080	334.2665	360.7913
368.1139	379.8273	413.2805
421.1622	433.0832	452.6586
478.5670	504.0803	517.1895
529.2156	538.7408	556.8217
603.0356	617.9194	626.4431
633.1733	654.3707	676.6976
691.9060	707.8197	711.9030
716.6398	739.1563	754.3336
758.9923	769.8868	780.5230
786.2439	800.0975	814.7363
844.3743	856.4203	873.2709
884.8787	893.3268	903.8936
925.1203	952.6279	970.7160

972.9336	973.5245	983.9640
992.4986	993.1607	1006.6909
1010.5016	1013.6218	1030.3315
1042.6135	1050.7359	1057.5164
1075.3056	1080.3171	1104.1491
1132.3119	1141.5082	1149.5904
1153.2494	1184.2752	1185.6655
1192.0928	1196.9288	1202.3767
1210.7552	1212.1005	1225.4109
1257.9249	1269.8947	1286.5815
1300.3256	1314.0182	1319.0032
1324.3589	1345.0816	1361.7496
1362.3387	1365.7783	1387.5991
1416.8325	1426.3814	1473.9913
1475.1231	1494.7329	1504.0449
1508.5640	1536.4196	1595.0103
1617.9336	1623.4855	1637.8275
1642.0422	1646.1071	1658.3936
1900.6276	3061.2752	3090.1574
3096.5235	3146.9175	3175.2702
3181.9647	3189.1165	3190.7779
3195.9033	3197.6379	3199.2501
3206.7252	3207.0795	3207.6117
3214.1082	3216.1003	3222.0461

M6SS

Zero-point correction= 0.352502

Thermal correction to Energy= 0.375299

Thermal correction to Enthalpy= 0.376243

Thermal correction to Gibbs Free Energy= 0.298245

Sum of electronic and zero-point Energies= -4083.010291

Sum of electronic and thermal Energies= -4082.987495

Sum of electronic and thermal Enthalpies= -4082.986550

Sum of electronic and thermal Free Energies= -4083.064548

Cartesian coordinates

C	0.442919	1.329333	0.239322
C	-0.404933	2.312260	-0.601538
H	0.118439	1.410391	1.281415
C	-0.994213	3.456063	0.216107
O	-0.589526	4.400153	0.838151
C	1.925039	1.651791	0.185133
C	2.623365	1.944548	1.362829
C	2.629717	1.624147	-1.026624
C	3.994895	2.205635	1.333511
H	2.088723	1.962728	2.308640
C	3.999722	1.882538	-1.059264
H	2.108007	1.389719	-1.949551
C	4.687287	2.174669	0.121535
H	4.520803	2.430815	2.257002
H	4.531055	1.852311	-2.006214
H	5.754430	2.375879	0.096334
H	0.115153	2.630351	-1.506265
C	-3.645738	0.094901	-0.256700
C	-3.687457	-1.279605	0.080569
C	-4.897972	-1.961906	0.233226
C	-6.080897	-1.253698	0.037204
C	-6.057980	0.111800	-0.300753
C	-4.853331	0.789390	-0.446512
C	-2.289236	0.580326	-0.355075
C	-1.348204	-0.374669	-0.099503

H	-4.917062	-3.015373	0.494878
H	-7.032622	-1.764414	0.149064
H	-6.994128	0.642514	-0.446170
H	-4.836629	1.845878	-0.696694
S	-2.063655	-1.940448	0.268654
C	-1.883049	1.930457	-0.819191
O	-2.295965	3.059794	0.074540
H	-2.262857	2.148785	-1.820465
C	0.142018	-0.145203	-0.190092
H	0.424868	-0.252946	-1.241596
C	0.972766	-1.116642	0.630857
C	2.013501	-1.888300	0.097065
C	0.744906	-1.224783	2.013125
C	2.796316	-2.728081	0.890917
C	1.513349	-2.057063	2.821937
H	-0.054942	-0.636325	2.453177
C	2.544560	-2.810925	2.258739
H	3.593170	-3.309928	0.441711
H	1.308600	-2.115267	3.886314
H	3.153920	-3.463349	2.876433
Br	2.433125	-1.835602	-1.782255

Vibrational frequencies

27.6720	29.1583	38.2538
46.9331	53.7293	58.6599
81.4393	98.0328	113.4164
132.8966	141.6443	164.8779
182.3179	196.6182	209.7780
229.1909	264.8200	278.3283
316.0274	318.6565	354.7709
367.2848	389.7989	420.4224

422.6389	433.2607	452.7764
480.9487	504.2609	507.5293
533.8751	550.2341	552.7962
582.4756	597.6170	622.5426
633.9807	655.3127	674.7430
695.0283	710.7835	718.2697
720.2918	744.9552	753.8287
766.7254	772.4037	775.0830
788.8239	801.4005	820.9184
850.8028	860.7457	876.9362
885.1515	896.1438	912.5766
928.2117	956.4736	969.3630
977.2093	978.2518	990.7438
997.3696	1002.7034	1010.3420
1015.7805	1026.5129	1037.8056
1048.5617	1060.0726	1069.8341
1078.9226	1086.9333	1113.4532
1124.5467	1146.7566	1149.7225
1154.6244	1185.6682	1187.8092
1193.7485	1195.8851	1207.2164
1215.1729	1226.6039	1232.6793
1259.6371	1271.4895	1289.1681
1292.3996	1300.7487	1321.0875
1337.7926	1347.8123	1363.6300
1365.1137	1373.6885	1393.1033
1419.2299	1428.2196	1473.5510
1474.1739	1496.8668	1504.7829
1514.6045	1539.0369	1591.7970
1617.6037	1620.8096	1639.3649
1645.4645	1646.1456	1659.5398

1898.8735	3068.2259	3082.3123
3102.8744	3136.1517	3180.7580
3186.1596	3190.7403	3192.2515
3194.2346	3198.7984	3200.7880
3201.5967	3207.4043	3210.6058
3213.5346	3215.4839	3223.3784

TS7SR

Zero-point correction= 0.611578

Thermal correction to Energy= 0.645847

Thermal correction to Enthalpy= 0.646791

Thermal correction to Gibbs Free Energy= 0.542060

Sum of electronic and zero-point Energies= -4545.390310

Sum of electronic and thermal Energies= -4545.356042

Sum of electronic and thermal Enthalpies= -4545.355097

Sum of electronic and thermal Free Energies= -4545.459829

Cartesian coordinates

C	1.125948	-0.575445	-0.344890
C	0.252536	-0.016196	0.802590
H	0.618773	-0.292373	-1.274565
C	-1.281030	-0.289007	0.473267
O	-1.613271	-1.460072	0.270664
C	1.273982	-2.085339	-0.347587
C	1.093017	-2.786739	-1.545510
C	1.664321	-2.796656	0.794271
C	1.302575	-4.163831	-1.608272
H	0.791293	-2.245203	-2.438470
C	1.878651	-4.173866	0.734539
H	1.818050	-2.274766	1.733470
C	1.701532	-4.862439	-0.467141

H	1.157048	-4.689843	-2.547678
H	2.187058	-4.708527	1.628595
H	1.870415	-5.934586	-0.512512
H	0.449115	-0.510870	1.762041
C	1.284151	3.693856	0.195993
C	2.417002	4.132876	-0.517067
C	2.699909	5.482637	-0.717144
C	1.812213	6.411997	-0.176095
C	0.676539	5.996038	0.536452
C	0.401432	4.643446	0.722245
C	1.214049	2.237495	0.243498
C	2.291396	1.620945	-0.433456
H	3.577306	5.800148	-1.270435
H	2.004790	7.471508	-0.311252
H	0.000631	6.740088	0.945663
H	-0.483490	4.323668	1.263525
S	3.382566	2.756154	-1.092148
C	0.352011	1.440195	0.976594
O	-1.994963	0.760697	0.428110
H	-0.293263	1.902956	1.715264
C	2.521879	0.139997	-0.443796
H	2.936164	-0.132141	-1.418043
C	3.539999	-0.273673	0.621245
C	4.501528	-1.269090	0.377695
C	3.516310	0.287436	1.907293
C	5.388639	-1.694808	1.366019
C	4.393908	-0.129029	2.906320
H	2.798711	1.067483	2.135790
C	5.333197	-1.123523	2.636074
H	6.113024	-2.469754	1.142955

H	4.343034	0.326282	3.890141
H	6.023880	-1.456799	3.404218
Br	4.627318	-2.135811	-1.329168
C	-5.555615	-2.128043	1.377215
C	-6.963796	-2.722331	1.248546
C	-8.032690	-1.761430	0.712459
C	-4.949428	-1.620473	0.049646
C	-7.709005	-1.189638	-0.673461
C	-5.452403	-0.260443	-0.358510
H	-5.547776	-1.315133	2.113978
H	-6.913054	-3.592023	0.579001
H	-8.190661	-0.928393	1.409146
H	-7.331952	-1.975000	-1.336342
H	-5.170185	-2.333610	-0.753672
H	-4.883210	-2.901388	1.763873
H	-7.281611	-3.100958	2.227046
H	-8.985438	-2.298386	0.638007
H	-3.860784	-1.565297	0.131383
H	-8.611298	-0.790856	-1.139574
C	-7.283906	1.277510	-0.908551
H	-8.281582	1.324344	-0.465587
H	-7.390664	1.401569	-1.992521
C	-6.389642	2.361183	-0.317264
H	-6.723914	3.340133	-0.669610
H	-6.466391	2.348773	0.775010
C	-4.943996	2.108863	-0.728605
H	-4.250612	2.771437	-0.205852
H	-4.813815	2.266327	-1.805993
N	-4.581713	0.733580	-0.389017
N	-6.743390	-0.071816	-0.639752

H	-3.596477	0.573904	-0.078227

Vibrational frequencies

-40.3923	15.2811	18.6254
31.2689	34.0731	37.5974
42.9117	46.9959	54.1317
56.8559	64.2127	69.5791
78.2046	87.0627	89.9586
105.8146	109.3102	127.0666
144.7314	146.8691	173.4001
185.8306	192.9158	203.5696
218.6027	237.2064	239.0819
269.9197	274.0912	299.0893
303.2301	318.6372	334.0333
352.4252	357.3569	368.0459
375.6785	384.7608	414.1177
417.1656	418.8978	434.2038
436.1581	459.4704	486.0122
490.9757	497.1853	516.1737
517.9793	527.5247	531.9694
534.7740	571.1304	591.3572
614.5015	631.7535	634.1692
649.1958	649.7370	663.6299
688.7461	700.8350	702.7268
710.4720	718.7780	720.2884
737.0712	744.7786	761.7215
763.0215	773.8595	776.8746
797.9083	803.5360	806.1796
837.9091	848.3702	857.1072
864.8251	870.2920	877.9438
885.4319	899.7500	900.7525

906.1999	909.0663	925.1271
925.9061	935.2013	962.5594
966.4944	972.8668	976.6939
983.2276	992.6162	993.7747
1001.0165	1009.0989	1013.0592
1014.7108	1016.7409	1024.5450
1028.0856	1037.6060	1047.7622
1060.3005	1061.7074	1071.6021
1081.1632	1092.7176	1105.4761
1108.4460	1114.9344	1120.3584
1131.4523	1135.5791	1149.6661
1155.4183	1166.2832	1183.3292
1188.8297	1191.6562	1197.2847
1201.7530	1217.0091	1218.2356
1220.9509	1226.9436	1232.1865
1246.1638	1259.3051	1259.4200
1272.0513	1273.8180	1295.8398
1302.1214	1314.3161	1322.3838
1323.3826	1324.6649	1328.3212
1334.4991	1348.5976	1354.4224
1358.9913	1366.0708	1370.3878
1371.4909	1378.0990	1382.1064
1386.8418	1396.0258	1402.5907
1406.9340	1416.2869	1417.4673
1439.6316	1459.5151	1471.4572
1479.7204	1488.0415	1488.4899
1489.8638	1492.6452	1496.4706
1500.5200	1503.7039	1504.3033
1511.6837	1518.7629	1529.3012
1541.1255	1578.5172	1618.4324

1619.4338	1639.9049	1640.4669
1644.3148	1646.4683	1661.0151
1684.7449	1741.3066	2977.6292
3026.4920	3039.7543	3046.7587
3051.9038	3052.2066	3055.3033
3056.8663	3063.5627	3072.8731
3073.6829	3078.2860	3086.6334
3089.2001	3094.1863	3113.3951
3118.0587	3125.8014	3133.8119
3137.2823	3175.7536	3182.0750
3192.0309	3198.8345	3200.9362
3201.4886	3208.8739	3209.2798
3209.4222	3218.1353	3218.3483
3224.8894	3224.9974	3229.4021

TS7SR'

Zero-point correction= 0.348529

Thermal correction to Energy= 0.371703

Thermal correction to Enthalpy= 0.372648

Thermal correction to Gibbs Free Energy= 0.293362

Sum of electronic and zero-point Energies= -4082.976557

Sum of electronic and thermal Energies= -4082.953382

Sum of electronic and thermal Enthalpies= -4082.952438

Sum of electronic and thermal Free Energies= -4083.031724

Cartesian coordinates

O	-0.399936	4.180276	0.001207
C	0.616665	3.551495	0.296351
O	1.829524	3.879609	0.266625
C	-0.446175	1.274576	-0.316454
C	0.369566	2.002857	0.774501

H	-0.128187	1.702516	-1.273176
C	-1.945171	1.480086	-0.207014
C	-2.677053	1.832863	-1.347603
C	-2.638600	1.255749	0.989947
C	-4.065031	1.956322	-1.299604
H	-2.151484	2.009218	-2.282522
C	-4.028069	1.374158	1.041294
H	-2.095822	0.970704	1.885641
C	-4.747082	1.722201	-0.103664
H	-4.613759	2.232122	-2.195880
H	-4.548413	1.190830	1.977336
H	-5.828858	1.813988	-0.063346
H	-0.140090	2.075079	1.739817
C	3.691847	0.145055	0.024530
C	3.834619	-1.051238	-0.707904
C	5.080262	-1.623558	-0.964805
C	6.205756	-0.972635	-0.462365
C	6.084486	0.221206	0.267478
C	4.837001	0.788538	0.510294
C	2.295066	0.538797	0.139208
C	1.425731	-0.352725	-0.506111
H	5.172736	-2.543392	-1.532613
H	7.189082	-1.395211	-0.643269
H	6.977406	0.710699	0.643225
H	4.743873	1.720831	1.058253
S	2.254578	-1.676652	-1.221289
C	1.739826	1.546130	0.932965
H	2.348480	2.003530	1.703907
C	-0.070278	-0.246417	-0.451628
H	-0.466866	-0.572339	-1.416752

C	-0.658586	-1.164274	0.619948
C	-1.853689	-1.873951	0.416449
C	-0.050930	-1.292928	1.878286
C	-2.420534	-2.668671	1.412611
C	-0.605551	-2.078939	2.886283
H	0.876175	-0.766667	2.074945
C	-1.794170	-2.770296	2.653481
H	-3.346305	-3.198427	1.218717
H	-0.106975	-2.150962	3.847693
H	-2.236673	-3.388491	3.428343
Br	-2.806677	-1.760946	-1.246606

Vibrational frequencies

-290.8045	21.6388	31.9577
39.6145	46.5976	49.9767
61.8917	68.4497	77.9008
94.5425	123.4465	139.6850
144.9232	169.0462	187.5210
200.9710	229.4207	236.7174
268.4292	300.8179	333.0160
357.9619	361.3177	387.3615
414.9461	417.8776	434.0223
456.2495	480.6526	496.2495
513.3592	530.1431	533.9320
556.7959	590.2137	602.1022
614.2187	631.9396	643.3161
662.8790	670.6197	695.1453
709.9128	715.4726	725.9264
734.5566	741.5134	760.1333
765.3115	772.0070	775.7124
798.9776	814.0197	859.9358

865.1543	880.9380	897.7966
900.4130	927.3406	952.4330
961.8089	975.1586	976.8681
990.0711	993.9902	1003.1470
1010.0654	1013.9487	1025.1170
1032.7709	1045.7493	1053.2791
1059.7489	1073.2393	1075.7676
1081.7453	1116.1339	1149.7124
1152.9588	1165.0409	1187.8968
1189.7331	1198.1036	1203.9435
1215.7963	1221.3035	1226.9159
1261.4709	1269.8058	1296.3848
1309.3083	1315.0946	1320.5572
1334.5219	1351.8581	1362.3306
1366.8608	1369.4873	1380.4379
1421.8792	1453.3757	1473.9651
1492.1483	1495.6147	1504.0513
1510.4607	1541.2628	1558.9409
1616.6305	1618.5175	1639.2707
1641.1770	1646.6043	1660.9462
1763.7292	3059.5657	3087.5403
3093.9811	3175.6238	3182.2248
3191.0932	3196.9921	3198.2638
3200.0519	3205.5871	3207.9404
3210.6507	3214.7325	3220.9146
3222.4011	3226.4724	3240.4291

TS7SR"

Zero-point correction= 0.744570

Thermal correction to Energy= 0.790175

Thermal correction to Enthalpy= 0.791119

Thermal correction to Gibbs Free Energy= 0.662097

Sum of electronic and zero-point Energies= -5135.529128

Sum of electronic and thermal Energies= -5135.483524

Sum of electronic and thermal Enthalpies= -5135.482580

Sum of electronic and thermal Free Energies= -5135.611601

Cartesian coordinates

O	-1.062651	-0.082396	-1.295525
C	-0.081995	-0.852252	-1.270204
C	-4.005189	-2.690068	2.620322
C	-3.426194	-2.708978	1.342612
C	-2.045337	-2.737793	1.162849
C	-1.234614	-2.745076	2.302479
C	-1.801612	-2.721674	3.582374
C	-3.190453	-2.696081	3.751011
C	-5.512187	-2.665177	2.533577
C	-5.762440	-3.148889	1.082018
C	-4.501711	-2.708386	0.284687
H	-1.597487	-2.745407	0.172324
H	-1.155946	-2.731889	4.456015
H	-3.625305	-2.687749	4.746262
H	-5.884800	-1.644691	2.684782
H	-5.774009	-4.240976	1.070957
H	-6.007825	-3.306470	3.266502
H	-4.294908	-3.348269	-0.574151
N	-4.754364	-1.339238	-0.247502
O	-6.985908	-2.765332	0.467156
C	-3.872850	-0.489731	-0.797842
C	-5.973987	-0.704831	-0.238546
N	-4.551130	0.614774	-1.085790

N	-5.878606	0.500179	-0.741646
C	-7.187476	-1.364882	0.341879
H	-7.430525	-0.896150	1.304741
H	-8.041062	-1.220033	-0.324334
C	-4.020734	1.840757	-1.622634
C	-4.416086	2.231928	-2.912114
C	-3.134477	2.581918	-0.829476
C	-3.882112	3.422442	-3.407163
C	-2.624871	3.763688	-1.380336
C	-2.986950	4.199580	-2.657890
H	-4.166844	3.748795	-4.404172
H	-1.930155	4.354356	-0.789460
C	-2.715844	2.130387	0.545245
H	-3.548523	1.689981	1.102785
H	-1.922177	1.379786	0.472193
H	-2.326289	2.970125	1.121975
C	-2.447233	5.490449	-3.221654
H	-3.227112	6.261471	-3.242330
H	-1.615328	5.873831	-2.624514
H	-2.099514	5.358245	-4.251716
C	-5.373457	1.402308	-3.729040
H	-5.075508	0.348417	-3.748694
H	-6.385756	1.441751	-3.312925
H	-5.414642	1.764225	-4.758896
O	-0.031416	-2.101415	-1.262175
H	-2.795609	-0.621894	-0.963175
C	1.766779	-0.122574	0.307406
C	1.361989	-0.136828	-1.183799
H	1.449397	-1.094970	0.700335
C	1.082754	0.957148	1.123516

C	0.459474	0.615463	2.329826
C	1.126839	2.307955	0.749773
C	-0.084015	1.597013	3.159062
H	0.409180	-0.427760	2.626138
C	0.599034	3.292981	1.583832
H	1.601449	2.596413	-0.182524
C	-0.001729	2.942090	2.795231
H	-0.562256	1.310265	4.091338
H	0.658954	4.336251	1.286965
H	-0.411058	3.710695	3.444583
H	1.257957	0.858112	-1.624272
C	4.167408	-2.624249	-2.238444
C	5.340594	-2.909468	-1.512836
C	6.286630	-3.834212	-1.950995
C	6.037260	-4.483790	-3.159582
C	4.874097	-4.214857	-3.897768
C	3.933269	-3.293550	-3.444353
C	3.341842	-1.635523	-1.553676
C	3.910882	-1.207135	-0.331203
H	7.183494	-4.042218	-1.376985
H	6.754316	-5.208867	-3.530935
H	4.703125	-4.736671	-4.833968
H	3.028334	-3.095318	-4.009986
S	5.415986	-1.947495	-0.020033
C	2.217447	-0.979993	-2.021697
H	1.933842	-1.106545	-3.064184
C	3.322388	-0.125983	0.526198
H	3.480410	-0.404414	1.571829
C	4.024074	1.211813	0.294745
C	4.291368	2.101277	1.349031

C	4.380826	1.627951	-0.997001
C	4.887306	3.343147	1.132212
C	4.973029	2.867369	-1.230811
H	4.189072	0.972033	-1.838731
C	5.230474	3.726909	-0.163161
H	5.075806	4.004162	1.970412
H	5.233728	3.156060	-2.244013
H	5.695952	4.693220	-0.330050
Br	3.802066	1.677705	3.155233
H	-0.155254	-2.780086	2.190216

Vibrational frequencies

-110.4301	13.9645	16.2603
21.9898	25.6649	31.5221
34.8033	38.3681	42.0222
45.9305	48.9468	58.8313
66.1418	69.2962	74.3970
81.1701	85.1788	87.2380
89.0717	103.8815	111.3013
125.0361	130.0389	132.5011
143.5991	144.5217	149.4783
167.1651	173.2025	176.1851
190.3011	194.9986	203.3847
208.5997	219.8226	229.1789
237.6328	238.9185	256.8358
268.0744	271.4203	284.3757
291.4523	302.9470	323.8917
331.6705	343.8800	349.6746
350.6200	362.7535	374.6620
394.5330	414.1666	416.0375
422.2461	436.0533	456.7204

458.8635	469.1433	483.7459
495.0431	499.8054	514.6727
515.9469	520.6088	524.5727
529.9963	534.1872	541.0540
566.2483	567.0367	581.4403
589.2090	594.7629	601.7062
614.2153	614.9924	629.1679
629.8257	640.8924	649.8347
651.1016	678.6896	688.4671
691.2584	708.0733	713.0908
717.5897	724.1609	729.6907
740.5402	744.7201	748.9458
753.1560	761.9815	773.9788
774.8020	778.4695	787.9142
790.0622	808.7396	814.5357
820.2616	839.8290	862.7726
869.0233	874.3232	883.1741
885.2105	886.1364	899.2815
903.4353	915.9074	922.6025
932.7706	961.7230	967.3314
968.4524	969.7025	971.3283
975.9093	976.5662	988.6729
989.3301	994.5356	995.5298
1005.2403	1011.2765	1011.3875
1011.9576	1015.0003	1030.8290
1036.6090	1043.4122	1045.9912
1047.3714	1048.0993	1048.5709
1052.9497	1056.3474	1059.7238
1063.6443	1064.2597	1066.2084
1069.8865	1073.3064	1074.4726

1075.1945	1080.4845	1102.8281
1117.7684	1126.6518	1137.8260
1151.3203	1156.8624	1162.3934
1165.2477	1183.5464	1184.1765
1186.0797	1195.2975	1196.8143
1198.7456	1205.5075	1211.7840
1220.1207	1224.8138	1228.7389
1232.2350	1248.5353	1256.0782
1256.9577	1271.6537	1275.6666
1282.2508	1294.9029	1295.2739
1300.1228	1320.4861	1321.1746
1321.5431	1325.9527	1328.5703
1337.9614	1341.6860	1349.1522
1350.8514	1351.0506	1360.3770
1364.6089	1370.5341	1370.9133
1378.7161	1388.7837	1411.5676
1414.1529	1416.7307	1419.0194
1419.9058	1424.2444	1440.1475
1448.6372	1456.7128	1473.7063
1476.8263	1479.8761	1482.0154
1486.9024	1488.8049	1489.0486
1492.9258	1494.5312	1497.3006
1499.4466	1505.0978	1508.9675
1511.2073	1520.7994	1526.4360
1537.0213	1562.6329	1584.0867
1618.6437	1620.2711	1624.1574
1636.7258	1637.0572	1640.6241
1642.7664	1646.0950	1653.9984
1658.8913	1662.2531	1729.1977
2993.3325	3039.1283	3042.1744

3049.7875	3053.3518	3060.6381
3061.2366	3086.3530	3101.9748
3102.9743	3109.8914	3113.6055
3118.6939	3125.3645	3128.5045
3131.1334	3136.7827	3140.8353
3155.4366	3178.1305	3179.1813
3183.2587	3185.1191	3187.2951
3187.3545	3197.0243	3198.3352
3198.8750	3199.5227	3202.5423
3204.4947	3207.3002	3209.9980
3210.5192	3211.0461	3218.3155
3221.0606	3224.8088	3225.5689

NHC-H+

Cartesian coordinates

C	-3.711814	0.634170	-0.432446
C	-2.924194	0.647923	0.728416
C	-2.738156	1.808604	1.475489
C	-3.361775	2.980365	1.034856
C	-4.146212	2.979155	-0.124809
C	-4.328802	1.806285	-0.865761
C	-3.751825	-0.744858	-1.045527
C	-3.294253	-1.639172	0.135345
C	-2.374121	-0.730436	0.999506
H	-2.122000	1.819833	2.371030
H	-4.626198	3.898112	-0.449413
H	-4.946233	1.808705	-1.759329
H	-3.052427	-0.806611	-1.888216
H	-4.162748	-1.881601	0.751667
H	-4.737763	-1.035234	-1.416606

H	-2.360256	-1.015377	2.052329
N	-0.980297	-0.880000	0.493037
O	-2.712073	-2.896482	-0.184473
C	0.092284	-0.128878	0.787979
C	-0.568038	-1.836925	-0.403830
N	1.097501	-0.619189	0.072408
N	0.702849	-1.697486	-0.686069
C	-1.531419	-2.834177	-0.971721
H	-1.746841	-2.576607	-2.017253
H	-1.082412	-3.830004	-0.959391
C	2.437439	-0.098856	-0.007426
C	3.488224	-0.877177	0.504575
C	2.624603	1.160779	-0.592371
C	4.775177	-0.344645	0.416908
C	3.935947	1.647769	-0.646630
C	5.017900	0.913261	-0.153555
H	5.608316	-0.922678	0.808522
H	4.108771	2.625085	-1.088940
C	1.476527	1.980800	-1.120081
H	0.730765	1.361563	-1.628556
H	0.977852	2.506723	-0.299487
H	1.834562	2.731095	-1.826054
C	6.426480	1.444919	-0.246872
H	6.998266	0.898852	-1.007126
H	6.439799	2.504382	-0.517028
H	6.959006	1.324950	0.702568
C	3.239121	-2.228294	1.124760
H	2.429218	-2.188814	1.861201
H	2.948298	-2.963862	0.367253
H	4.138288	-2.593586	1.626102

H	0.164539	0.743886	1.450031
H	-3.243154	3.896097	1.606004

Vibrational frequencies

M7SR

Zero-point correction= 0.336028

Thermal correction to Energy= 0.356589

Thermal correction to Enthalpy= 0.357534

Thermal correction to Gibbs Free Energy= 0.284699

Sum of electronic and zero-point Energies= -3894.457690

Sum of electronic and thermal Energies= -3894.437129

Sum of electronic and thermal Enthalpies= -3894.436185

Sum of electronic and thermal Free Energies= -3894.509020

Cartesian coordinates

C	-0.435017	1.617038	-0.489992
C	0.392821	2.458169	0.462459
H	-0.182987	1.970671	-1.501359
C	-1.932720	1.783012	-0.310620
C	-2.768572	1.874877	-1.430275
C	-2.515989	1.812260	0.964256
C	-4.151219	1.993026	-1.285457
H	-2.330425	1.849078	-2.424794
C	-3.898696	1.926409	1.114142
H	-1.883364	1.733147	1.843382
C	-4.721646	2.016958	-0.011120
H	-4.781905	2.064597	-2.167211
H	-4.332622	1.943695	2.110052
H	-5.798023	2.107817	0.104836
H	-0.079102	3.326564	0.912467
C	3.713504	0.681132	0.022912

C	3.941010	-0.581721	-0.579013
C	5.228802	-1.101841	-0.737120
C	6.305074	-0.346774	-0.278133
C	6.099768	0.907522	0.324773
C	4.818237	1.424304	0.474903
C	2.305457	1.015493	0.067956
C	1.513401	0.047580	-0.489942
H	5.386488	-2.068906	-1.204694
H	7.314037	-0.732863	-0.388038
H	6.954371	1.479274	0.674253
H	4.664890	2.395363	0.936156
S	2.424797	-1.331821	-1.078469
C	1.693185	2.197280	0.671105
H	2.304661	2.841483	1.296459
C	0.006448	0.099198	-0.494916
H	-0.361944	-0.314207	-1.435716
C	-0.597979	-0.724447	0.640054
C	-1.758168	-1.497410	0.483666
C	-0.030631	-0.691492	1.923986
C	-2.337557	-2.195386	1.543868
C	-0.595172	-1.377600	2.996850
H	0.872510	-0.111346	2.075415
C	-1.754456	-2.131268	2.807958
H	-3.234260	-2.782176	1.379575
H	-0.129009	-1.324734	3.975930
H	-2.204913	-2.672652	3.634289
Br	-2.631270	-1.646673	-1.226266

Vibrational frequencies

17.3654	35.0103	46.2345
50.9181	62.0928	71.5060

113.9881	119.6838	144.4027
153.3721	173.4528	201.0711
222.3858	239.0218	265.9574
291.2371	333.6856	342.6373
370.4060	407.0401	417.4639
427.8455	436.3959	459.8913
470.7301	503.8933	515.7647
523.4126	535.5648	563.4597
595.5076	613.4572	626.4504
632.4643	665.4857	685.3103
704.8197	716.0475	722.9637
733.2292	747.8374	761.0692
766.6586	772.7149	781.3846
793.7373	814.6867	862.5570
869.2780	870.3498	895.8007
923.8772	936.2703	948.2117
968.4546	976.9344	980.6112
989.5888	993.9807	999.6680
1004.2127	1014.7215	1027.0405
1044.1695	1050.6018	1054.9684
1062.5385	1076.4593	1080.0701
1111.0256	1145.5025	1152.0715
1176.1967	1184.8374	1190.5110
1193.7754	1198.7517	1209.4081
1220.3944	1233.1315	1251.0921
1286.3200	1292.0183	1307.5227
1321.3026	1325.2351	1356.9112
1360.9434	1363.6933	1370.4827
1378.0958	1445.5783	1471.9014
1473.0585	1491.6199	1504.0345

1509.3005	1536.8257	1577.9323
1608.5409	1617.8197	1636.5852
1642.3240	1644.8107	1659.6711
1689.4000	3003.3422	3099.6766
3173.6526	3179.7840	3184.2207
3186.7928	3188.0738	3194.0398
3195.2195	3195.6475	3203.5097
3204.1212	3205.3166	3207.5995
3211.9395	3222.3139	3225.4626

TS8R

Zero-point correction= 0.395395

Thermal correction to Energy= 0.429184

Thermal correction to Enthalpy= 0.430129

Thermal correction to Gibbs Free Energy= 0.327767

Sum of electronic and zero-point Energies= -5379.530097

Sum of electronic and thermal Energies= -5379.496308

Sum of electronic and thermal Enthalpies= -5379.495364

Sum of electronic and thermal Free Energies= -5379.597725

Cartesian coordinates

C	-0.988968	1.257363	0.302158
C	0.070240	1.310991	1.280831
H	-0.191625	1.426776	-0.701152
C	-1.929876	2.411981	0.123861
C	-2.979047	2.329797	-0.813756
C	-1.775114	3.615903	0.834542
C	-3.844022	3.401571	-1.019027
H	-3.146804	1.421829	-1.381431
C	-2.639539	4.688043	0.625669
H	-0.981673	3.730077	1.562508

C	-3.678436	4.588578	-0.302445
H	-4.647226	3.307149	-1.743589
H	-2.498925	5.603763	1.192010
H	-4.350429	5.425749	-0.465268
H	0.354825	2.260089	1.716726
C	1.307959	-2.302928	1.169141
C	0.671122	-3.384655	0.518666
C	1.223797	-4.665618	0.503620
C	2.440228	-4.859785	1.155887
C	3.088934	-3.796776	1.806271
C	2.533327	-2.521870	1.816361
C	0.548314	-1.076608	1.028839
C	-0.602304	-1.242716	0.277781
H	0.725359	-5.485961	-0.002585
H	2.891988	-5.846874	1.156296
H	4.037985	-3.971725	2.303220
H	3.041979	-1.701023	2.311887
S	-0.839221	-2.879054	-0.251557
C	0.861622	0.213980	1.551309
H	1.719927	0.325418	2.205900
C	-1.584871	-0.139990	0.002318
H	-1.821272	-0.176365	-1.063209
C	-2.881894	-0.409867	0.776565
C	-4.002862	-0.992246	0.172521
C	-2.969945	-0.108712	2.142539
C	-5.176575	-1.251223	0.879382
C	-4.131390	-0.362890	2.867240
H	-2.113411	0.337330	2.637500
C	-5.238513	-0.931459	2.234504
H	-6.027033	-1.697178	0.376317

H	-4.171946	-0.115017	3.923111
H	-6.150420	-1.129236	2.789084
Br	-3.964512	-1.476091	-1.690912
C	2.648553	0.107020	-1.292994
C	1.917864	1.352882	-1.097084
C	2.591550	2.407283	-0.373106
C	3.881175	2.253860	0.104769
C	4.626705	0.996317	-0.067792
C	3.920743	-0.061841	-0.822116
Cl	4.808575	-1.530558	-1.059607
Cl	1.819094	-1.124864	-2.184803
O	5.761418	0.846862	0.387463
O	0.753349	1.535292	-1.597669
C	4.541721	3.296800	0.812055
N	5.077631	4.149157	1.395743
C	1.885954	3.640296	-0.210566
N	1.309068	4.639026	-0.067389

Vibrational frequencies

-1166.6039	16.7377	25.9375
37.6470	39.3951	43.2073
44.2195	50.6530	52.3473
72.7910	73.1770	77.5300
87.6959	92.5067	103.9288
122.2605	129.7217	144.5983
144.9493	150.7463	161.9313
182.3453	191.0516	207.8315
213.3275	235.5461	247.7515
260.9282	266.6279	279.2014
298.9388	303.3926	329.1780
346.9024	352.3744	352.6026

366.8533	379.5789	406.2468
413.9163	431.1028	436.6570
453.8075	457.6752	460.4743
482.9579	485.9726	500.6912
503.7768	511.0767	513.9704
519.3086	527.0801	540.8761
544.6875	576.2882	602.9144
623.9420	631.4073	640.2454
649.2676	665.1123	692.4966
707.5185	712.6877	720.2743
730.2091	738.9551	749.0279
768.0078	769.8570	773.7826
774.8862	786.0051	789.3166
795.6156	814.7995	844.2273
861.0593	879.0252	882.2127
890.0127	899.4066	948.5421
960.3387	967.8830	979.5700
991.4020	1000.6767	1002.9389
1007.4885	1009.6039	1014.3864
1015.0032	1016.9078	1027.3381
1050.1153	1059.9480	1073.5414
1074.6563	1076.0254	1081.0713
1109.1195	1124.9660	1146.4766
1152.5426	1163.4154	1191.6148
1192.6104	1197.7964	1208.6356
1215.6795	1221.7375	1236.0892
1263.4492	1263.8642	1267.2256
1289.5969	1297.8520	1320.9292
1331.3766	1342.3847	1354.9478
1361.6145	1365.5085	1378.4748

1381.7181	1409.6348	1462.9678
1475.5989	1479.7697	1489.1351
1503.5615	1509.3753	1523.6369
1531.6370	1546.3765	1554.8660
1586.0448	1615.2217	1620.1900
1627.6371	1633.8002	1641.1588
1644.4485	1654.2365	1682.8215
2335.5454	2353.1996	3092.1913
3191.4789	3196.3264	3199.5457
3200.5316	3205.4672	3208.7638
3211.0178	3212.0146	3214.9018
3218.3208	3221.6198	3224.5503
3227.2259	3229.2407	3241.8551

TS8R'

Zero-point correction= 0.393716

Thermal correction to Energy= 0.427953

Thermal correction to Enthalpy= 0.428897

Thermal correction to Gibbs Free Energy= 0.324066

Sum of electronic and zero-point Energies= -5379.520825

Sum of electronic and thermal Energies= -5379.486588

Sum of electronic and thermal Enthalpies= -5379.485644

Sum of electronic and thermal Free Energies= -5379.590475

Cartesian coordinates

C	-1.351402	-0.816497	-1.482384
C	-1.596109	0.286306	-2.462909
H	-0.381891	-1.258668	-1.727484
C	-2.386713	-1.941106	-1.639076
C	-1.961805	-3.274361	-1.640337
C	-3.754592	-1.654257	-1.712379

C	-2.893962	-4.310323	-1.722871
H	-0.902989	-3.500312	-1.549494
C	-4.685974	-2.690287	-1.793199
H	-4.088939	-0.621154	-1.703078
C	-4.257960	-4.020549	-1.800390
H	-2.553331	-5.341622	-1.722043
H	-5.745630	-2.458199	-1.849866
H	-4.983885	-4.825995	-1.863029
H	-1.420636	0.049103	-3.507540
C	-2.840163	3.028365	-0.195876
C	-2.894032	3.020008	1.222005
C	-3.373158	4.113463	1.941947
C	-3.796285	5.233234	1.227466
C	-3.751112	5.262495	-0.179856
C	-3.280018	4.172343	-0.894342
C	-2.313593	1.805163	-0.723430
C	-2.008836	0.862305	0.283332
H	-3.411810	4.099467	3.026140
H	-4.167470	6.097930	1.768832
H	-4.090756	6.148029	-0.707179
H	-3.250749	4.190482	-1.979040
S	-2.309987	1.499724	1.895896
C	-2.063066	1.502432	-2.104642
H	-2.243790	2.269927	-2.849758
C	-1.284833	-0.342307	-0.005042
H	-0.094765	0.309922	0.029892
C	-1.242729	-1.445326	1.016126
C	-0.155092	-2.319051	1.174732
C	-2.378789	-1.715850	1.801304
C	-0.159071	-3.363226	2.093563

C	-2.405743	-2.758617	2.724447
H	-3.269396	-1.115064	1.659075
C	-1.289524	-3.576968	2.883169
H	0.709529	-4.004294	2.189788
H	-3.303018	-2.932539	3.309430
H	-1.293292	-4.388311	3.604020
Br	1.408824	-2.165753	0.063499
C	2.735511	1.050608	-1.233039
C	1.999027	1.021344	0.009918
C	2.724778	0.726827	1.212726
C	4.097413	0.542495	1.205126
C	4.879781	0.611568	-0.039627
C	4.093550	0.865416	-1.263526
Cl	5.001785	0.923541	-2.740381
Cl	1.799852	1.336424	-2.670401
O	6.103722	0.458342	-0.048938
O	0.729698	1.234112	0.051449
C	4.815147	0.252949	2.398519
N	5.400070	0.015696	3.376376
C	1.947102	0.565287	2.400495
N	1.291656	0.407835	3.347343

Vibrational frequencies

-1640.3711	15.4388	21.0528
23.4520	32.7605	38.5901
41.2758	43.1734	52.6501
60.0237	65.7317	68.6371
73.3483	86.9796	93.3280
114.5326	122.2016	129.1095
148.5576	154.5747	157.8976
182.4731	189.0048	209.4006

211.4956	227.7051	240.4152
256.5402	269.0903	275.5372
292.9382	301.5751	324.1296
332.3588	347.7665	354.2907
362.5700	374.9627	383.3846
418.8487	420.4121	433.6508
436.1820	441.2051	449.7018
477.4424	485.8393	490.1887
502.7353	507.1296	514.4362
524.1942	529.3637	533.3657
552.2217	580.7885	597.6697
622.0426	632.3014	639.2180
653.0880	663.7087	689.7065
708.1228	715.8948	721.7024
730.4967	735.9124	749.0798
763.8440	766.9705	767.2828
771.2625	774.2924	784.6483
793.5963	818.2987	838.3756
865.8964	876.7506	880.4223
889.5983	893.9333	941.4376
956.5154	966.3518	977.2698
987.3856	997.2258	1003.3587
1006.2485	1011.8521	1013.0850
1014.1054	1015.8648	1031.0325
1046.9259	1055.7937	1057.6246
1068.7963	1077.2947	1080.9569
1088.0300	1117.5765	1120.2607
1151.1295	1161.5705	1188.8295
1192.0134	1192.7502	1196.5032
1215.3944	1218.3293	1220.7793

1233.7899	1251.7520	1261.7469
1278.8430	1302.9136	1312.1806
1326.5373	1345.5287	1356.6875
1358.8099	1364.5894	1374.6877
1385.5152	1423.6396	1448.6670
1465.3977	1469.6735	1491.7190
1494.3846	1507.8724	1510.0839
1514.9827	1530.4634	1536.0691
1595.6192	1603.2139	1611.2676
1631.8742	1638.0105	1638.8866
1647.9043	1654.7266	1673.2115
2334.3891	2353.0949	3079.4604
3183.6677	3188.6272	3196.9885
3197.6471	3200.2939	3203.7835
3204.2641	3207.4260	3212.2849
3215.0880	3215.1679	3218.2693
3222.5842	3224.7078	3229.2354

TS8R'‘

Zero-point correction= 0.950363

Thermal correction to Energy= 1.004078

Thermal correction to Enthalpy= 1.005022

Thermal correction to Gibbs Free Energy= 0.863210

Sum of electronic and zero-point Energies= -5135.500757

Sum of electronic and thermal Energies= -5135.447043

Sum of electronic and thermal Enthalpies= -5135.446099

Sum of electronic and thermal Free Energies= -5135.587911

Cartesian coordinates

C	2.276306	1.021672	1.113334
C	3.224666	2.078629	1.395424

H	1.856746	1.536444	-0.212529
C	0.936724	0.990328	1.739016
C	-0.010940	0.020522	1.334119
C	0.523176	1.928950	2.711238
C	-1.306856	0.017237	1.840997
H	0.261252	-0.749314	0.623188
C	-0.774674	1.926338	3.213263
H	1.229284	2.657385	3.092747
C	-1.704652	0.979286	2.771174
H	-2.012125	-0.733581	1.499914
H	-1.059842	2.660629	3.961261
H	-2.717332	0.976716	3.162648
H	2.867415	2.987601	1.865718
C	6.313131	0.698973	-0.359663
C	6.447662	-0.582893	-0.947428
C	7.610387	-0.966009	-1.620728
C	8.656993	-0.050398	-1.701980
C	8.543226	1.225841	-1.122661
C	7.382764	1.604476	-0.456762
C	5.018830	0.872451	0.271476
C	4.220592	-0.239161	0.143194
H	7.696404	-1.951096	-2.068758
H	9.569980	-0.327636	-2.220274
H	9.371274	1.924189	-1.198827
H	7.296656	2.592913	-0.015231
S	4.992109	-1.554907	-0.715926
C	4.522696	2.033134	0.970837
H	5.184034	2.877948	1.132335
C	2.857550	-0.364384	0.764578
H	2.199707	-0.835061	0.035898

C	2.915307	-1.299171	1.982530
C	2.461065	-2.621604	1.948583
C	3.457400	-0.843195	3.193940
C	2.516749	-3.461242	3.061639
C	3.526921	-1.663284	4.316574
H	3.822023	0.177413	3.245779
C	3.051334	-2.975052	4.253037
H	2.148209	-4.478794	2.996400
H	3.948987	-1.278809	5.239937
H	3.095115	-3.622300	5.123469
Br	1.736158	-3.365402	0.321713
C	0.191231	1.663823	-1.428709
C	-0.773692	2.621681	-0.923478
C	-2.064273	2.181353	-0.766071
C	-2.494328	0.877870	-1.181039
C	-1.584421	0.137221	-2.002594
C	-0.272701	0.507580	-2.173540
H	-2.805582	2.853986	-0.361292
H	-1.937964	-0.762362	-2.483933
C	-3.776140	0.369098	-0.822271
C	-4.327970	-0.808142	-1.427209
C	-4.539167	0.989441	0.221443
C	-5.527364	-1.350411	-1.060426
H	-3.774170	-1.267234	-2.232976
C	-5.734632	0.505952	0.670761
H	-4.108649	1.851000	0.710242
C	-6.298165	-0.710290	0.033998
C	0.637737	-0.169601	-3.219029
C	-0.112054	-1.270830	-3.992910
H	-0.997164	-0.884559	-4.509047

H	0.554143	-1.693000	-4.751900
H	-0.424729	-2.092071	-3.338634
C	1.061155	0.923136	-4.233279
H	1.668818	1.694867	-3.754491
H	1.655257	0.473669	-5.036866
H	0.186635	1.403693	-4.685177
C	1.907525	-0.801022	-2.616764
H	2.524969	-0.058283	-2.115480
H	1.657111	-1.594987	-1.909485
H	2.506356	-1.253085	-3.415372
C	-0.389504	4.107648	-0.752205
C	0.095555	4.607098	-2.137130
H	0.997623	4.076811	-2.453332
H	-0.675337	4.462659	-2.901790
H	0.329852	5.676576	-2.089267
C	-1.604945	4.956521	-0.332049
H	-1.994139	4.652117	0.645659
H	-1.302224	6.005638	-0.255062
H	-2.419680	4.903338	-1.061550
C	0.729869	4.356851	0.278669
H	0.931119	5.432489	0.340706
H	0.431199	4.011800	1.269955
H	1.654880	3.858214	-0.002924
C	-6.096422	-2.601771	-1.747696
C	-5.172345	-3.118605	-2.867075
H	-4.187706	-3.412554	-2.486984
H	-5.622799	-4.004095	-3.327300
H	-5.026863	-2.375931	-3.659314
C	-6.256499	-3.739550	-0.709854
H	-6.942973	-3.453457	0.087395

H	-6.645385	-4.639970	-1.199663
H	-5.289081	-3.992961	-0.261253
C	-7.469100	-2.276891	-2.385043
H	-8.187961	-1.953884	-1.631619
H	-7.371927	-1.483488	-3.135146
H	-7.866158	-3.166506	-2.887673
C	-6.497100	1.176552	1.824029
C	-5.753780	2.412725	2.367114
H	-5.621474	3.184702	1.601159
H	-6.337065	2.855113	3.181197
H	-4.766792	2.159218	2.769987
C	-7.886785	1.645340	1.327431
H	-8.431273	2.131338	2.145405
H	-7.782429	2.373720	0.514976
H	-8.480678	0.805748	0.965284
C	-6.667268	0.178943	2.995418
H	-7.236463	-0.698993	2.688595
H	-5.691368	-0.153538	3.367610
H	-7.194785	0.663918	3.824965
O	1.475526	1.863548	-1.258522
O	-7.390131	-1.183014	0.412055

Vibrational frequencies

-1460.2616	11.4314	18.2047
22.0190	27.6547	31.1303
34.1695	38.6409	40.7736
47.5132	50.8576	55.6780
58.8401	66.1219	70.4210
81.9803	84.1609	93.1549
94.3310	103.3219	113.5787
116.7575	129.3577	137.7081

143.4744	151.9158	155.0586
163.9909	167.4600	170.4031
173.4206	186.6585	206.1239
212.7272	225.5168	228.6320
237.2033	243.0131	246.1257
255.3818	261.1964	269.1593
272.4071	273.6869	275.9834
287.1125	287.3787	292.9838
301.0492	303.7187	309.5718
310.6698	320.1264	324.9003
327.5251	334.4916	341.5980
349.4372	352.6243	361.7686
367.9104	369.7574	372.0173
373.9830	379.5417	387.3967
390.7880	402.4570	403.6930
408.3157	413.0102	418.3408
420.6378	421.4849	431.2880
447.3469	453.2026	453.5372
455.4672	458.2658	465.1718
473.3627	481.5434	489.8427
503.6723	510.3992	521.5315
529.7728	536.2594	540.0765
542.4647	568.9105	573.8664
577.4267	596.3980	600.7048
602.9506	626.4943	631.0840
638.5552	647.0213	665.4292
669.2021	680.7470	685.9243
691.1880	704.8346	715.6397
725.3658	734.6871	750.1747
756.8704	761.6598	764.7109

768.7451	783.5546	787.4917
790.3941	800.6023	809.5867
814.5620	819.9268	821.8650
832.5578	843.1886	858.4077
873.3673	877.5628	891.5045
895.5511	897.2292	899.5774
900.8343	907.5357	918.6528
931.0824	937.4395	941.9704
943.1522	944.5213	946.5068
947.1596	947.5045	950.7406
953.5927	954.9210	964.0037
972.4216	974.5976	975.0584
976.7900	976.9757	986.8753
987.4943	991.7250	1000.7087
1007.4691	1010.1913	1011.4706
1024.1422	1039.8285	1041.5684
1049.0191	1054.5542	1054.6891
1057.5610	1059.9569	1061.3823
1063.1004	1064.2870	1067.3026
1070.4981	1074.6183	1079.8259
1088.5269	1113.6134	1118.1257
1130.9948	1141.4626	1148.4543
1163.0439	1189.8955	1190.9808
1192.9989	1202.6570	1208.3911
1213.5456	1222.6581	1223.8030
1224.2791	1228.3106	1228.9639
1230.3095	1237.6861	1239.3176
1241.6844	1248.5297	1260.6552
1273.1331	1278.6401	1279.6984
1283.2150	1287.2723	1292.4134

1296.1073	1322.7880	1332.5603
1337.4227	1340.5160	1351.4288
1361.9246	1362.4318	1364.3792
1369.1912	1375.1605	1379.6701
1383.1657	1396.9506	1398.6069
1403.8559	1406.3145	1408.2647
1409.4736	1412.8194	1416.0626
1429.0687	1431.8688	1435.3912
1437.5382	1438.1666	1469.6647
1471.6319	1472.6121	1476.4522
1479.6315	1481.3715	1481.9862
1485.2332	1486.9689	1487.7752
1494.0190	1495.4600	1497.6858
1499.0091	1499.3850	1500.8251
1501.6942	1502.0619	1505.0102
1506.3719	1506.8677	1507.6767
1509.5065	1510.8278	1512.6758
1513.1301	1514.4237	1515.2276
1529.3089	1530.2897	1531.1193
1531.7233	1535.9562	1542.0470
1548.9039	1550.3179	1580.8592
1597.3727	1614.6839	1615.5119
1618.4776	1625.1979	1633.2222
1641.2292	1644.4920	1650.2198
1666.6558	3033.6987	3034.8990
3035.6192	3035.7134	3037.0192
3037.1889	3041.0883	3041.1907
3041.3011	3041.5434	3053.9152
3054.8880	3097.8854	3098.1528
3098.9765	3099.1144	3106.0300

3106.0567	3107.3551	3108.1658
3108.9050	3109.8457	3111.4957
3112.4951	3114.5115	3114.8442
3125.9546	3128.2784	3132.8357
3135.3917	3135.5444	3157.7777
3159.2188	3159.5781	3161.4384
3182.7740	3187.3480	3187.4516
3188.8891	3194.0117	3195.5812
3199.6861	3201.3671	3204.2046
3205.5525	3212.3509	3212.7155
3215.7517	3216.7809	3223.0989
3224.0682	3232.3419	3243.6832
3244.5683	3259.2484	3260.6943

TS8R‘’‘

Zero-point correction= 0.949387

Thermal correction to Energy= 1.003464

Thermal correction to Enthalpy= 1.004408

Thermal correction to Gibbs Free Energy= 0.860178

Sum of electronic and zero-point Energies= -5135.489261

Sum of electronic and thermal Energies= -5135.435184

Sum of electronic and thermal Enthalpies= -5135.434240

Sum of electronic and thermal Free Energies= -5135.578470

Cartesian coordinates

C	4.007393	-1.001190	1.069873
C	4.338811	0.128496	2.028852
H	3.397535	-1.731362	1.609495
C	5.341440	-1.705279	0.758953
C	5.640231	-2.915403	1.397848
C	6.291896	-1.145186	-0.106841

C	6.857877	-3.561556	1.170498
H	4.908613	-3.358803	2.068637
C	7.504619	-1.793175	-0.340802
H	6.077014	-0.206583	-0.606768
C	7.792927	-3.003841	0.296983
H	7.071239	-4.501143	1.672657
H	8.226312	-1.351945	-1.022523
H	8.737458	-3.507545	0.112682
H	4.576899	-0.157836	3.048861
C	4.485402	2.991172	-0.414396
C	4.112327	2.970660	-1.784454
C	4.309735	4.074485	-2.615477
C	4.882839	5.221353	-2.067859
C	5.256707	5.263235	-0.711473
C	5.064948	4.162978	0.113278
C	4.190945	1.751639	0.244624
C	3.583389	0.809295	-0.592363
H	4.020569	4.044917	-3.661543
H	5.041535	6.091650	-2.697424
H	5.700393	6.167922	-0.306686
H	5.357383	4.197640	1.158246
S	3.407353	1.423614	-2.239589
C	4.449334	1.407731	1.625906
H	4.751985	2.188275	2.317457
C	3.163328	-0.491124	-0.126758
H	1.942748	-0.270440	0.821841
C	2.637940	-1.471851	-1.137415
C	1.418165	-1.290409	-1.827679
C	3.332419	-2.660848	-1.443246
C	0.939502	-2.202148	-2.767592

C	2.860544	-3.589520	-2.367394
H	4.270834	-2.859857	-0.946715
C	1.662326	-3.361384	-3.042000
H	-0.004890	-2.012873	-3.265530
H	3.438407	-4.487895	-2.562242
H	1.284087	-4.074739	-3.767589
Br	0.269389	0.205614	-1.458721
C	-0.800603	-1.480471	1.594781
C	-2.116774	-1.360645	1.220498
C	-2.753809	-0.101440	0.996023
C	-2.000726	1.062589	1.332664
C	-0.672360	1.021321	1.689295
C	-0.011817	-0.267030	1.671180
H	-2.719744	-2.252492	1.143830
H	-2.487526	2.023377	1.266198
C	-4.097187	-0.020287	0.516173
C	-4.848677	1.199307	0.577427
C	-4.743089	-1.161812	-0.063980
C	-6.136883	1.312256	0.136501
H	-4.378182	2.059098	1.031053
C	-6.020751	-1.140094	-0.546782
H	-4.166696	-2.070935	-0.154272
C	-6.796814	0.122422	-0.456980
O	-7.973554	0.181365	-0.867972
O	1.297577	-0.343123	1.765727
C	-6.922452	2.627924	0.252547
C	-7.347597	3.111756	-1.155723
C	-8.176227	2.415595	1.135534
C	-6.083337	3.747392	0.898016
H	-6.468953	3.291238	-1.785602

H	-7.984643	2.378350	-1.650576
H	-7.899902	4.055051	-1.073495
H	-7.890289	2.083581	2.140124
H	-8.723980	3.359772	1.237320
H	-8.845310	1.671593	0.702423
H	-6.682920	4.661852	0.951468
H	-5.776932	3.496082	1.919295
H	-5.184252	3.978981	0.316274
C	-6.671749	-2.380164	-1.178454
C	-7.920384	-2.786113	-0.357727
C	-7.079016	-2.076622	-2.641028
C	-5.714689	-3.587835	-1.201951
H	-7.643665	-3.024981	0.675479
H	-8.660024	-1.985283	-0.342174
H	-8.381328	-3.678914	-0.796198
H	-6.202374	-1.800855	-3.238196
H	-7.526955	-2.968135	-3.095009
H	-7.801576	-1.261830	-2.689741
H	-6.225422	-4.442701	-1.657036
H	-4.815250	-3.389590	-1.795188
H	-5.404336	-3.888751	-0.195251
C	-0.211237	-2.849927	1.994501
C	0.442301	-2.733766	3.392921
C	-1.302926	-3.935801	2.082471
C	0.837875	-3.329858	0.973606
H	1.258873	-2.010422	3.395998
H	-0.293825	-2.425115	4.143580
H	0.843731	-3.707133	3.696339
H	-1.761082	-4.142705	1.109387
H	-0.849314	-4.868892	2.431634

H	-2.096249	-3.668238	2.788461
H	1.196671	-4.328781	1.247183
H	0.417457	-3.383133	-0.034867
H	1.693326	-2.663110	0.947233
C	0.079346	2.316670	2.055191
C	0.934923	2.110273	3.328661
C	0.985958	2.753377	0.886532
C	-0.900471	3.471515	2.350700
H	0.318055	1.751916	4.160682
H	1.741440	1.396179	3.165949
H	1.379014	3.066014	3.628382
H	0.397802	2.959935	-0.013213
H	1.529729	3.666257	1.154396
H	1.713499	1.984821	0.646699
H	-0.332086	4.346825	2.680750
H	-1.469974	3.776831	1.467049
H	-1.608616	3.212640	3.145411

Vibrational frequencies

-1398.0323	7.7180	12.5820
16.7720	21.5163	26.2532
27.0753	37.5148	41.9334
51.3448	55.0259	56.6061
59.8393	64.7641	69.2299
71.6462	81.6847	82.8600
87.5912	93.0329	103.3935
123.8472	128.3788	131.6795
136.0920	150.0895	154.2556
163.7570	168.4124	173.9583
176.3271	203.2408	208.1152
216.9615	223.4432	225.3469

228.7972	235.8674	240.4680
244.5082	249.7605	263.4210
267.3362	272.8630	276.2985
279.7602	287.2857	289.7067
295.0620	299.8249	302.4522
308.6929	312.9580	320.7401
323.2420	327.8809	336.5739
347.4348	349.0032	352.7192
363.0001	365.0980	369.9550
371.0789	373.2356	378.1117
388.1853	393.0118	406.2339
409.3616	410.7983	413.5224
414.6231	422.6600	423.2450
440.5536	445.2566	450.6094
454.7055	458.3713	467.3826
473.6996	481.2008	492.5823
504.7262	515.2944	525.0209
534.2887	536.5287	539.1418
542.8936	561.3703	579.0655
585.9842	595.9632	600.4059
614.2109	624.4985	634.6199
640.3599	651.0304	663.3883
664.3257	683.0055	686.0882
686.8952	712.9265	715.2439
729.0780	731.7675	746.6529
752.1264	756.4613	762.1762
763.2452	775.8669	783.9694
793.7481	796.1667	807.2882
816.7195	820.7180	823.6538
838.8640	859.9019	862.1684

871.6615	882.7408	887.5387
897.7339	900.4888	902.0466
906.0817	911.2678	925.0954
928.8434	940.2478	941.2000
943.2851	943.8708	946.1529
946.6080	946.7449	948.7934
950.0707	951.7859	959.0012
969.3133	971.0338	972.6706
973.5587	974.3956	976.1181
982.0203	988.3875	991.0513
1004.4891	1005.4332	1014.3464
1025.3312	1033.2205	1042.6556
1046.3896	1048.9403	1052.3387
1057.8999	1058.3155	1059.2346
1060.0691	1060.9838	1062.4165
1063.2301	1068.0849	1091.9040
1093.5050	1094.7222	1115.2602
1116.0579	1135.3391	1155.1553
1160.6098	1186.0119	1188.4745
1189.3694	1199.5958	1211.1757
1211.7035	1212.4618	1222.4210
1224.0503	1225.1027	1229.5890
1232.4941	1237.7593	1238.1134
1239.4458	1242.2900	1244.7372
1270.8795	1275.1804	1275.7644
1283.4699	1292.4947	1293.8437
1296.6388	1304.9181	1321.7020
1346.9032	1350.4192	1360.0087
1361.8212	1366.9349	1369.9538
1370.7726	1376.4924	1385.3684

1397.6185	1399.3909	1403.5935
1405.5646	1406.4599	1407.2519
1407.7007	1411.9573	1414.4076
1431.3327	1432.5896	1434.0161
1435.8846	1439.9453	1449.0395
1453.3945	1462.5764	1467.0714
1480.2802	1483.0611	1484.1486
1484.7550	1486.7927	1490.8836
1492.0566	1494.4960	1496.3815
1498.0220	1498.9786	1499.6129
1500.1230	1500.9191	1502.0306
1502.2835	1503.7483	1504.3695
1505.7341	1506.5463	1507.2371
1511.4351	1513.3926	1514.2213
1516.0702	1524.0910	1526.7073
1530.1410	1530.8197	1531.4625
1538.4785	1557.4713	1581.5263
1598.9486	1607.3195	1615.6466
1634.6101	1635.1161	1635.6460
1640.2748	1648.9784	1668.1265
1669.9267	3034.2049	3034.5100
3036.4942	3036.6905	3036.9525
3037.0756	3041.2816	3041.6462
3042.5294	3042.6665	3049.7591
3051.3260	3077.6281	3099.3226
3099.6748	3100.4215	3100.5253
3101.0009	3104.0640	3106.3872
3107.6768	3107.7948	3108.6490
3109.9038	3111.1758	3111.6763
3112.9411	3114.0451	3117.1062

3152.5451	3159.9953	3160.5871
3162.0592	3162.8217	3167.6416
3175.9159	3184.8945	3187.7716
3189.3718	3193.4557	3195.9726
3196.9079	3205.1202	3205.2498
3208.0847	3208.9966	3213.7168
3214.2852	3220.8348	3223.2385
3224.8457	3246.1524	3249.1094
3258.6678	3262.0140	3271.3275

M8R

Zero-point correction= 0.325081

Thermal correction to Energy= 0.345462

Thermal correction to Enthalpy= 0.346406

Thermal correction to Gibbs Free Energy= 0.274277

Sum of electronic and zero-point Energies= -3893.695450

Sum of electronic and thermal Energies= -3893.675070

Sum of electronic and thermal Enthalpies= -3893.674126

Sum of electronic and thermal Free Energies= -3893.746254

Cartesian coordinates

C	-0.861445	1.707508	-0.251274
C	-0.017984	2.803162	-0.146675
C	-2.311274	1.851252	-0.342066
C	-3.122428	0.834801	-0.899607
C	-2.944352	3.020044	0.142948
C	-4.499719	0.992441	-0.983770
H	-2.685289	-0.079992	-1.281732
C	-4.323774	3.165703	0.066704
H	-2.359222	3.800656	0.615126
C	-5.106577	2.156488	-0.501598

H	-5.102080	0.206420	-1.427482
H	-4.790874	4.063820	0.457767
H	-6.184024	2.273704	-0.563882
H	-0.423408	3.806816	-0.161929
C	3.437052	1.120031	-0.032743
C	3.671082	-0.266975	-0.142657
C	4.954993	-0.809632	-0.113931
C	6.025315	0.071802	0.031022
C	5.813345	1.455575	0.144103
C	4.527920	1.987042	0.114130
C	2.017158	1.420190	-0.093721
C	1.228215	0.275395	-0.231114
H	5.117866	-1.878987	-0.198075
H	7.036590	-0.321132	0.057883
H	6.664619	2.119031	0.257532
H	4.363965	3.056417	0.202777
S	2.154610	-1.172164	-0.317761
C	1.373911	2.666315	-0.056019
H	1.979402	3.564757	0.025516
C	-0.265221	0.316317	-0.290434
H	-0.534214	-0.085517	-1.280731
C	-0.863287	-0.612139	0.774458
C	-1.270251	-1.919904	0.485658
C	-0.964781	-0.168421	2.099450
C	-1.785992	-2.761696	1.469779
C	-1.474559	-0.998196	3.094651
H	-0.639522	0.838022	2.344348
C	-1.889212	-2.293283	2.778756
H	-2.098520	-3.768141	1.216351
H	-1.546933	-0.633734	4.114067

H	-2.290757	-2.945833	3.547381
Br	-1.116290	-2.609846	-1.301058

Vibrational frequencies

23.9998	40.0041	46.4893
48.2729	65.4881	80.4566
114.7924	126.6786	140.0704
154.7873	178.6123	203.2294
214.4461	242.7794	270.1814
293.5398	329.4366	354.2615
369.7544	403.3711	409.2479
438.2523	449.1129	455.5230
474.7558	494.0036	502.3733
518.6256	522.2168	561.9533
592.2797	617.2459	627.5311
644.2261	654.6316	690.5943
697.4246	702.7795	731.1636
737.8905	742.0910	768.0477
773.9122	781.7397	797.7525
833.7991	850.0286	864.3170
878.8144	890.1551	897.2167
966.5587	971.2623	974.9510
979.0630	1004.0388	1007.3703
1011.3673	1016.9604	1019.8844
1022.9969	1028.5226	1030.8235
1049.0615	1060.7676	1071.7765
1078.9500	1101.1088	1127.5346
1136.1820	1151.7174	1159.8385
1181.6828	1190.7179	1194.5827
1197.8752	1213.9528	1226.4734
1234.6679	1286.0500	1294.1600

1317.6304	1320.2229	1339.3166
1344.6936	1359.1883	1371.5133
1377.7247	1386.3062	1417.0746
1472.3777	1477.6395	1486.2451
1499.4042	1512.8772	1534.9613
1565.5545	1601.9383	1617.4224
1619.8519	1621.1444	1640.5486
1644.8965	1647.9838	2996.3428
3199.2195	3199.7467	3200.9439
3204.1943	3207.0137	3208.4932
3209.0460	3214.8212	3217.1407
3220.5250	3222.2813	3226.5105
3229.0530	3231.3698	3239.7304

M8R-1

Zero-point correction= 0.324496

Thermal correction to Energy= 0.344950

Thermal correction to Enthalpy= 0.345894

Thermal correction to Gibbs Free Energy= 0.273484

Sum of electronic and zero-point Energies= -3893.691047

Sum of electronic and thermal Energies= -3893.670593

Sum of electronic and thermal Enthalpies= -3893.669649

Sum of electronic and thermal Free Energies= -3893.742060

Cartesian coordinates

C	0.731137	1.551321	-1.186300
C	-0.232502	2.678504	-1.080188
C	2.010082	1.814717	-0.373271
C	1.922157	2.001455	1.011136
C	3.256705	1.844482	-1.003349
C	3.079323	2.219866	1.758641

H	0.953991	1.967498	1.500328
C	4.412965	2.063399	-0.252200
H	3.324249	1.689055	-2.076002
C	4.325936	2.251544	1.128777
H	3.006425	2.361858	2.832691
H	5.379212	2.084783	-0.747190
H	5.225987	2.420882	1.712243
H	0.161987	3.669540	-1.279863
C	-3.364897	0.807183	-0.217450
C	-3.503980	-0.605092	-0.073389
C	-4.739217	-1.179614	0.228892
C	-5.832192	-0.332939	0.385171
C	-5.716366	1.067715	0.243545
C	-4.497064	1.641393	-0.055722
C	-2.032284	1.188460	-0.524922
C	-1.151726	0.052312	-0.610942
H	-4.847842	-2.252777	0.340062
H	-6.800645	-0.763021	0.621110
H	-6.594255	1.691291	0.372694
H	-4.398280	2.715644	-0.167929
S	-2.001115	-1.475419	-0.325254
C	-1.538141	2.505686	-0.755629
H	-2.212383	3.351231	-0.682138
C	0.177116	0.185557	-0.902519
C	1.109950	-0.959649	-0.991069
C	1.497825	-1.712675	0.130052
C	1.664695	-1.290708	-2.239281
C	2.389069	-2.776587	0.011981
C	2.547573	-2.359068	-2.366730
H	1.380119	-0.709506	-3.110853

C	2.906194	-3.103224	-1.241525
H	2.682559	-3.336314	0.892617
H	2.954324	-2.607918	-3.341290
H	3.597794	-3.934834	-1.331059
Br	0.875035	-1.245261	1.879253
H	1.044231	1.519188	-2.247456

Vibrational frequencies

22.2728	31.4185	40.6983
49.3595	72.2275	84.8387
102.7838	111.2927	139.6821
168.2586	197.2170	215.5860
218.5843	246.1540	268.1834
278.7763	319.8529	322.6354
364.7897	401.2026	420.7814
433.0832	439.5155	449.5188
474.6482	497.7670	500.7891
515.6794	531.5311	573.0253
601.1351	616.3022	632.2935
649.8603	658.2100	681.5385
697.3980	714.7077	724.2363
733.0578	749.7813	762.1362
772.0234	776.7289	794.2535
826.1918	843.0462	855.6567
867.0536	882.2692	901.7696
930.7350	968.8433	977.0538
980.7208	987.3468	1001.8097
1007.7218	1012.8423	1016.6263
1019.5798	1020.1659	1038.2724
1047.5296	1055.8668	1072.9158
1082.8252	1094.0603	1106.8220

1108.9973	1145.0805	1160.3050
1171.5842	1188.5487	1190.9272
1197.1166	1198.0591	1208.3728
1220.2054	1268.0963	1287.0912
1301.5749	1333.0671	1348.5406
1349.7147	1360.3204	1364.5797
1384.1719	1395.4111	1465.0942
1469.3625	1490.1222	1496.7541
1506.6856	1524.4713	1531.2469
1553.5460	1592.9229	1610.5604
1628.2602	1638.7257	1639.0512
1648.5260	1653.7333	2966.1040
3188.7431	3194.1900	3196.2101
3202.1262	3206.2576	3207.6671
3208.9529	3212.4206	3215.9099
3218.0384	3220.0753	3223.4488
3228.3121	3228.6257	3235.9553

TS9R

Zero-point correction= 0.570657

Thermal correction to Energy= 0.601843

Thermal correction to Enthalpy= 0.602787

Thermal correction to Gibbs Free Energy= 0.504170

Sum of electronic and zero-point Energies= -4355.631106

Sum of electronic and thermal Energies= -4355.599920

Sum of electronic and thermal Enthalpies= -4355.598975

Sum of electronic and thermal Free Energies= -4355.697592

Cartesian coordinates

C	-0.244601	1.044326	1.778493
C	-0.952967	0.486341	2.839461

C	1.004935	1.777181	2.010678
C	1.945652	1.968708	0.976241
C	1.297810	2.327707	3.278934
C	3.131598	2.657553	1.202864
H	1.756104	1.573956	-0.010661
C	2.482435	3.021081	3.500996
H	0.583186	2.245964	4.090862
C	3.407896	3.184782	2.467140
H	3.840789	2.780663	0.390798
H	2.680589	3.442724	4.481342
H	4.332516	3.725376	2.642933
H	-0.564894	0.557481	3.848067
C	-3.944568	-1.062806	1.024636
C	-4.133206	-1.074369	-0.372232
C	-5.240005	-1.681339	-0.965850
C	-6.174402	-2.288858	-0.127753
C	-6.002689	-2.291099	1.265958
C	-4.894598	-1.683530	1.848592
C	-2.719626	-0.374586	1.386991
C	-2.015462	0.114028	0.273292
H	-5.372617	-1.682570	-2.042563
H	-7.045916	-2.767631	-0.562596
H	-6.743162	-2.772197	1.896123
H	-4.759533	-1.686957	2.925263
S	-2.807602	-0.255933	-1.220064
C	-2.172218	-0.170234	2.658911
H	-2.699474	-0.548490	3.529934
C	-0.728428	0.836633	0.379090
H	0.073868	0.038465	-0.000805
C	-0.735762	2.108180	-0.477874

C	-0.347235	2.169106	-1.821245
C	-1.226044	3.287679	0.104900
C	-0.408420	3.357073	-2.552311
C	-1.295082	4.480084	-0.609489
H	-1.555447	3.261993	1.139213
C	-0.878165	4.516521	-1.941627
H	-0.093153	3.367568	-3.589843
H	-1.675153	5.375197	-0.127907
H	-0.923267	5.441179	-2.509236
Br	0.264053	0.601064	-2.733059
C	4.350605	-0.522287	-0.092545
C	5.505239	-1.516290	-0.275630
C	5.146743	-2.986204	-0.022917
C	3.139036	-0.774459	-1.016266
C	3.987471	-3.491761	-0.893096
C	2.184620	-1.823906	-0.490127
H	4.012920	-0.515827	0.951090
H	5.881161	-1.424975	-1.304945
H	4.884938	-3.145398	1.031514
H	4.114990	-3.155568	-1.928456
H	3.491241	-1.057788	-2.015947
H	4.726697	0.485850	-0.298246
H	6.333597	-1.229573	0.383182
H	6.028018	-3.605588	-0.228017
H	2.563982	0.138223	-1.147954
H	3.991623	-4.583863	-0.923521
C	1.914928	-4.149513	0.312989
H	2.628628	-4.719881	0.916894
H	1.475286	-4.841758	-0.416915
C	0.833767	-3.542745	1.196357

H	0.153279	-4.325926	1.543564
H	1.287487	-3.077347	2.078650
C	0.086842	-2.475630	0.398129
H	-0.658845	-1.993504	1.031535
H	-0.460013	-2.942234	-0.435652
N	0.991679	-1.451287	-0.118501
N	2.658863	-3.100726	-0.400609

Vibrational frequencies

-57.6069	6.3892	7.9975
22.6478	30.7740	42.3543
46.4276	63.6524	67.3466
76.4962	82.0036	87.0624
98.3637	107.7066	116.0694
121.9297	136.2165	153.8411
169.5528	185.7744	204.2347
218.1648	248.7920	253.2172
255.1205	276.3184	299.4209
305.7629	332.0501	352.8031
356.8897	365.7263	379.2270
402.0691	406.3262	418.2332
435.1068	437.9553	452.3799
460.0743	478.6018	487.2365
502.7505	506.4242	517.4105
522.5161	525.2103	526.4878
578.9637	599.3747	622.2018
629.9547	643.3980	646.0480
658.4493	692.4548	695.8782
700.3346	703.4456	706.3631
731.7466	735.3113	739.2650
767.5921	773.3175	779.6873

801.4583	805.1029	831.9761
846.4129	847.9834	856.7660
861.7272	875.8090	877.0716
884.9755	895.3446	903.2134
911.9514	932.4402	945.6759
958.0746	960.8973	975.2033
976.8477	991.7145	996.5752
1004.4832	1007.3084	1011.7597
1013.3151	1013.9238	1019.9525
1020.8218	1025.5024	1037.2383
1047.6283	1060.3325	1072.7276
1080.9400	1083.2953	1101.9196
1109.1838	1112.5419	1118.8292
1126.8249	1128.7170	1131.8109
1150.4936	1161.0817	1177.1115
1182.9770	1191.4450	1193.2941
1194.4943	1212.1193	1223.2112
1228.2568	1236.1402	1237.0739
1245.5545	1261.8566	1264.5570
1288.6185	1290.0805	1294.1626
1314.6007	1317.3076	1321.6288
1330.7404	1340.6380	1345.8382
1355.7850	1362.0524	1365.3964
1369.8248	1374.9366	1380.5192
1384.4861	1384.9099	1391.7829
1398.6118	1405.3509	1416.5189
1418.7596	1468.5003	1469.9348
1479.9165	1480.4325	1481.9972
1485.8013	1489.4047	1491.4656
1494.0861	1500.6743	1500.9559

1508.7598	1510.0606	1530.3423
1536.9317	1569.9882	1603.9980
1618.1677	1618.4241	1623.5151
1632.4768	1640.8027	1643.6893
1651.3202	1833.0292	3003.2146
3016.9396	3027.7082	3035.2833
3042.0627	3050.4102	3056.0751
3057.3566	3072.8312	3080.1797
3082.4558	3088.1788	3112.9079
3115.1563	3134.7680	3183.1980
3196.4601	3196.9796	3201.1082
3202.5714	3203.1653	3205.7605
3209.9656	3212.7228	3215.8044
3217.6406	3221.3806	3222.4560
3224.9787	3237.3977	3266.1247

TS10

Zero-point correction= 0.311908

Thermal correction to Energy= 0.331218

Thermal correction to Enthalpy= 0.332162

Thermal correction to Gibbs Free Energy= 0.263461

Sum of electronic and zero-point Energies= -3893.243269

Sum of electronic and thermal Energies= -3893.223959

Sum of electronic and thermal Enthalpies= -3893.223015

Sum of electronic and thermal Free Energies= -3893.291716

Cartesian coordinates

C	3.476953	-0.375371	-0.501866
C	3.121133	-1.508129	0.249475
C	4.108594	-2.456060	0.564915
C	5.414239	-2.252440	0.131418

C	5.750765	-1.114787	-0.622968
C	4.786199	-0.163990	-0.946301
H	3.854789	-3.338277	1.145087
H	6.182255	-2.979346	0.377752
H	6.774730	-0.971598	-0.955049
H	5.044630	0.717964	-1.524256
C	1.699379	-1.534641	0.542518
C	1.009706	-2.641001	1.038147
C	0.993691	-0.362927	0.139292
C	-0.365200	-2.652041	0.913704
H	1.546134	-3.520093	1.379148
C	-0.430965	-0.251800	0.291584
C	-1.080304	-1.529987	0.462333
H	-0.908354	-3.574553	1.088531
S	2.112626	0.702623	-0.753790
C	-1.292470	0.993625	0.311413
C	-1.004701	2.364783	0.049857
C	-2.648151	0.819182	0.715151
C	-2.011277	3.322797	-0.143488
C	-3.649678	1.768313	0.592196
H	-2.935537	-0.117949	1.156786
C	-3.348413	3.024817	0.072350
H	-1.719434	4.332321	-0.408617
H	-4.657445	1.517551	0.907811
H	-4.111504	3.781076	-0.080937
C	-2.462603	-1.859495	-0.008979
C	-3.354804	-2.606991	0.777967
C	-2.845002	-1.519701	-1.318819
C	-4.603592	-2.980038	0.279254
H	-3.077405	-2.872315	1.793948

C	-4.090572	-1.897072	-1.816180
H	-2.157420	-0.956329	-1.941959
C	-4.978430	-2.624935	-1.018255
H	-5.284666	-3.546533	0.908025
H	-4.366781	-1.626759	-2.831474
H	-5.950178	-2.916288	-1.405983
Br	0.708491	3.230185	0.226386

Vibrational frequencies

-48.3312	32.7378	38.1045
63.2210	75.7296	99.2234
120.3363	124.3456	138.6952
162.2319	194.1966	209.0421
222.6448	238.3601	260.7372
315.6266	327.2593	352.5302
380.9820	398.8001	418.8522
435.4184	450.4079	478.4172
489.9519	505.5230	510.8854
526.8679	535.0698	577.3527
609.5173	627.3161	631.4576
645.1909	654.1418	679.5022
705.9537	713.4249	719.3826
732.3679	740.3839	753.5279
769.6592	778.5573	786.9757
798.6105	835.1722	842.2221
863.7042	866.3120	873.3397
933.7325	950.9261	956.9850
967.0586	983.7617	989.3012
997.1465	1002.5614	1004.9361
1011.4024	1026.7871	1034.9759
1053.4744	1067.5614	1081.1158

1102.7881	1109.5178	1117.4159
1155.7326	1161.9029	1168.6617
1186.8468	1190.0194	1196.9608
1209.6921	1213.7753	1263.8013
1277.9263	1282.5672	1307.6179
1314.4550	1321.1816	1346.3039
1359.6547	1362.6407	1392.5795
1426.1828	1451.6272	1482.6408
1487.0184	1498.8275	1504.5058
1530.4185	1590.1726	1597.1175
1609.2128	1621.5750	1625.2204
1636.3793	1643.4644	1650.4312
3182.5677	3187.2879	3188.4648
3195.6845	3197.2783	3199.3535
3202.7579	3203.8251	3204.8060
3211.4903	3212.2544	3212.4984
3218.8638	3224.4231	3301.2270

TS11

Zero-point correction= 0.301880

Thermal correction to Energy= 0.322653

Thermal correction to Enthalpy= 0.323598

Thermal correction to Gibbs Free Energy= 0.250371

Sum of electronic and zero-point Energies= -6464.361172

Sum of electronic and thermal Energies= -6464.340399

Sum of electronic and thermal Enthalpies= -6464.339455

Sum of electronic and thermal Free Energies= -6464.412681

Cartesian coordinates

C	4.177937	-1.257927	-0.679455
C	3.600624	-2.191286	0.198128

C	4.306645	-3.365455	0.507597
C	5.558824	-3.578912	-0.058641
C	6.117848	-2.636444	-0.939477
C	5.434207	-1.465824	-1.257847
H	3.878308	-4.097701	1.185378
H	6.111048	-4.482503	0.181333
H	7.095728	-2.819043	-1.375015
H	5.867087	-0.734286	-1.933091
C	2.272475	-1.783545	0.619246
C	1.353461	-2.609700	1.265627
C	1.893002	-0.480110	0.183205
C	0.028255	-2.221707	1.268077
H	1.649281	-3.588415	1.628337
C	0.588475	0.055015	0.458054
C	-0.378381	-0.963217	0.793887
H	-0.733738	-2.933480	1.566559
S	3.158376	0.155831	-0.901129
C	0.133641	1.497998	0.458711
C	0.778021	2.705382	0.059767
C	-1.160272	1.756445	0.997172
C	0.077911	3.906672	-0.125528
C	-1.850026	2.952545	0.883685
H	-1.654395	0.973702	1.544419
C	-1.256531	4.031042	0.231987
H	0.619103	4.767950	-0.499794
H	-2.845253	3.032095	1.309436
H	-1.780300	4.969519	0.081436
C	-1.840027	-0.890041	0.483217
C	-2.815210	-1.313441	1.400717
C	-2.257933	-0.502330	-0.801917

C	-4.167448	-1.329370	1.060663
H	-2.520082	-1.609654	2.402536
C	-3.603788	-0.516382	-1.156987
H	-1.519280	-0.185022	-1.530669
C	-4.548900	-0.927859	-0.217251
H	-4.909068	-1.647069	1.784919
H	-3.909570	-0.217301	-2.153357
Br	2.677452	3.028738	0.022201
Br	-6.407159	-0.947349	-0.695635

Vibrational frequencies

-47.9630	22.5853	34.2089
37.3923	77.1190	85.9634
107.0375	122.6808	134.9927
151.2260	164.4724	172.3782
192.7283	208.3186	226.9884
267.1970	284.1708	314.5101
338.3567	351.7746	376.8863
393.1881	407.8282	426.6408
441.0286	468.2128	477.5755
488.1338	506.1000	515.2910
531.1900	539.9307	575.9869
609.9569	635.9495	640.9030
649.6586	658.8260	686.2006
709.8611	713.5720	735.2320
740.5114	748.6564	754.6361
770.2971	781.6738	799.6396
827.0173	842.7484	849.3219
859.6903	865.6521	874.3725
952.4147	957.4122	968.5209
981.5831	986.8425	990.6046

995.6627	1002.2470	1016.1087
1026.4537	1046.0536	1055.3105
1081.0458	1093.5467	1103.0550
1116.5594	1145.3186	1156.5270
1164.9055	1168.3800	1190.3261
1198.0969	1212.1369	1218.7599
1264.8916	1279.5131	1283.1358
1306.6202	1312.2812	1317.6227
1336.4379	1346.1132	1363.2865
1393.2453	1422.1627	1441.7007
1452.0569	1485.9559	1497.8269
1504.8652	1524.9279	1588.6989
1596.5860	1605.3951	1612.7270
1622.0333	1634.4711	1636.1714
1643.9720	3187.4049	3195.0237
3199.3299	3199.7860	3203.3179
3205.1237	3206.6497	3211.7287
3212.4587	3219.1480	3222.4079
3223.7691	3225.0214	3301.9897

TS12

Zero-point correction= 0.302448

Thermal correction to Energy= 0.322944

Thermal correction to Enthalpy= 0.323889

Thermal correction to Gibbs Free Energy= 0.252174

Sum of electronic and zero-point Energies= -4352.850554

Sum of electronic and thermal Energies= -4352.830058

Sum of electronic and thermal Enthalpies= -4352.829114

Sum of electronic and thermal Free Energies= -4352.900828

Cartesian coordinates

C	3.775373	-1.018416	-0.617119
C	3.244102	-2.012809	0.221526
C	4.025095	-3.140442	0.524032
C	5.305851	-3.246675	-0.007276
C	5.819662	-2.242892	-0.846936
C	5.060553	-1.118198	-1.159936
H	3.631362	-3.921020	1.167980
H	5.915229	-4.114147	0.227511
H	6.821108	-2.341914	-1.255111
H	5.457133	-0.340390	-1.805258
C	1.876510	-1.716713	0.608132
C	1.008166	-2.621223	1.218562
C	1.407926	-0.439926	0.178993
C	-0.343667	-2.342470	1.179839
H	1.370645	-3.576145	1.584128
C	0.054964	-0.017445	0.413292
C	-0.835550	-1.117465	0.699187
H	-1.054450	-3.117709	1.444852
S	2.656859	0.317133	-0.845502
C	-0.519883	1.382293	0.413318
C	0.036271	2.645984	0.059096
C	-1.851572	1.522168	0.901659
C	-0.753662	3.789183	-0.133122
C	-2.633652	2.659104	0.780122
H	-2.300508	0.690695	1.414533
C	-2.106393	3.796427	0.173061
H	-0.272774	4.699625	-0.471750
H	-3.648205	2.647041	1.165433
H	-2.699166	4.692178	0.018179
C	-2.283468	-1.163566	0.324409

C	-3.259738	-1.673419	1.195656
C	-2.673986	-0.800380	-0.976188
C	-4.590370	-1.794754	0.797059
H	-2.984326	-1.954294	2.207332
C	-3.997392	-0.919188	-1.390936
H	-1.931574	-0.418587	-1.669324
C	-4.945772	-1.412160	-0.494512
H	-5.337512	-2.176898	1.483955
H	-4.286093	-0.638096	-2.397782
Br	1.902751	3.123693	0.091802
Cl	-6.629594	-1.559756	-1.010072

Vibrational frequencies

-45.9651	29.0027	38.7730
42.3431	80.8190	89.7413
109.5955	124.2235	136.5531
157.4819	174.4336	189.3237
200.7400	213.3997	231.0556
277.4613	301.5508	326.0461
340.4928	364.9183	391.7925
404.2248	424.4220	425.4119
440.9224	478.9348	481.2470
490.6187	505.9662	518.6156
533.4000	543.7733	576.5558
610.7366	637.3997	643.4960
651.4820	662.3251	691.0279
712.1996	716.4679	734.9505
737.2815	748.5927	755.8436
771.4572	783.6319	801.4778
830.2320	843.4858	845.3832
858.9097	865.2514	873.2919

951.8053	961.7026	967.0975
973.4081	981.2497	991.7356
995.3109	1002.8630	1019.8164
1027.4808	1047.7507	1054.5353
1081.0701	1102.8949	1104.5514
1116.9810	1146.5324	1156.1021
1160.9861	1168.9836	1190.9610
1196.6398	1213.0592	1218.8263
1264.8304	1276.0794	1283.7776
1307.0993	1313.3494	1318.6300
1335.0540	1345.8143	1362.0795
1391.2836	1423.0317	1444.7205
1451.8086	1486.0237	1499.1947
1504.4363	1527.3575	1589.2393
1596.8310	1607.3330	1614.6804
1621.7763	1635.9095	1639.5253
1643.4094	3188.6590	3195.6883
3200.5662	3202.4165	3204.2208
3205.4758	3205.7325	3212.6251
3213.6081	3219.8384	3222.3950
3223.8231	3224.5116	3305.4034

TS13

Zero-point correction= 0.303640

Thermal correction to Energy= 0.323768

Thermal correction to Enthalpy= 0.324713

Thermal correction to Gibbs Free Energy= 0.254214

Sum of electronic and zero-point Energies= -3992.482942

Sum of electronic and thermal Energies= -3992.462814

Sum of electronic and thermal Enthalpies= -3992.461869

Sum of electronic and thermal Free Energies= -3992.532368

Cartesian coordinates

C	3.612470	-0.762296	-0.566968
C	3.144911	-1.811986	0.241881
C	4.015604	-2.866349	0.562992
C	5.318279	-2.849396	0.076420
C	5.766513	-1.793520	-0.736424
C	4.919153	-0.738575	-1.065349
H	3.674141	-3.685228	1.188859
H	5.996433	-3.659651	0.326476
H	6.786119	-1.796271	-1.110070
H	5.265342	0.080265	-1.688502
C	1.744110	-1.644750	0.584392
C	0.937296	-2.635059	1.145091
C	1.179821	-0.405607	0.160814
C	-0.431437	-2.472917	1.063454
H	1.368357	-3.564276	1.502855
C	-0.211713	-0.105595	0.357908
C	-1.012864	-1.283775	0.592555
H	-1.081064	-3.311928	1.288061
S	2.388767	0.473669	-0.813536
C	-0.902666	1.242050	0.373892
C	-0.446750	2.556694	0.064864
C	-2.252809	1.258389	0.830502
C	-1.323771	3.637272	-0.113777
C	-3.123299	2.330298	0.720741
H	-2.644355	0.376991	1.305448
C	-2.678593	3.525146	0.159774
H	-0.912075	4.593493	-0.415619
H	-4.142258	2.223176	1.078923

H	-3.339960	4.373504	0.016469
C	-2.440114	-1.442199	0.171214
C	-3.395151	-2.058053	0.997555
C	-2.819843	-1.072926	-1.131848
C	-4.698193	-2.279415	0.552173
H	-3.125499	-2.343292	2.009503
C	-4.115751	-1.289460	-1.592198
H	-2.089554	-0.610949	-1.788004
C	-5.034362	-1.887309	-0.736823
H	-5.444842	-2.743085	1.187852
H	-4.415802	-1.010888	-2.596665
Br	1.373321	3.185242	0.143890
F	-6.298502	-2.098666	-1.178018

Vibrational frequencies

-47.1510	33.2697	40.6451
50.2469	77.3076	91.9571
111.9087	123.7511	138.7999
158.6739	186.6177	199.6295
208.5367	223.8797	237.4077
290.1069	321.9748	343.1552
362.7215	378.0529	415.4730
418.5447	429.5196	442.7029
453.0571	478.3924	488.7127
505.6191	506.3418	531.4372
537.7053	573.4351	584.3822
612.8704	639.1637	647.0335
655.2908	669.7192	700.1563
712.5076	731.4168	732.5468
737.5616	754.4327	771.6915
783.1974	786.5176	828.2280

831.3943	833.4107	853.7482
856.8976	865.4479	873.8871
952.4278	957.0797	962.1368
965.7316	974.2716	991.3585
994.8341	1002.6412	1025.7349
1027.0038	1046.9196	1054.9989
1081.2386	1103.4025	1114.6487
1127.0769	1154.2489	1159.0303
1169.0628	1186.6628	1189.9802
1195.1561	1212.7373	1262.2453
1264.4555	1276.9413	1283.9209
1306.9714	1314.4135	1321.1962
1327.9044	1346.1502	1361.6843
1390.2216	1423.5235	1448.6838
1451.4498	1486.1999	1499.5121
1503.7447	1543.1221	1589.2949
1596.2820	1607.8039	1621.1387
1634.1898	1636.6871	1643.1010
1653.9085	3188.5387	3196.3609
3198.1989	3201.6780	3204.7562
3205.5090	3207.5424	3210.5731
3213.6208	3217.7251	3222.3169
3222.4310	3223.6092	3305.3947

P-Ph

Zero-point correction= 0.312916

Thermal correction to Energy= 0.333094

Thermal correction to Enthalpy= 0.334038

Thermal correction to Gibbs Free Energy= 0.262442

Sum of electronic and zero-point Energies= -3893.305843

Sum of electronic and thermal Energies= -3893.285665

Sum of electronic and thermal Enthalpies= -3893.284721

Sum of electronic and thermal Free Energies= -3893.356317

Cartesian coordinates

C	3.829255	0.532684	-0.121308
C	3.608602	-0.862805	-0.092888
C	4.707346	-1.724150	0.049427
C	5.987867	-1.191611	0.158545
C	6.189166	0.198230	0.128204
C	5.113023	1.072773	-0.012142
H	4.551882	-2.798691	0.072503
H	6.839811	-1.855684	0.268271
H	7.194390	0.599688	0.214646
H	5.270793	2.146593	-0.035218
C	2.200216	-1.197643	-0.220198
C	1.590607	-2.458626	-0.206791
C	1.383783	-0.053479	-0.355364
C	0.211382	-2.552639	-0.328107
H	2.195335	-3.354601	-0.104392
C	-0.011068	-0.131909	-0.472334
C	-0.605410	-1.411008	-0.467307
H	-0.260427	-3.530084	-0.331539
S	2.325493	1.449225	-0.310145
C	-0.809732	1.124621	-0.565576
C	-1.621721	1.588556	0.480126
C	-0.748807	1.905224	-1.731845
C	-2.368169	2.760716	0.368005
C	-1.483847	3.082355	-1.858446
H	-0.122625	1.563066	-2.550205
C	-2.299562	3.507058	-0.808386

H	-2.990599	3.088625	1.193107
H	-1.423689	3.660867	-2.774931
H	-2.880693	4.419880	-0.896293
C	-2.078134	-1.593091	-0.585454
C	-2.761840	-2.372867	0.361722
C	-2.809547	-1.016508	-1.636116
C	-4.139058	-2.569065	0.263050
H	-2.209050	-2.808409	1.188463
C	-4.187465	-1.211524	-1.733871
H	-2.294304	-0.421752	-2.382828
C	-4.857384	-1.986898	-0.784225
H	-4.652320	-3.169425	1.008924
H	-4.736491	-0.760959	-2.555846
H	-5.930579	-2.136777	-0.859944
Br	-1.714181	0.615420	2.129580

Vibrational frequencies

28.5794	35.6362	47.0721
51.4775	66.0628	79.1263
97.4279	126.1672	141.2320
178.5528	198.5049	212.8537
231.8083	241.1024	262.5137
289.4823	322.4196	359.8482
379.3871	413.0847	420.0748
437.9107	452.0807	455.7123
484.7849	500.1378	523.3234
525.7523	540.6716	587.3047
615.3633	628.3440	632.0321
646.9805	657.0213	687.9228
700.5263	717.0246	733.7888
737.8945	752.4826	762.8409

773.9076	775.6073	794.1657
818.5889	849.2675	857.2167
863.7767	878.5882	896.8636
938.4273	955.4233	969.8479
974.3965	981.0920	993.5243
1002.8368	1008.9661	1013.3677
1015.5123	1039.7551	1043.4020
1052.3007	1069.2603	1077.9415
1091.2271	1110.5131	1135.9435
1144.0650	1163.1578	1169.8489
1185.9234	1189.0679	1189.8645
1212.7216	1259.3811	1281.2676
1296.1669	1305.2035	1323.5389
1331.8612	1341.9582	1351.2712
1356.4784	1362.8256	1414.5814
1462.7107	1473.8192	1486.2869
1488.1673	1506.1137	1520.4204
1540.1878	1599.7307	1610.5416
1612.9534	1630.0011	1632.7168
1642.4517	1645.0101	1655.6631
3180.7236	3188.1609	3188.5777
3192.8425	3193.6921	3196.3855
3198.7451	3201.5701	3205.1157
3206.1992	3209.6366	3212.9923
3213.1465	3214.0515	3222.3798

P-PhBr

Zero-point correction= 0.302956

Thermal correction to Energy= 0.324623

Thermal correction to Enthalpy= 0.325567

Thermal correction to Gibbs Free Energy= 0.249471

Sum of electronic and zero-point Energies= -6464.424116

Sum of electronic and thermal Energies= -6464.402449

Sum of electronic and thermal Enthalpies= -6464.401505

Sum of electronic and thermal Free Energies= -6464.477601

Cartesian coordinates

C	4.836591	0.017528	-0.282311
C	4.389750	-1.315940	-0.143510
C	5.337614	-2.339374	0.011221
C	6.692547	-2.024603	0.024465
C	7.118856	-0.693401	-0.114810
C	6.195887	0.339243	-0.269667
H	5.008701	-3.368782	0.118525
H	7.427986	-2.814546	0.143007
H	8.179904	-0.462670	-0.102289
H	6.526858	1.367596	-0.376781
C	2.940497	-1.414480	-0.183394
C	2.131615	-2.550481	-0.052716
C	2.319957	-0.158486	-0.363190
C	0.751186	-2.416854	-0.102307
H	2.584304	-3.527784	0.084791
C	0.927414	-0.006203	-0.409196
C	0.131028	-1.163305	-0.284862
H	0.123717	-3.298163	-0.014566
S	3.498650	1.162455	-0.467872
C	0.342956	1.358666	-0.553925
C	-0.320039	2.016920	0.492789
C	0.464987	2.043510	-1.774508
C	-0.865914	3.289739	0.332924
C	-0.070810	3.317954	-1.949462

H	0.977393	1.550281	-2.594845
C	-0.741611	3.939448	-0.894940
H	-1.375646	3.769243	1.160873
H	0.031485	3.820543	-2.906097
H	-1.166572	4.930700	-1.019633
C	-1.355032	-1.096218	-0.314351
C	-2.100274	-1.684734	0.719379
C	-2.045200	-0.464499	-1.360071
C	-3.493300	-1.646130	0.717245
H	-1.583591	-2.162320	1.545649
C	-3.438175	-0.415002	-1.377203
H	-1.491874	-0.011111	-2.174829
C	-4.147478	-1.007654	-0.334454
H	-4.056282	-2.098339	1.526011
H	-3.959267	0.073051	-2.193111
Br	-0.482618	1.177681	2.209371
Br	-6.066635	-0.946848	-0.349647

Vibrational frequencies

22.8052	29.3679	32.0252
50.3981	61.9146	73.5125
95.6326	107.3851	135.2959
138.8108	160.5377	172.5713
211.2690	217.6897	233.3216
267.0989	283.4297	293.7342
333.7415	354.1766	366.7117
399.6407	417.1731	424.0411
445.2743	457.0354	470.0419
493.0334	502.2128	524.1566
528.5049	543.1901	585.5873
616.9347	635.4192	640.7393

649.5914	663.3803	695.7449
706.0026	735.0235	739.3744
742.1075	755.7336	763.3427
774.3010	787.0899	816.3640
841.2785	849.9824	857.6158
862.0590	877.7409	896.9796
955.5109	970.8053	974.5330
980.4974	985.9385	995.1052
1007.7068	1014.1737	1020.0853
1040.4911	1051.6997	1063.8565
1071.9126	1093.1731	1093.7275
1136.6185	1144.6435	1147.1124
1165.3627	1171.8229	1192.8398
1192.9732	1218.0714	1260.3427
1282.4917	1297.6441	1306.1744
1323.6722	1330.5437	1334.7599
1343.4793	1352.1839	1357.5751
1414.3464	1434.3034	1465.7496
1482.5135	1488.5647	1507.1057
1520.3161	1535.4586	1597.3679
1611.3745	1613.2526	1618.2916
1632.8296	1642.1731	1643.4024
1645.7728	3189.8541	3194.2476
3194.5398	3198.0539	3202.3114
3204.1454	3206.6423	3209.6190
3212.3253	3214.8659	3214.9239
3222.3756	3223.7290	3226.2423

P-PhCl

Zero-point correction= 0.303462

Thermal correction to Energy= 0.324860

Thermal correction to Enthalpy= 0.325805

Thermal correction to Gibbs Free Energy= 0.251166

Sum of electronic and zero-point Energies= -4352.913533

Sum of electronic and thermal Energies= -4352.892135

Sum of electronic and thermal Enthalpies= -4352.891191

Sum of electronic and thermal Free Energies= -4352.965829

Cartesian coordinates

C	4.348046	0.201263	-0.222054
C	3.976895	-1.158459	-0.120210
C	4.979222	-2.130431	0.021765
C	6.313814	-1.740157	0.059229
C	6.665073	-0.383972	-0.043636
C	5.686900	0.598561	-0.185876
H	4.707894	-3.179160	0.099194
H	7.091588	-2.489977	0.167629
H	7.711164	-0.094149	-0.013334
H	5.961392	1.645762	-0.266437
C	2.536556	-1.339232	-0.183915
C	1.793742	-2.523147	-0.092571
C	1.846541	-0.117797	-0.346652
C	0.409027	-2.469186	-0.165489
H	2.300026	-3.475290	0.033298
C	0.448264	-0.045958	-0.416813
C	-0.280568	-1.250489	-0.333825
H	-0.166586	-3.387689	-0.108845
S	2.948083	1.271485	-0.399177
C	-0.212593	1.284656	-0.552219
C	-0.942652	1.883513	0.485334
C	-0.099391	1.996753	-1.758034

C	-1.560385	3.123781	0.329779
C	-0.706545	3.239347	-1.928453
H	0.463705	1.549048	-2.571217
C	-1.442761	3.800751	-0.883935
H	-2.120975	3.557633	1.150171
H	-0.609148	3.763020	-2.874222
H	-1.924683	4.765983	-1.005512
C	-1.767269	-1.271370	-0.396255
C	-2.499386	-1.924775	0.607366
C	-2.470026	-0.659988	-1.445625
C	-3.891761	-1.969180	0.573658
H	-1.973953	-2.387901	1.436268
C	-3.862653	-0.692713	-1.495680
H	-1.926278	-0.157833	-2.237912
C	-4.558181	-1.347072	-0.480502
H	-4.447806	-2.468988	1.359028
H	-4.396157	-0.220537	-2.313072
Br	-1.101967	1.006006	2.183018
Cl	-6.325301	-1.388358	-0.530949

Vibrational frequencies

28.5494	31.5037	37.4332
51.1724	64.0438	74.7300
95.7732	114.4168	138.9259
142.9483	180.4285	188.4742
213.0616	224.9540	236.0030
274.4571	296.4099	307.0428
336.1773	367.2074	397.2565
411.3011	420.7972	423.3647
447.0028	457.7114	478.7929
498.8562	510.6806	524.1081

530.0221	542.9965	584.7009
617.2515	636.2601	643.6251
650.1795	666.6454	697.1086
711.5058	728.7513	740.6838
744.2400	754.4031	763.3060
774.5546	787.5960	817.5896
839.3172	843.6588	857.3095
860.0767	878.9371	893.9370
956.5316	969.0808	972.2987
972.4653	979.7214	995.1944
1007.7512	1014.5998	1023.4106
1040.4549	1051.7724	1065.8359
1071.9080	1092.8260	1104.5018
1136.7176	1146.0953	1148.0483
1165.1407	1174.6285	1189.9586
1192.0718	1218.5540	1260.9017
1282.3778	1298.1818	1307.5403
1323.9441	1331.8994	1334.2469
1343.5981	1352.4166	1357.9925
1414.5887	1437.0516	1465.3619
1482.3281	1489.1449	1506.9869
1521.0553	1537.7146	1598.4236
1611.2325	1613.3712	1620.8005
1632.9518	1642.8845	1645.2185
1646.6405	3189.8455	3195.0687
3195.5355	3197.4441	3202.8667
3204.9484	3205.9965	3210.9953
3213.0912	3214.5389	3214.9064
3222.1422	3223.3186	3227.0497

P-PhF

Zero-point correction= 0.304634

Thermal correction to Energy= 0.325678

Thermal correction to Enthalpy= 0.326623

Thermal correction to Gibbs Free Energy= 0.252921

Sum of electronic and zero-point Energies= -3992.545997

Sum of electronic and thermal Energies= -3992.524952

Sum of electronic and thermal Enthalpies= -3992.524008

Sum of electronic and thermal Free Energies= -3992.597709

Cartesian coordinates

C	4.088286	0.352938	-0.180670
C	3.781567	-1.024476	-0.106608
C	4.827417	-1.948955	0.038236
C	6.140780	-1.495386	0.104354
C	6.427814	-0.122390	0.028081
C	5.405411	0.813982	-0.115270
H	4.605842	-3.010518	0.095836
H	6.951893	-2.208654	0.215149
H	7.458053	0.216859	0.080546
H	5.628955	1.874735	-0.174437
C	2.352713	-1.273440	-0.197889
C	1.666115	-2.493011	-0.138428
C	1.606767	-0.084098	-0.350905
C	0.281672	-2.503871	-0.233054
H	2.215253	-3.422272	-0.020947
C	0.207564	-0.077973	-0.439126
C	-0.464297	-1.317205	-0.389277
H	-0.250371	-3.449486	-0.201667
S	2.641316	1.356759	-0.366441
C	-0.516380	1.221331	-0.555995

C	-1.286430	1.760042	0.485609
C	-0.427723	1.964105	-1.745026
C	-1.968435	2.968300	0.348187
C	-1.097632	3.176612	-1.896918
H	0.166943	1.564190	-2.560698
C	-1.874946	3.675502	-0.850424
H	-2.560345	3.354059	1.170792
H	-1.017653	3.724537	-2.830516
H	-2.406423	4.616022	-0.958344
C	-1.947173	-1.407570	-0.474279
C	-2.661149	-2.110068	0.510435
C	-2.663328	-0.815507	-1.527152
C	-4.049455	-2.221948	0.454279
H	-2.124081	-2.558361	1.339956
C	-4.052273	-0.914801	-1.598478
H	-2.131129	-0.277666	-2.303780
C	-4.718817	-1.616814	-0.601954
H	-4.609737	-2.755099	1.214695
H	-4.613691	-0.464814	-2.410048
Br	-1.408796	0.842941	2.164880
F	-6.068347	-1.716269	-0.663404

Vibrational frequencies

26.7257	31.8665	40.7631
50.9371	63.4553	73.3238
96.0613	121.6601	138.6356
154.1777	188.8735	204.6913
212.3775	233.8653	243.0531
281.1484	304.8289	339.2877
356.8565	393.5627	410.9354
427.1134	429.2286	443.1036

450.0362	459.8616	487.1193
500.6456	524.5695	528.3301
544.0195	582.0098	585.3368
618.6698	638.4835	649.9317
654.1335	676.1551	698.6818
723.3645	728.0325	739.6121
754.4192	763.9219	775.4340
789.8273	797.8242	829.4694
839.0420	840.5929	855.8464
865.2230	878.1135	894.7043
955.3966	955.8814	968.9660
971.1864	972.9644	994.4321
1009.4762	1014.9911	1028.7232
1039.9811	1051.3949	1065.1435
1071.5334	1091.3960	1125.2223
1137.0536	1145.3961	1165.0160
1172.8787	1187.5949	1190.1569
1191.8950	1259.9829	1264.6765
1281.0056	1297.1126	1307.7220
1322.9673	1325.5687	1337.6531
1343.1780	1352.1833	1357.8098
1414.4908	1441.0994	1464.2931
1482.5860	1489.0553	1506.8777
1521.7952	1553.1235	1600.4148
1610.9409	1613.4123	1632.8008
1639.7296	1642.3331	1646.2117
1657.8986	3188.8905	3193.9390
3194.5904	3197.0937	3202.0218
3205.2731	3205.5684	3210.2691
3210.5944	3213.8832	3213.9313

3221.8843 3222.5411 3224.8368

PR

Zero-point correction= 0.312916

Thermal correction to Energy= 0.333094

Thermal correction to Enthalpy= 0.334038

Thermal correction to Gibbs Free Energy= 0.262442

Sum of electronic and zero-point Energies= -3893.305843

Sum of electronic and thermal Energies= -3893.285665

Sum of electronic and thermal Enthalpies= -3893.284721

Sum of electronic and thermal Free Energies= -3893.356317

Cartesian coordinates

C	3.829255	0.532684	-0.121308
C	3.608602	-0.862805	-0.092888
C	4.707346	-1.724150	0.049427
C	5.987867	-1.191611	0.158545
C	6.189166	0.198230	0.128204
C	5.113023	1.072773	-0.012142
H	4.551882	-2.798691	0.072503
H	6.839811	-1.855684	0.268271
H	7.194390	0.599688	0.214646
H	5.270793	2.146593	-0.035218
C	2.200216	-1.197643	-0.220198
C	1.590607	-2.458626	-0.206791
C	1.383783	-0.053479	-0.355364
C	0.211382	-2.552639	-0.328107
H	2.195335	-3.354601	-0.104392
C	-0.011068	-0.131909	-0.472334
C	-0.605410	-1.411008	-0.467307
H	-0.260427	-3.530084	-0.331539

S	2.325493	1.449225	-0.310145
C	-0.809732	1.124621	-0.565576
C	-1.621721	1.588556	0.480126
C	-0.748807	1.905224	-1.731845
C	-2.368169	2.760716	0.368005
C	-1.483847	3.082355	-1.858446
H	-0.122625	1.563066	-2.550205
C	-2.299562	3.507058	-0.808386
H	-2.990599	3.088625	1.193107
H	-1.423689	3.660867	-2.774931
H	-2.880693	4.419880	-0.896293
C	-2.078134	-1.593091	-0.585454
C	-2.761840	-2.372867	0.361722
C	-2.809547	-1.016508	-1.636116
C	-4.139058	-2.569065	0.263050
H	-2.209050	-2.808409	1.188463
C	-4.187465	-1.211524	-1.733871
H	-2.294304	-0.421752	-2.382828
C	-4.857384	-1.986898	-0.784225
H	-4.652320	-3.169425	1.008924
H	-4.736491	-0.760959	-2.555846
H	-5.930579	-2.136777	-0.859944
Br	-1.714181	0.615420	2.129580

Vibrational frequencies

28.5794	35.6362	47.0721
51.4775	66.0628	79.1263
97.4279	126.1672	141.2320
178.5528	198.5049	212.8537
231.8083	241.1024	262.5137
289.4823	322.4196	359.8482

379.3871	413.0847	420.0748
437.9107	452.0807	455.7123
484.7849	500.1378	523.3234
525.7523	540.6716	587.3047
615.3633	628.3440	632.0321
646.9805	657.0213	687.9228
700.5263	717.0246	733.7888
737.8945	752.4826	762.8409
773.9076	775.6073	794.1657
818.5889	849.2675	857.2167
863.7767	878.5882	896.8636
938.4273	955.4233	969.8479
974.3965	981.0920	993.5243
1002.8368	1008.9661	1013.3677
1015.5123	1039.7551	1043.4020
1052.3007	1069.2603	1077.9415
1091.2271	1110.5131	1135.9435
1144.0650	1163.1578	1169.8489
1185.9234	1189.0679	1189.8645
1212.7216	1259.3811	1281.2676
1296.1669	1305.2035	1323.5389
1331.8612	1341.9582	1351.2712
1356.4784	1362.8256	1414.5814
1462.7107	1473.8192	1486.2869
1488.1673	1506.1137	1520.4204
1540.1878	1599.7307	1610.5416
1612.9534	1630.0011	1632.7168
1642.4517	1645.0101	1655.6631
3180.7236	3188.1609	3188.5777
3192.8425	3193.6921	3196.3855

3198.7451	3201.5701	3205.1157
3206.1992	3209.6366	3212.9923
3213.1465	3214.0515	3222.3798

PS

Zero-point correction= 0.312916

Thermal correction to Energy= 0.333095

Thermal correction to Enthalpy= 0.334040

Thermal correction to Gibbs Free Energy= 0.262432

Sum of electronic and zero-point Energies= -3893.305843

Sum of electronic and thermal Energies= -3893.285664

Sum of electronic and thermal Enthalpies= -3893.284720

Sum of electronic and thermal Free Energies= -3893.356327

Cartesian coordinates

C	-3.828720	0.532765	-0.122043
C	-3.608325	-0.862764	-0.093083
C	-4.707229	-1.723875	0.049485
C	-5.987657	-1.191078	0.158324
C	-6.188715	0.198780	0.127446
C	-5.112426	1.073096	-0.013155
H	-4.551961	-2.798426	0.072996
H	-6.839725	-1.854945	0.268259
H	-7.193877	0.600416	0.213661
H	-5.270032	2.146922	-0.036673
C	-2.200010	-1.197876	-0.220136
C	-1.590585	-2.458962	-0.206315
C	-1.383416	-0.053867	-0.355644
C	-0.211346	-2.553217	-0.327297
H	-2.195442	-3.354814	-0.103715
C	0.011461	-0.132584	-0.472273

C	0.605632	-1.411731	-0.466541
H	0.260358	-3.530701	-0.330320
S	-2.324837	1.449058	-0.311232
C	0.810466	1.123695	-0.566224
C	1.621437	1.588740	0.479756
C	0.750867	1.902935	-1.733456
C	2.368171	2.760666	0.367015
C	1.486272	3.079757	-1.860740
H	0.125489	1.559897	-2.552038
C	2.301013	3.505545	-0.810381
H	2.989693	3.089517	1.192401
H	1.427212	3.657155	-2.777990
H	2.882365	4.418166	-0.898792
C	2.078402	-1.593825	-0.584532
C	2.761975	-2.374425	0.362064
C	2.810015	-1.016186	-1.634452
C	4.139202	-2.570603	0.263398
H	2.209037	-2.810756	1.188265
C	4.187949	-1.211117	-1.732173
H	2.294867	-0.420568	-2.380549
C	4.857711	-1.987403	-0.783163
H	4.652328	-3.171712	1.008753
H	4.737130	-0.759733	-2.553589
H	5.930911	-2.137222	-0.858862
Br	1.711605	0.617802	2.130646

Vibrational frequencies

28.4353	35.4723	47.0356
51.4788	66.0492	79.1346
97.4141	126.0909	141.1706
178.4963	198.4893	212.8301

231.8204 241.1170 262.5543

289.5184 322.3948 359.8108

379.3892 413.0794 420.0906

437.9033 452.0680 455.6704

484.7656 500.1242 523.3187

525.7292 540.6352 587.3012

615.3535 628.3442 632.0444

646.9830 657.0224 687.9120

700.5169 717.0087 733.7696

737.8811 752.4624 762.7927

773.8597 775.5614 794.1634

818.5792 849.2438 857.2087

863.7543 878.4984 896.8219

938.4414 955.3470 969.8300

974.3720 981.0809 993.4686

1002.8139 1008.9517 1013.3771

1015.5215 1039.7562 1043.4161

1052.2945 1069.2724 1077.9448

1091.2255 1110.5466 1135.9314

1144.0719 1163.1357 1169.8143

1185.9248 1189.0841 1189.8404

1212.7442 1259.3730 1281.2323

1296.1931 1305.1773 1323.5497

1331.8731 1341.9784 1351.2614

1356.4719 1362.8538 1414.5552

1462.7094 1473.8010 1486.2846

1488.1448 1506.1234 1520.4491

1540.1939 1599.7342 1610.5575

1612.9548 1630.0377 1632.6904

1642.4770 1644.9956 1655.6574

3180.7842	3188.2366	3188.6532
3192.9583	3193.7905	3196.4570
3198.8413	3201.6935	3205.1851
3206.2782	3209.7425	3213.0986
3213.2237	3214.0835	3222.5160

pre-R2+DBU

Zero-point correction= 0.472116

Thermal correction to Energy= 0.499422

Thermal correction to Enthalpy= 0.500366

Thermal correction to Gibbs Free Energy= 0.412168

Sum of electronic and zero-point Energies= -4123.234851

Sum of electronic and thermal Energies= -4123.207545

Sum of electronic and thermal Enthalpies= -4123.206601

Sum of electronic and thermal Free Energies= -4123.294799

Cartesian coordinates

C	-3.258000	-1.071357	0.437659
C	-3.826008	0.048865	-0.211935
C	-5.028432	-0.030291	-0.919666
C	-5.673047	-1.262717	-0.979713
C	-5.123372	-2.390136	-0.345206
C	-3.927888	-2.306136	0.360147
C	-2.006922	-0.735678	1.099330
C	-1.647625	0.585974	0.932819
H	-5.447845	0.842263	-1.410854
H	-6.608179	-1.351174	-1.524542
H	-5.641062	-3.342869	-0.407280
H	-3.500021	-3.170881	0.850883
S	-2.820941	1.480162	-0.007479
C	-1.186502	-1.670598	1.867563

O	-1.464245	-2.855187	2.042369
H	-0.256370	-1.257802	2.295325
C	-0.428632	1.293677	1.477286
H	-0.624178	1.572264	2.518882
H	0.405433	0.583515	1.496080
C	-0.027170	2.534124	0.708738
C	0.473357	2.483583	-0.601297
C	-0.140701	3.801086	1.298280
C	0.854523	3.626738	-1.299473
C	0.231222	4.959851	0.616658
H	-0.528476	3.868918	2.310750
C	0.730228	4.872767	-0.683236
H	1.242187	3.545788	-2.308821
H	0.131708	5.926221	1.101033
H	1.024111	5.767678	-1.223053
Br	0.663229	0.784418	-1.479161
C	0.881123	-2.885227	-0.489410
C	1.609074	-3.231288	-1.795671
C	2.823851	-2.353748	-2.127903
C	1.765997	-2.953884	0.773685
C	3.897593	-2.338455	-1.027865
C	2.599851	-1.708873	1.005473
H	0.436646	-1.885584	-0.556021
H	1.946218	-4.276083	-1.737037
H	2.513444	-1.318794	-2.318314
H	4.076020	-3.357176	-0.663701
H	2.411211	-3.840260	0.720351
H	0.045430	-3.581544	-0.358102
H	0.894403	-3.184019	-2.626959
H	3.280654	-2.722932	-3.054525

H	1.137545	-3.074011	1.656230
H	4.847440	-1.994232	-1.444772
C	4.324670	-0.172962	0.125746
H	4.445440	0.178912	-0.904964
H	5.332048	-0.338257	0.533802
C	3.570976	0.866270	0.945614
H	4.208955	1.737398	1.125697
H	2.702787	1.195464	0.370892
C	3.095028	0.232660	2.252884
H	2.492009	0.948097	2.824883
H	3.965576	-0.011811	2.882298
N	2.294273	-0.971031	2.030786
N	3.591971	-1.446149	0.094950

Vibrational frequencies

19.8851	23.6033	30.4458
39.0201	42.6339	52.3196
62.6322	79.0414	80.3904
95.3029	103.5243	122.0352
124.9133	134.5364	173.2113
188.7867	196.7260	211.4349
221.3552	249.5965	255.7392
258.5415	263.3205	313.3212
319.8284	346.7173	355.5837
379.0972	384.5058	395.1123
408.0219	429.0829	434.9701
438.2774	454.1867	484.5825
499.2451	503.0568	514.4612
518.8818	528.9826	536.5183
602.3959	616.3972	644.0643
647.8468	667.8887	695.6190

707.9154	708.9188	748.3387
749.0642	761.8091	773.9938
776.4471	802.7374	803.2511
850.9100	866.3162	876.5865
879.3111	885.2823	892.1769
899.4473	906.1725	933.6932
941.3176	964.5336	968.1029
969.6116	996.3480	1004.1958
1007.0343	1014.8326	1020.5775
1031.5947	1040.4288	1048.1305
1060.9345	1071.5328	1077.6460
1088.8622	1107.2059	1111.2396
1123.8523	1134.6300	1146.3456
1150.2694	1179.4797	1185.9271
1190.9431	1195.3954	1213.8297
1223.1226	1227.4168	1234.6565
1237.1204	1258.0531	1263.9409
1295.2328	1300.0545	1308.7900
1316.2414	1317.6355	1346.3093
1347.7388	1354.7956	1359.0912
1365.4874	1379.5634	1383.0695
1393.6475	1397.1671	1402.1380
1405.0123	1408.8155	1464.2774
1465.4591	1471.3825	1477.8787
1478.7912	1482.8116	1491.0595
1492.5824	1495.0043	1499.7849
1502.3124	1506.9092	1510.3968
1517.4012	1531.1709	1565.7353
1610.2347	1618.8526	1643.8949
1644.3721	1661.3631	1729.5041

2988.5073	2998.8054	3008.7404
3016.1902	3036.3734	3040.8305
3048.8081	3049.2313	3051.1082
3052.4249	3065.5156	3067.3146
3078.6109	3082.6838	3093.7027
3097.6674	3107.9256	3140.2967
3142.8602	3189.4939	3189.7455
3199.3789	3199.5863	3211.4036
3212.4423	3221.4448	3242.9321

TS_{DBU}

Zero-point correction= 0.466802

Thermal correction to Energy= 0.493675

Thermal correction to Enthalpy= 0.494619

Thermal correction to Gibbs Free Energy= 0.408281

Sum of electronic and zero-point Energies= -4123.213768

Sum of electronic and thermal Energies= -4123.186895

Sum of electronic and thermal Enthalpies= -4123.185951

Sum of electronic and thermal Free Energies= -4123.272288

Cartesian coordinates

C	-3.536634	-0.179692	0.464236
C	-3.431323	0.451222	-0.796708
C	-4.416350	0.335139	-1.777450
C	-5.547737	-0.430034	-1.492018
C	-5.676589	-1.063567	-0.246493
C	-4.687768	-0.945430	0.728281
C	-2.382038	0.079805	1.309187
C	-1.414009	0.901722	0.696675
H	-4.306495	0.829892	-2.738000
H	-6.329264	-0.532708	-2.239118

H	-6.562628	-1.656450	-0.036668
H	-4.782927	-1.434165	1.689569
S	-1.926487	1.360418	-0.931456
C	-2.209758	-0.461711	2.635864
O	-3.014854	-1.186367	3.231529
H	-1.256837	-0.194920	3.135542
C	-0.142385	1.328571	1.236767
H	-0.229778	1.480884	2.315292
H	0.719644	0.200561	1.303960
C	0.601239	2.475520	0.631702
C	1.344050	2.428648	-0.562914
C	0.650415	3.703319	1.327927
C	2.061399	3.520715	-1.053768
C	1.372493	4.800163	0.866733
H	0.093897	3.781504	2.257902
C	2.078709	4.714311	-0.335155
H	2.613201	3.430030	-1.982878
H	1.376791	5.722671	1.439848
H	2.643224	5.561819	-0.711633
Br	1.443706	0.808788	-1.603564
C	-0.074501	-2.626359	-0.896790
C	0.539002	-3.888700	-1.511660
C	2.069672	-3.955773	-1.455931
C	0.247761	-2.415483	0.596328
C	2.640279	-3.888324	-0.031767
C	1.611787	-1.834134	0.886396
H	0.237834	-1.738146	-1.454538
H	0.133034	-4.766067	-0.988692
H	2.513948	-3.145776	-2.048948
H	2.061538	-4.529313	0.642934

H	0.148103	-3.366483	1.135268
H	-1.164670	-2.680043	-0.991864
H	0.213795	-3.971793	-2.555544
H	2.399956	-4.898849	-1.907415
H	-0.480754	-1.733867	1.031752
H	3.662962	-4.270322	-0.022120
C	4.060711	-1.949935	0.666033
H	4.640716	-2.237531	-0.216128
H	4.545027	-2.399126	1.542600
C	4.004932	-0.432829	0.790775
H	4.987773	-0.051528	1.081480
H	3.734572	0.005438	-0.173086
C	2.939035	-0.051966	1.815539
H	2.788155	1.031005	1.847723
H	3.245137	-0.369243	2.821249
N	1.654097	-0.667392	1.487020
N	2.710563	-2.524319	0.519632

Vibrational frequencies

-1568.3790	24.0851	30.5421
33.0928	39.1514	45.6756
66.8443	76.6524	78.1492
98.0898	112.3460	114.4554
124.3989	132.0667	140.4970
166.6358	181.0950	200.6909
213.5996	219.3294	251.2389
259.7484	269.4587	284.7934
317.4505	322.9770	357.8675
363.4325	382.4002	385.4739
405.4183	423.5624	431.3371
444.8092	457.0998	477.1514

497.6874	501.6930	517.6748
523.2366	526.8158	540.4011
550.2758	608.1628	632.8567
644.7218	653.8303	664.9723
708.1132	709.0847	722.8228
745.9047	749.3365	760.9216
772.7784	775.3065	804.0571
808.6843	845.3890	864.5516
870.8322	881.0653	883.2665
900.1346	908.9151	915.3074
934.5720	936.0116	951.0795
964.9016	984.9719	997.2875
998.7093	1002.6596	1011.1432
1017.6401	1024.6113	1026.2712
1049.4762	1064.2114	1073.4372
1089.3560	1109.6614	1110.7725
1118.0591	1129.9674	1137.5079
1144.5847	1151.4450	1184.3085
1186.1172	1189.0809	1210.2304
1226.4331	1234.1583	1245.1644
1250.4180	1263.7307	1266.5016
1271.5378	1297.0073	1299.3001
1317.2535	1323.3313	1326.0051
1337.8191	1357.2757	1360.4300
1363.8256	1367.7067	1379.8096
1393.6042	1394.6612	1396.3688
1400.0882	1407.2562	1419.4135
1436.5105	1462.9831	1470.6861
1477.2289	1479.8576	1492.2146
1494.5630	1496.4226	1499.1392

1500.8729	1504.4397	1506.5928
1515.8197	1517.7561	1531.2240
1604.6134	1608.3328	1610.4184
1636.6987	1638.2215	1673.5062
1701.0876	2934.3698	3023.0829
3032.2433	3035.2977	3037.3557
3051.1313	3059.0926	3060.1432
3072.8540	3080.4437	3083.4874
3092.3933	3093.9433	3100.5256
3108.0677	3123.7964	3137.6268
3171.3333	3183.2152	3183.3512
3194.0892	3195.2469	3206.6800
3206.7655	3219.7515	3239.1967

pre-R2+DQH$^-$

Zero-point correction= 0.853146

Thermal correction to Energy= 0.903544

Thermal correction to Enthalpy= 0.904488

Thermal correction to Gibbs Free Energy= 0.767233

Sum of electronic and zero-point Energies= -4903.106532

Sum of electronic and thermal Energies= -4903.056134

Sum of electronic and thermal Enthalpies= -4903.055190

Sum of electronic and thermal Free Energies= -4903.192445

Cartesian coordinates

C	-6.139704	-1.976626	0.984206
C	-6.893902	-2.148462	-0.200924
C	-7.979627	-3.025538	-0.272591
C	-8.317476	-3.744617	0.870607
C	-7.582460	-3.588631	2.058928
C	-6.501659	-2.716564	2.125117

C	-5.058453	-1.021883	0.806614
C	-5.000977	-0.501634	-0.468670
H	-8.542741	-3.144327	-1.193134
H	-9.156966	-4.432892	0.840799
H	-7.862087	-4.160654	2.938842
H	-5.930083	-2.591602	3.036040
S	-6.263975	-1.137779	-1.499288
C	-4.108841	-0.603587	1.844528
O	-4.138102	-1.005710	3.005111
H	-3.330397	0.101602	1.519032
C	-4.027862	0.497898	-1.019144
H	-3.971025	0.392835	-2.108159
C	-4.314136	1.953037	-0.687157
C	-3.452701	2.961860	-1.147391
C	-5.401168	2.358425	0.097927
C	-3.651084	4.307633	-0.846839
C	-5.619004	3.701453	0.409004
H	-6.082248	1.604754	0.479082
C	-4.743769	4.679443	-0.062413
H	-2.956220	5.053183	-1.217067
H	-6.470899	3.978883	1.022494
H	-4.901075	5.726641	0.177544
Br	-1.920854	2.494511	-2.205592
C	6.343671	-1.608619	-0.088415
C	4.948620	-1.532649	0.000158
C	4.256028	-0.329032	0.196703
C	5.027847	0.837497	0.322626
C	6.424384	0.840392	0.261559
C	7.071211	-0.401118	0.046597
H	4.366140	-2.441754	-0.064522

H	4.503062	1.775440	0.446451
C	2.777820	-0.292643	0.258715
C	2.093319	0.623492	1.078230
C	1.992220	-1.171221	-0.509257
C	0.704837	0.685559	1.159233
H	2.691096	1.287550	1.693652
C	0.600514	-1.167656	-0.488881
H	2.510934	-1.858042	-1.169877
C	-0.105287	-0.225133	0.365126
O	-1.392956	-0.201541	0.424601
O	8.449590	-0.361246	-0.023517
C	0.009704	1.687449	2.104944
C	-0.955086	2.592355	1.304482
C	-0.778562	0.911090	3.186579
C	1.005244	2.610675	2.834683
H	-0.410627	3.177592	0.554629
H	-1.688514	1.986624	0.778769
H	-1.473212	3.293482	1.972218
H	-0.091466	0.350975	3.832865
H	-1.350963	1.598523	3.823581
H	-1.468991	0.202992	2.728396
H	0.453956	3.304617	3.480353
H	1.698630	2.052853	3.474270
H	1.597717	3.212432	2.135820
C	-0.204739	-2.116432	-1.401163
C	-1.191799	-2.966770	-0.565990
C	-0.982807	-1.273312	-2.438669
C	0.688343	-3.100293	-2.183575
H	-0.645996	-3.615083	0.130840
H	-1.853472	-2.321058	0.010613

H	-1.794614	-3.611561	-1.218922
H	-0.288001	-0.789141	-3.135829
H	-1.664161	-1.902319	-3.027289
H	-1.558555	-0.491965	-1.947654
H	0.059522	-3.751621	-2.802272
H	1.384200	-2.586815	-2.856554
H	1.274495	-3.744128	-1.517609
C	7.041337	-2.973552	-0.307576
C	7.968657	-3.309412	0.888759
C	6.029808	-4.134094	-0.408722
C	7.829702	-2.970169	-1.643057
H	8.749039	-2.565935	1.077871
H	7.381828	-3.387066	1.809725
H	8.470721	-4.268896	0.722324
H	5.341027	-4.004979	-1.249374
H	6.572627	-5.071868	-0.566835
H	5.439308	-4.244530	0.505815
H	8.325980	-3.935400	-1.792406
H	7.147062	-2.802976	-2.482400
H	8.601486	-2.197285	-1.707548
C	7.220820	2.158936	0.402251
C	8.177641	2.080936	1.616465
C	8.022779	2.440589	-0.890960
C	6.296853	3.371288	0.636818
H	7.611662	1.923547	2.541712
H	8.899767	1.270072	1.516060
H	8.731152	3.022110	1.719881
H	7.346739	2.540283	-1.747849
H	8.578538	3.380944	-0.792261
H	8.734491	1.643507	-1.108750

H	6.907798	4.274873	0.737173
H	5.605980	3.534404	-0.196769
H	5.708281	3.268986	1.554574
H	8.808147	-1.244236	-0.164000
H	-3.025400	0.248817	-0.636360

Vibrational frequencies

7.5518	10.9990	15.4041
26.5234	28.5575	38.2030
39.8577	43.5798	50.8148
52.9556	58.5590	62.2393
67.4132	69.3798	78.7424
88.7644	92.9229	97.9377
108.0613	120.5218	129.6624
132.0687	141.8599	152.6722
162.8495	164.7975	175.9371
182.9783	193.5223	201.4387
205.0311	211.7341	213.2041
223.8714	227.1333	231.7616
235.3014	243.5237	261.5675
266.6469	272.4668	276.0295
289.0436	290.9515	294.1971
299.2362	302.8482	311.4082
315.6272	323.3514	328.8144
329.8789	343.2443	352.2989
357.1806	359.3368	365.2648
369.5874	376.6417	376.9232
381.4985	384.5142	385.7700
392.8230	396.5748	412.0590
413.3645	416.3441	421.3575
431.5453	437.1144	447.8523

449.7965	452.1630	457.0660
460.2730	473.0256	483.6472
503.2331	511.9183	525.7187
533.2690	536.2699	538.9821
548.2041	558.3270	586.6069
588.9805	615.6547	624.5227
633.0355	635.3771	638.5184
659.6724	673.0850	680.7184
704.3998	711.9546	726.7158
750.0230	763.7098	765.4820
766.1320	768.4923	768.8831
773.6579	778.3378	793.9696
813.5681	821.6302	822.0557
828.8324	865.5455	882.9236
887.5543	887.7956	900.3171
905.7965	906.6930	916.5478
919.0853	933.9661	936.0524
938.4129	938.8996	939.8312
941.8412	947.3527	951.2171
959.5611	959.9769	961.7210
964.8691	965.5951	975.3804
980.5307	1001.9220	1005.4044
1009.1749	1017.5032	1032.1390
1044.3920	1048.4531	1050.5163
1052.2486	1054.5395	1056.1392
1057.6779	1058.8333	1062.0617
1066.2602	1074.0269	1084.5525
1130.4011	1136.9596	1142.8825
1144.4118	1151.1280	1170.8465
1179.8701	1191.2705	1194.3313

1209.0062	1215.9433	1222.5798
1223.9599	1224.1214	1225.6917
1229.5415	1232.0662	1234.9150
1235.7568	1260.3089	1269.8182
1276.5402	1284.5922	1294.8167
1296.0247	1299.4423	1306.5823
1313.2293	1324.9668	1328.1743
1338.5372	1350.4075	1361.1701
1373.5685	1384.5683	1385.2575
1387.0663	1391.6425	1398.1227
1405.9342	1407.6649	1409.1681
1412.1426	1419.5496	1425.0478
1425.1354	1428.4668	1435.6389
1448.6091	1466.5774	1469.9699
1473.4914	1475.3757	1476.4998
1478.1386	1482.9827	1484.7413
1485.5644	1486.0115	1491.2929
1494.1505	1498.8238	1499.6659
1500.0219	1501.4917	1501.7304
1502.3217	1503.3943	1504.0703
1504.7063	1506.0116	1510.3496
1515.5790	1516.1036	1516.2815
1517.8093	1522.1994	1525.5849
1529.6969	1532.0838	1532.8224
1539.0240	1560.9324	1574.5006
1610.3286	1619.1014	1621.2021
1636.6789	1643.2393	1644.6027
1648.9283	1736.7682	2959.8097
3016.0907	3018.1410	3019.2840
3020.5897	3027.6757	3028.7768

3033.9325	3034.4527	3040.5738
3041.7138	3042.4227	3049.0597
3056.7749	3071.2376	3076.0628
3077.4288	3078.3601	3084.9653
3090.6518	3091.7609	3095.7506
3096.7497	3097.4666	3097.5843
3106.7248	3109.5219	3110.8643
3112.4531	3114.8926	3118.0518
3118.6666	3122.0162	3154.7056
3156.7361	3159.3731	3166.7775
3187.7714	3190.4050	3190.8779
3192.9479	3195.8477	3197.7534
3199.0088	3203.0441	3210.5716
3212.6608	3220.3339	3231.2763
3233.2498	3243.7682	3860.3966

TS_{DQH^-}

Zero-point correction= 0.848067

Thermal correction to Energy= 0.897712

Thermal correction to Enthalpy= 0.898656

Thermal correction to Gibbs Free Energy= 0.765199

Sum of electronic and zero-point Energies= -4903.092619

Sum of electronic and thermal Energies= -4903.042974

Sum of electronic and thermal Enthalpies= -4903.042029

Sum of electronic and thermal Free Energies= -4903.175487

Cartesian coordinates

C	-6.114498	-1.455289	0.934067
C	-6.236527	-2.257431	-0.225889
C	-7.058660	-3.383641	-0.272632
C	-7.789151	-3.718645	0.867891

C	-7.686069	-2.937469	2.029288
C	-6.858274	-1.818044	2.072607
C	-5.180680	-0.355129	0.754427
C	-4.635404	-0.292735	-0.534714
H	-7.131416	-3.983467	-1.175059
H	-8.439988	-4.588018	0.852497
H	-8.259758	-3.210351	2.910797
H	-6.768724	-1.217476	2.968815
S	-5.242824	-1.617954	-1.535941
C	-4.731783	0.520185	1.818712
O	-5.156176	0.514033	2.977932
H	-3.930194	1.223234	1.537473
C	-3.616385	0.569442	-1.099331
H	-3.346966	0.262182	-2.112274
C	-3.736792	2.052565	-1.056403
C	-2.680564	2.868138	-1.511257
C	-4.881171	2.738520	-0.602688
C	-2.739677	4.259372	-1.514276
C	-4.958581	4.129277	-0.589525
H	-5.727549	2.156314	-0.253190
C	-3.887293	4.900457	-1.046046
H	-1.890093	4.833860	-1.867440
H	-5.862686	4.610428	-0.226922
H	-3.936421	5.985079	-1.037484
Br	-1.047294	2.041484	-2.098929
C	6.029817	-1.579222	0.024294
C	4.633758	-1.562794	0.124931
C	3.896223	-0.384940	0.296435
C	4.609490	0.819343	0.381702
C	6.003507	0.883143	0.305352

C	6.701095	-0.335319	0.118312
H	4.089756	-2.497011	0.089102
H	4.042304	1.734294	0.490179
C	2.414857	-0.406798	0.376041
C	1.715425	0.470255	1.217189
C	1.660345	-1.314319	-0.378000
C	0.322119	0.497154	1.289265
H	2.295955	1.131553	1.848745
C	0.263649	-1.355111	-0.348169
H	2.197273	-1.999176	-1.022558
C	-0.434196	-0.390119	0.451333
O	-1.767938	-0.363505	0.498891
O	8.071835	-0.236304	0.031192
C	-0.385007	1.455537	2.274572
C	-1.238125	2.474615	1.493822
C	-1.284412	0.651361	3.244130
C	0.610351	2.258824	3.135715
H	-0.622482	3.040721	0.787760
H	-2.011110	1.969845	0.923737
H	-1.717641	3.183976	2.180179
H	-0.676319	-0.001618	3.882001
H	-1.845744	1.330296	3.898256
H	-1.993567	0.032835	2.694875
H	0.051928	2.899689	3.827504
H	1.257306	1.611602	3.738007
H	1.248328	2.912196	2.530030
C	-0.483049	-2.412369	-1.194437
C	-1.560330	-3.141605	-0.355966
C	-1.133951	-1.725927	-2.412884
C	0.463345	-3.506109	-1.736665

H	-1.096736	-3.675523	0.482599
H	-2.289895	-2.443407	0.050466
H	-2.080567	-3.882016	-0.975942
H	-0.369484	-1.279076	-3.058543
H	-1.702960	-2.450041	-3.009907
H	-1.805292	-0.931165	-2.102630
H	-0.125984	-4.259172	-2.271673
H	1.200290	-3.114060	-2.445443
H	1.002863	-4.018068	-0.931958
C	6.788105	-2.916306	-0.166770
C	7.733924	-3.183615	1.032090
C	5.827197	-4.121703	-0.234636
C	7.571223	-2.911243	-1.505422
H	8.487071	-2.406893	1.197884
H	7.155859	-3.260686	1.958520
H	8.272123	-4.126405	0.885759
H	5.129478	-4.043480	-1.074253
H	6.409715	-5.038458	-0.373084
H	5.246735	-4.235938	0.685949
H	8.100928	-3.861142	-1.635920
H	6.880865	-2.786296	-2.345765
H	8.315477	-2.113509	-1.587954
C	6.742739	2.237408	0.410075
C	7.703856	2.228018	1.623623
C	7.529248	2.522761	-0.891815
C	5.766255	3.412898	0.618040
H	7.145921	2.068182	2.553304
H	8.459451	1.446254	1.540310
H	8.217041	3.193834	1.703930
H	6.848340	2.570087	-1.749236

H	8.040872	3.489837	-0.817216
H	8.277596	1.755241	-1.091937
H	6.337033	4.344585	0.692822
H	5.066780	3.523550	-0.217105
H	5.185953	3.308083	1.540751
H	8.470662	-1.108761	-0.057948
H	-2.499298	0.134636	-0.335690

Vibrational frequencies

-1634.2828	12.9865	15.2892
22.8007	26.7811	33.5122
40.8750	42.3261	46.6912
53.1032	55.3902	64.5973
72.6357	75.7472	82.2334
85.0289	94.1335	102.3506
109.6135	123.5711	128.8620
133.3041	137.4828	141.5570
158.3131	168.0511	171.7697
178.8134	182.3685	202.6093
205.1827	210.7829	216.2071
220.4958	228.3352	228.9241
246.2817	257.9476	262.8734
264.6448	268.6176	277.4414
284.9623	285.8806	291.2945
302.6524	305.8530	314.1694
315.6058	321.9907	329.3080
330.5466	339.1290	345.7143
357.4981	358.5096	365.7291
369.2254	374.3061	379.0013
381.6587	384.8258	386.9207
390.1336	401.2265	408.1505

418.1358	420.4575	422.2973
424.9515	428.7401	441.8615
450.5202	457.2184	458.7716
459.5080	472.2746	478.9351
501.0256	505.8016	526.0404
539.3255	541.4108	544.5269
550.6624	560.5127	565.2051
591.9619	595.2651	626.1992
636.2203	637.8967	639.0630
640.2339	670.4501	673.7582
675.9368	698.1500	708.4393
738.9394	745.3525	764.4474
765.5605	766.1342	768.5921
770.2231	772.5915	775.7563
797.0410	819.6368	824.7145
841.4642	848.3350	868.9799
879.4128	883.8801	891.8825
900.2832	906.0416	910.7018
919.7263	923.6930	934.9844
937.7333	940.9815	942.9412
945.4262	946.3622	948.2311
948.2936	951.3554	954.9458
963.7204	967.6089	975.5754
979.7452	980.2541	981.8682
993.6000	996.7260	1012.0071
1025.7414	1045.6943	1049.5589
1053.7491	1055.9505	1055.9704
1057.7839	1061.6873	1064.7900
1064.8606	1068.0092	1074.6405
1090.0147	1138.4061	1143.3842

1145.6557	1147.9818	1149.5997
1164.7939	1183.1979	1190.4641
1198.1154	1216.0586	1221.7451
1224.8874	1227.4459	1228.5036
1230.6583	1233.2806	1234.9430
1236.3559	1239.1113	1257.1198
1262.6433	1270.9057	1280.9839
1291.0287	1296.3357	1297.4650
1304.7557	1313.9817	1320.2986
1322.2016	1327.7444	1346.0201
1354.4580	1357.1964	1368.2438
1396.5918	1398.6586	1404.2256
1407.0641	1408.2747	1409.9467
1416.3156	1417.2539	1424.5616
1425.2498	1430.1270	1430.8921
1436.3345	1440.2623	1448.2381
1459.7948	1468.6790	1470.7046
1477.9617	1481.1445	1482.0000
1483.4755	1484.1529	1486.2485
1486.3104	1490.1605	1493.1268
1498.3063	1498.8737	1499.0391
1499.9944	1502.5203	1503.0691
1506.0353	1506.7957	1507.3050
1508.2400	1511.3115	1511.8563
1515.6885	1516.1728	1520.8066
1522.7684	1526.4849	1531.0115
1532.1242	1532.6065	1538.0818
1583.7973	1604.2681	1607.2995
1625.5512	1636.9840	1637.7364
1644.5423	1649.8439	1709.9779

3013.5167	3025.2988	3026.0645
3029.2733	3029.3752	3035.0801
3035.2719	3036.0337	3037.5431
3040.9234	3042.2870	3042.5483
3048.9129	3084.6632	3084.9208
3090.2806	3090.3958	3096.5450
3096.5814	3097.8481	3099.5625
3102.7563	3103.8244	3105.5333
3108.6093	3108.6500	3110.5509
3112.4026	3113.6214	3116.9090
3119.4293	3122.0694	3156.3236
3158.9694	3165.2879	3176.7339
3180.5066	3183.4412	3191.6865
3198.1844	3204.0582	3204.9091
3214.9835	3215.2156	3219.1077
3219.5849	3221.9211	3235.3671
3237.2776	3241.4957	3862.2789

TS4RR-m062x

Zero-point correction= 0.735728

Thermal correction to Energy= 0.781403

Thermal correction to Enthalpy= 0.782347

Thermal correction to Gibbs Free Energy= 0.655156

Sum of electronic and zero-point Energies= -5134.079098

Sum of electronic and thermal Energies= -5134.033424

Sum of electronic and thermal Enthalpies= -5134.032479

Sum of electronic and thermal Free Energies= -5134.159670

Cartesian coordinates

C	0.902893	1.214471	1.203763
C	0.114883	0.107317	0.953119

H	0.432202	2.185549	1.064920
C	-1.233365	0.280753	0.536767
O	-1.820987	1.323054	0.229596
C	2.134734	1.192957	1.988144
C	2.740046	2.412589	2.332893
C	2.768275	-0.000107	2.366448
C	3.930713	2.440636	3.047269
H	2.268718	3.339206	2.011224
C	3.966544	0.029554	3.073143
H	2.333626	-0.959689	2.098207
C	4.551246	1.246915	3.417274
H	4.387332	3.392706	3.299829
H	4.452486	-0.902929	3.344392
H	5.489105	1.266656	3.963309
C	-2.117991	-0.943313	0.680502
C	-3.832747	-2.176085	1.232803
C	-4.247021	0.255581	1.450906
H	-3.606875	1.084611	1.750021
N	-2.936796	-3.019442	0.810014
N	-1.873918	-2.236271	0.461434
N	-3.372670	-0.891631	1.159234
C	-5.167699	-2.392541	1.867748
H	-5.236867	-3.407165	2.260776
H	-5.976854	-2.234496	1.142157
C	-5.279475	-0.120354	2.579355
O	-5.235237	-1.489404	2.954091
C	-6.449851	0.590535	0.572720
C	-5.097107	0.582321	0.241405
C	-4.662429	0.826474	-1.059082
C	-5.620985	1.072170	-2.039363

C	-6.981206	1.079762	-1.716102
C	-7.404652	0.843815	-0.410220
C	-6.663454	0.303758	2.035663
H	-3.599964	0.837910	-1.290379
H	-7.715908	1.268971	-2.492728
H	-8.462406	0.848611	-0.163418
H	-7.396935	-0.489185	2.213272
H	-7.017112	1.196021	2.561532
C	-0.786956	-2.844800	-0.265017
C	0.171258	-3.576595	0.433575
C	-0.834754	-2.760414	-1.661455
C	1.137664	-4.240520	-0.327024
C	0.150072	-3.439132	-2.371244
C	1.134195	-4.191636	-1.722237
H	1.897645	-4.823342	0.187869
H	0.136521	-3.399366	-3.457842
C	-1.932203	-2.001159	-2.354880
H	-1.891882	-0.935044	-2.109449
H	-2.918349	-2.375254	-2.057435
H	-1.839199	-2.103000	-3.437846
C	2.156589	-4.940415	-2.536417
H	2.784790	-4.247715	-3.106697
H	1.665677	-5.600454	-3.257985
H	2.804749	-5.550297	-1.902687
C	0.136275	-3.679404	1.934479
H	-0.713500	-4.288639	2.260003
H	0.028924	-2.697323	2.406525
H	1.051974	-4.141709	2.306915
H	-5.025186	0.416365	3.492818
H	-5.310951	1.261270	-3.062495

H	0.467593	-0.895447	1.156959
C	4.927530	-0.484639	-0.270418
C	4.083043	-1.529129	-0.696542
C	4.477696	-2.863604	-0.662877
C	5.747181	-3.171300	-0.183903
C	6.601194	-2.150135	0.249285
C	6.206450	-0.818955	0.211015
C	4.304085	0.812839	-0.396763
C	2.977398	0.753438	-0.884559
H	3.806929	-3.647785	-0.996233
H	6.071463	-4.206473	-0.147103
H	7.589440	-2.402029	0.622868
H	6.862605	-0.027516	0.550234
S	2.522550	-0.921722	-1.231763
C	4.978610	2.045690	-0.077582
O	6.108232	2.136421	0.400967
H	4.424846	2.973827	-0.316635
C	2.067958	1.821365	-0.899729
H	2.476002	2.735524	-0.488293
C	0.842464	2.008450	-1.641867
C	0.096057	3.204434	-1.500250
C	0.281041	1.056528	-2.520314
C	-1.102890	3.436874	-2.147029
C	-0.917347	1.284137	-3.189915
H	0.819420	0.137251	-2.723890
C	-1.624748	2.466640	-3.001530
H	-1.629552	4.370817	-1.983467
H	-1.292441	0.531113	-3.876588
H	-2.559898	2.649002	-3.520843
Br	0.704953	4.588093	-0.329066

Vibrational frequencies

-153.2223	8.0427	17.2592
27.8262	31.4790	36.7110
37.8639	44.8296	46.3256
52.9397	65.0976	67.2906
68.6128	75.9218	82.0805
83.7385	94.0076	107.4868
112.1827	119.1407	127.5386
128.3574	134.8735	143.5744
150.6495	151.7183	160.8516
164.0855	181.6260	191.6020
200.0448	207.2513	213.6578
223.1901	229.2086	233.7913
234.9792	248.5066	252.9825
259.1535	261.4132	279.2466
287.0677	289.1636	302.6119
323.1883	329.2048	342.6883
354.1630	366.1602	376.6806
387.8908	390.9380	405.9928
408.4338	414.1199	431.5924
444.6145	446.6033	449.9126
462.5345	466.9435	492.8957
500.8271	504.3613	514.0272
517.8861	526.9076	533.3523
539.9262	540.4860	555.2758
561.6289	580.1453	583.8809
588.9025	599.5057	608.0539
611.6849	620.6781	626.2452
633.0228	637.2912	672.0255
683.5329	700.6053	701.7347

709.3378	711.5941	720.1700
739.4573	746.2758	748.5016
750.9375	757.9340	761.4082
773.1975	777.3627	777.9937
784.8904	793.3017	802.9489
815.7963	816.8942	836.5412
843.5680	861.8295	864.8657
876.1507	878.8422	882.4260
890.3175	891.3793	910.7592
914.3127	916.7530	921.2134
941.6744	961.5098	964.6562
964.9974	968.5648	981.0016
996.2915	997.7711	1009.5836
1012.2635	1015.0818	1018.0629
1019.1612	1020.2571	1026.4936
1027.9959	1030.3310	1034.8513
1043.4239	1053.1782	1056.2645
1059.7619	1061.9764	1062.7181
1063.4905	1064.9798	1065.2427
1067.0325	1068.1918	1071.8117
1093.9995	1116.4596	1118.5081
1125.1401	1134.0155	1142.4061
1149.7032	1157.6348	1170.8179
1171.1951	1172.8062	1173.5601
1185.1319	1195.3062	1197.9131
1199.9660	1209.2894	1222.9503
1233.5799	1238.3788	1241.3648
1255.9162	1275.6319	1276.0504
1276.4761	1293.9766	1304.9968
1309.5855	1311.8282	1321.9260

1326.8800	1333.2755	1336.8415
1344.3207	1348.9846	1352.3797
1362.7120	1364.5447	1368.4709
1369.4499	1379.4877	1381.4185
1385.8746	1412.9165	1413.5309
1415.2811	1422.1119	1427.9094
1456.4938	1463.4003	1471.1129
1472.3370	1473.0835	1483.0352
1483.6117	1484.2351	1488.7239
1493.4116	1495.2538	1497.5237
1498.4085	1513.0396	1514.0944
1515.7021	1517.8457	1524.6803
1533.1999	1536.8333	1545.4852
1555.2245	1578.2662	1588.5219
1639.3305	1644.5265	1666.5337
1669.4134	1675.6388	1678.8535
1680.0435	1686.6245	1688.0907
1692.0360	1696.4026	1714.0666
1746.0230	3003.2908	3067.0458
3067.5237	3071.0512	3076.9425
3091.2785	3136.1117	3136.5443
3136.7309	3138.5731	3163.8272
3169.0655	3172.0732	3172.8148
3176.6726	3185.5086	3189.9538
3191.9161	3195.5259	3198.9117
3201.6056	3205.9217	3207.4659
3211.4396	3211.6873	3215.5152
3221.2244	3221.4845	3222.4855
3224.9950	3227.6342	3228.2582
3233.1952	3234.6684	3237.2741

3238.7006 3249.0866 3251.3416

TS4SR-m062x

Zero-point correction= 0.736435

Thermal correction to Energy= 0.782163

Thermal correction to Enthalpy= 0.783107

Thermal correction to Gibbs Free Energy= 0.646500

Sum of electronic and zero-point Energies= -5134.081374

Sum of electronic and thermal Energies= -5134.035646

Sum of electronic and thermal Enthalpies= -5134.034702

Sum of electronic and thermal Free Energies= -5134.161753

Cartesian coordinates

C	-1.363377	0.308217	-0.553732
C	-0.092908	0.760361	-0.241135
H	-1.434509	-0.604585	-1.142850
C	1.045810	-0.036458	-0.502622
O	1.095821	-1.204763	-0.912478
C	-2.528292	1.193234	-0.568973
C	-3.591702	0.920655	-1.440463
C	-2.620896	2.312448	0.276971
C	-4.700989	1.761186	-1.495628
H	-3.539017	0.044515	-2.082486
C	-3.730701	3.144843	0.226666
H	-1.836157	2.496121	1.005862
C	-4.772670	2.874878	-0.664575
H	-5.516417	1.532103	-2.174809
H	-3.792846	3.999878	0.892955
H	-5.642204	3.523838	-0.696176
C	2.390823	0.634075	-0.291965
C	4.524480	0.917838	0.072312
C	3.809891	-1.445461	0.188614

H	2.876457	-1.913310	0.502540
N	4.066971	2.111557	-0.176507
N	2.739961	1.917661	-0.413410
N	3.529558	-0.014926	0.001130
C	5.857664	0.456760	0.562191
H	6.429514	1.301428	0.946867
H	6.429189	-0.029656	-0.238575
C	4.941176	-1.633914	1.266190
O	5.581832	-0.421181	1.638540
C	5.555700	-2.747660	-0.802335
C	4.369668	-2.068105	-1.070798
C	3.827650	-2.027379	-2.352287
C	4.507183	-2.680113	-3.378330
C	5.698584	-3.363057	-3.117555
C	6.229415	-3.404214	-1.830084
C	5.925143	-2.657384	0.655483
H	2.891367	-1.508175	-2.534588
H	6.215658	-3.867201	-3.928201
H	7.155690	-3.935403	-1.630837
H	6.956329	-2.328076	0.818203
H	5.813287	-3.628820	1.147439
C	1.909799	3.036170	-0.778788
C	1.508583	3.908184	0.237859
C	1.522742	3.168075	-2.112062
C	0.656755	4.948809	-0.122755
C	0.668589	4.228040	-2.419576
C	0.218265	5.114202	-1.440506
H	0.315278	5.638534	0.645267
H	0.343007	4.355759	-3.448728
C	1.972708	2.190177	-3.163007

H	1.396174	1.259523	-3.100300
H	3.031580	1.936634	-3.051876
H	1.821233	2.609128	-4.159417
C	-0.752708	6.211804	-1.782863
H	-1.771126	5.912369	-1.511523
H	-0.743419	6.432069	-2.852577
H	-0.523116	7.128948	-1.234376
C	1.931883	3.682356	1.663163
H	3.021031	3.657905	1.761187
H	1.542363	2.726471	2.033542
H	1.543358	4.474458	2.305864
H	4.498476	-1.997983	2.193779
H	4.106688	-2.662201	-4.386922
H	0.045243	1.746724	0.179161
C	-5.389123	-1.869353	-0.373278
C	-4.703112	-2.931801	-0.993420
C	-5.309152	-3.778531	-1.917159
C	-6.641616	-3.550453	-2.245284
C	-7.343189	-2.495246	-1.648955
C	-6.734987	-1.657843	-0.722561
C	-4.553741	-1.147686	0.564319
C	-3.236597	-1.641972	0.643752
H	-4.754896	-4.593137	-2.373647
H	-7.135076	-4.193772	-2.966784
H	-8.382712	-2.327324	-1.914498
H	-7.277033	-0.841852	-0.261398
S	-3.039364	-3.028764	-0.442863
C	-5.024677	-0.027589	1.347434
O	-6.129357	0.496032	1.233632
H	-4.325603	0.358147	2.113558

C	-2.160728	-1.026977	1.314883
H	-2.434704	-0.113813	1.826163
C	-0.908593	-1.596859	1.763704
C	0.015730	-0.816835	2.498087
C	-0.500728	-2.931232	1.529699
C	1.243934	-1.299379	2.939144
C	0.716711	-3.427716	1.962707
H	-1.175541	-3.612157	1.026304
C	1.606819	-2.613451	2.665943
H	1.897928	-0.650205	3.512585
H	0.967666	-4.464867	1.763066
H	2.556486	-3.000978	3.020990
Br	-0.447226	0.947559	3.069556

Vibrational frequencies

-165.6318	13.0479	20.0805
27.7274	32.0695	35.0410
41.8866	44.7187	45.9595
46.9170	59.3790	64.2514
72.7810	73.6889	77.1226
80.0579	95.1874	106.7596
109.8187	113.7876	126.1126
128.3547	132.6778	140.0504
142.8880	151.0190	157.1147
179.1257	189.9867	192.3997
200.9214	206.1545	210.4179
216.8819	221.8737	227.6387
230.2503	240.3658	253.9370
255.0647	270.5362	277.4637
282.0844	287.2414	312.5689
322.4019	326.8414	332.9532

356.9960	364.0131	375.2107
386.8255	396.0597	402.1949
409.1019	425.6611	430.1347
441.5191	444.0777	450.9822
452.0988	475.5463	494.1310
501.7117	502.2633	513.5029
526.2963	529.7552	534.3307
538.6780	542.0220	548.5249
555.1297	577.7929	583.5953
589.0881	600.6086	608.5083
611.3113	621.5183	631.0769
633.3384	645.3613	672.8865
681.4720	693.3207	710.2374
712.2440	715.9072	724.2714
735.1629	743.8538	747.4478
757.4679	759.1156	763.7429
772.6282	777.3143	778.1918
783.4064	798.9806	806.8124
813.8615	817.4426	838.0560
853.2412	863.6903	870.6729
871.9261	879.3151	888.5961
891.4330	895.4349	905.5840
913.5869	922.7937	926.3872
953.8030	960.6756	965.2367
967.2422	970.9416	981.1927
994.9906	998.3060	1005.1299
1011.0165	1014.7096	1014.8773
1017.3735	1020.0381	1026.7512
1031.7515	1032.8228	1039.1948
1041.7717	1050.3928	1053.7681

1059.1586	1060.1750	1062.6072
1065.3729	1069.2531	1070.1034
1070.1879	1072.6120	1073.0691
1089.1769	1119.7477	1122.1548
1124.3992	1139.3245	1146.3509
1151.8890	1159.6079	1167.2832
1174.8853	1178.7357	1183.4215
1183.7391	1198.1328	1202.7095
1210.5594	1215.5091	1228.9836
1231.8636	1245.6900	1246.8445
1263.9433	1277.1996	1277.4474
1280.6037	1288.1625	1305.5845
1306.5998	1310.0161	1326.7966
1328.5605	1331.5763	1340.6273
1342.3763	1343.4020	1350.8535
1358.3815	1368.2467	1373.6755
1374.6252	1384.3879	1384.9802
1398.2395	1411.3789	1416.7692
1418.3015	1420.0137	1431.6386
1460.7117	1463.5763	1466.1364
1473.5069	1479.6803	1482.2214
1483.9228	1486.4953	1487.0361
1490.8124	1492.7847	1493.6251
1501.7206	1511.7690	1516.4809
1517.0565	1519.9695	1527.8552
1535.0734	1539.7248	1545.7522
1552.7436	1575.9739	1592.7978
1629.2756	1642.1058	1664.8932
1672.2673	1673.9971	1679.0891
1683.1555	1689.3227	1690.6898

1694.1378	1699.1440	1706.9991
1759.0629	3002.8005	3064.4775
3071.2632	3072.4619	3089.4045
3091.0078	3133.1472	3137.0910
3143.5216	3143.9709	3168.6512
3168.7895	3171.6321	3175.3104
3181.0464	3192.4229	3196.0046
3198.0917	3198.2399	3201.0478
3203.7001	3207.1882	3208.4038
3212.0301	3213.8064	3214.4549
3217.9410	3223.2860	3224.0162
3224.9816	3228.4578	3232.0621
3237.0968	3242.5069	3243.0047
3243.7813	3266.5041	3281.5271

TS4RR-wb97xd

Zero-point correction= 0.738256

Thermal correction to Energy= 0.783821

Thermal correction to Enthalpy= 0.784766

Thermal correction to Gibbs Free Energy= 0.657989

Sum of electronic and zero-point Energies= -5134.251731

Sum of electronic and thermal Energies= -5134.206166

Sum of electronic and thermal Enthalpies= -5134.205222

Sum of electronic and thermal Free Energies= -5134.331998

Cartesian coordinates

C	0.817993	1.223996	1.127012
C	0.052561	0.088434	0.894176
H	0.328137	2.172390	0.926393
C	-1.272813	0.222277	0.423738
O	-1.873098	1.249106	0.074199

C	1.963110	1.281118	2.032632
C	2.458051	2.536572	2.417966
C	2.603498	0.133401	2.520375
C	3.540877	2.643212	3.280385
H	1.988530	3.431676	2.018283
C	3.694473	0.240670	3.375074
H	2.258294	-0.852380	2.224836
C	4.164956	1.493459	3.761617
H	3.908938	3.623524	3.566230
H	4.184581	-0.658823	3.734105
H	5.017900	1.573727	4.428015
C	-2.139540	-1.016720	0.532140
C	-3.852279	-2.281564	1.014420
C	-4.218385	0.114271	1.506274
H	-3.542054	0.900346	1.839546
N	-2.968639	-3.095161	0.515408
N	-1.904657	-2.288426	0.212148
N	-3.388526	-0.997799	1.028710
C	-5.156941	-2.542629	1.687404
H	-5.238891	-3.594814	1.958715
H	-5.997977	-2.277924	1.034028
C	-5.148378	-0.371650	2.682590
O	-5.133799	-1.778231	2.877957
C	-6.479937	0.626920	0.914908
C	-5.172138	0.603092	0.438397
C	-4.865286	1.001947	-0.859214
C	-5.904078	1.415917	-1.688226
C	-7.219862	1.437979	-1.218742
C	-7.515719	1.049054	0.085405
C	-6.556959	0.168397	2.345673

H	-3.834969	1.004610	-1.199597
H	-8.019377	1.763100	-1.877440
H	-8.539011	1.069514	0.448633
H	-7.307814	-0.611525	2.504513
H	-6.811132	0.999553	3.010803
C	-0.787023	-2.860823	-0.488864
C	0.164874	-3.577110	0.235447
C	-0.777076	-2.753992	-1.883487
C	1.184837	-4.191435	-0.492286
C	0.265168	-3.378722	-2.560395
C	1.249897	-4.103155	-1.882916
H	1.940737	-4.758154	0.044474
H	0.301571	-3.311952	-3.644601
C	-1.875444	-2.033524	-2.615224
H	-1.928280	-0.979230	-2.328561
H	-2.849103	-2.487318	-2.400792
H	-1.710796	-2.081172	-3.693272
C	2.360405	-4.765645	-2.653765
H	3.048940	-4.017048	-3.061201
H	1.964138	-5.334334	-3.500333
H	2.937705	-5.446305	-2.022965
C	0.079225	-3.710149	1.731518
H	-0.792800	-4.306195	2.020687
H	-0.019968	-2.736263	2.221693
H	0.972459	-4.198221	2.125829
H	-4.777887	0.032170	3.624002
H	-5.689071	1.727561	-2.705517
H	0.406677	-0.898356	1.161760
C	4.987644	-0.431265	0.016615
C	4.229507	-1.505924	-0.483565

C	4.672234	-2.824200	-0.421032
C	5.905268	-3.081621	0.167493
C	6.674390	-2.029239	0.677665
C	6.230242	-0.715693	0.607477
C	4.325928	0.844260	-0.162478
C	3.051934	0.730442	-0.762604
H	4.066918	-3.632988	-0.815629
H	6.268550	-4.102549	0.231774
H	7.634276	-2.241851	1.139189
H	6.819456	0.101136	1.004529
S	2.704149	-0.954928	-1.151249
C	4.923779	2.105366	0.188616
O	6.015548	2.254282	0.739018
H	4.345588	3.005096	-0.097545
C	2.091067	1.753748	-0.865480
H	2.427244	2.697949	-0.456589
C	0.971406	1.886740	-1.778194
C	0.193781	3.068996	-1.791265
C	0.553764	0.891711	-2.685085
C	-0.905764	3.246844	-2.611815
C	-0.539792	1.062822	-3.525664
H	1.117316	-0.029542	-2.767348
C	-1.286067	2.234617	-3.489461
H	-1.466307	4.173944	-2.567464
H	-0.803577	0.270150	-4.218308
H	-2.143923	2.372849	-4.139064
Br	0.617367	4.519935	-0.618474

Vibrational frequencies

-211.9330	14.9893	25.8282
27.4489	32.0892	34.4599

37.2589 41.5598 46.2363

50.3817 61.7702 63.0836

70.5674 73.1124 75.6136

82.8367 86.5636 90.5578

103.5561 114.8296 123.2631

129.4582 136.4838 140.8787

145.0768 148.6059 154.8553

163.2227 188.2211 191.1096

194.2916 201.7598 211.3497

219.4647 224.6596 225.7408

239.3117 245.9644 251.5428

257.4373 262.8285 284.9376

290.5227 296.1886 305.3179

326.6694 327.7552 342.4336

356.0024 369.9084 384.1442

390.5647 395.0558 409.4771

413.8527 426.3972 437.4927

449.8944 451.8769 455.1736

464.3257 476.4888 497.6392

507.9201 514.0370 519.2757

528.5476 534.1477 537.4195

543.9294 545.2445 557.0923

572.8996 587.1420 588.6052

592.4144 606.7331 612.1771

617.1093 624.3329 635.7136

640.6736 646.8573 677.2362

696.8453 707.1398 712.1676

713.9048 717.8091 726.0073

747.5806 751.0611 752.7366

760.7192 765.2387 770.1408

771.1335	774.0901	777.3141
793.6615	800.1995	817.7731
820.5137	832.7122	839.7514
861.8341	866.5944	873.9687
878.2853	879.9111	882.7419
890.8319	894.4454	910.9178
914.2638	921.6322	927.4123
948.9176	962.3743	963.5213
967.2991	971.2690	986.0880
993.3090	999.9142	1010.5753
1013.7652	1013.8992	1021.1957
1023.9197	1028.4364	1031.8643
1034.9290	1042.7746	1048.5157
1053.8811	1055.4705	1060.5291
1062.3779	1064.8528	1066.5756
1068.4394	1069.1971	1071.9558
1073.4561	1078.6580	1083.5574
1089.9491	1118.1550	1120.9011
1127.0438	1129.5999	1140.6470
1150.5108	1160.8165	1175.0220
1180.5862	1182.5623	1184.9593
1188.2679	1198.6509	1203.7422
1211.0625	1217.6879	1231.0416
1232.5046	1244.5014	1244.7915
1260.7488	1282.9869	1287.7925
1292.2223	1302.7200	1309.8101
1316.6726	1318.7508	1322.8643
1325.6419	1339.4923	1341.4854
1348.6947	1351.3685	1356.7860
1365.4741	1369.2274	1370.3607

1374.5499	1386.6631	1397.4377
1397.9830	1424.3962	1427.2725
1427.9876	1430.0523	1437.2403
1459.8200	1468.8990	1469.5340
1480.0613	1482.6822	1484.0580
1487.2197	1488.6877	1489.8306
1493.3308	1495.4154	1499.0528
1504.3773	1512.4208	1514.4653
1517.3727	1517.8321	1522.1874
1534.3750	1537.9863	1550.2241
1559.1481	1578.8812	1588.6400
1633.2104	1640.2551	1660.4928
1668.6573	1670.3913	1673.1959
1674.5743	1680.3631	1683.6254
1687.9634	1691.1639	1700.5628
1737.8807	2967.8836	3065.0207
3066.6651	3070.4254	3076.3312
3093.4052	3133.9538	3139.0326
3140.4528	3143.3031	3163.3575
3163.6086	3176.8488	3178.6663
3182.5657	3190.4984	3210.8545
3214.9513	3214.9855	3217.3536
3218.5210	3220.8964	3221.7778
3227.4013	3228.5557	3228.8187
3231.4095	3237.4521	3237.5457
3238.7894	3244.7657	3246.2848
3246.9146	3253.7408	3257.6537
3257.8721	3271.6028	3285.6347

TS4SR-wb97xd

Zero-point correction= 0.738159

Thermal correction to Energy= 0.783788

Thermal correction to Enthalpy= 0.784732

Thermal correction to Gibbs Free Energy= 0.656056

Sum of electronic and zero-point Energies= -5134.256335

Sum of electronic and thermal Energies= -5134.210706

Sum of electronic and thermal Enthalpies= -5134.209762

Sum of electronic and thermal Free Energies= -5134.336438

Cartesian coordinates

C	-1.363966	0.306422	-0.578261
C	-0.087621	0.755166	-0.267994
H	-1.433467	-0.585179	-1.195746
C	1.050590	-0.016907	-0.566807
O	1.106858	-1.166776	-1.033726
C	-2.518869	1.206640	-0.603649
C	-3.562981	0.961580	-1.503894
C	-2.613744	2.318497	0.249144
C	-4.654681	1.822365	-1.579745
H	-3.511046	0.093377	-2.154538
C	-3.705417	3.171620	0.178447
H	-1.846999	2.481794	1.000093
C	-4.726760	2.931045	-0.743161
H	-5.453556	1.615522	-2.284742
H	-3.768445	4.020810	0.851881
H	-5.580745	3.599191	-0.793839
C	2.389693	0.651785	-0.328471
C	4.516888	0.944256	0.063490
C	3.807734	-1.417980	0.172341
H	2.873070	-1.889857	0.473413
N	4.060231	2.136652	-0.189700
N	2.733405	1.936906	-0.442151

N	3.527705	0.007767	-0.022602
C	5.843680	0.491216	0.571770
H	6.403615	1.337320	0.969088
H	6.433101	0.017063	-0.222788
C	4.917745	-1.602108	1.271273
O	5.562953	-0.391207	1.641931
C	5.562172	-2.739576	-0.773084
C	4.389392	-2.051211	-1.070596
C	3.878304	-2.011545	-2.363491
C	4.575414	-2.671171	-3.371996
C	5.754754	-3.361855	-3.082257
C	6.253818	-3.403988	-1.782410
C	5.896940	-2.647608	0.691561
H	2.949113	-1.489347	-2.566322
H	6.287253	-3.871361	-3.879558
H	7.171615	-3.940896	-1.561434
H	6.930753	-2.343002	0.878982
H	5.750837	-3.613376	1.186106
C	1.891129	3.050680	-0.782186
C	1.466385	3.886702	0.253908
C	1.497584	3.209096	-2.112060
C	0.579044	4.907194	-0.078715
C	0.606978	4.244211	-2.389895
C	0.126701	5.088479	-1.387530
H	0.219495	5.566341	0.706858
H	0.273401	4.386163	-3.414380
C	1.974930	2.277154	-3.192064
H	1.433021	1.325420	-3.152581
H	3.042503	2.057914	-3.095763
H	1.803750	2.716033	-4.177005

C	-0.894748	6.147801	-1.702213
H	-1.901844	5.716711	-1.673720
H	-0.744298	6.567806	-2.700340
H	-0.862457	6.961286	-0.973081
C	1.892099	3.645073	1.675499
H	2.979806	3.585459	1.770593
H	1.473998	2.702343	2.047254
H	1.533204	4.445736	2.325368
H	4.456730	-1.949709	2.195014
H	4.196683	-2.652863	-4.389024
H	0.046816	1.731999	0.171228
C	-5.371035	-1.914013	-0.364280
C	-4.686685	-2.967456	-0.996074
C	-5.301850	-3.821885	-1.906890
C	-6.642260	-3.608138	-2.207704
C	-7.342435	-2.559661	-1.599337
C	-6.723910	-1.716511	-0.686336
C	-4.528008	-1.178756	0.558257
C	-3.203004	-1.653975	0.606402
H	-4.750666	-4.632269	-2.373890
H	-7.144230	-4.258036	-2.917478
H	-8.388825	-2.402456	-1.843625
H	-7.261459	-0.903879	-0.214454
S	-3.011034	-3.038027	-0.479635
C	-5.001639	-0.091554	1.381100
O	-6.127237	0.401619	1.336807
H	-4.278922	0.299307	2.121983
C	-2.118975	-1.021261	1.255542
H	-2.409568	-0.124028	1.784974
C	-0.873537	-1.589153	1.735528

C	0.016132	-0.815498	2.515762
C	-0.438185	-2.907672	1.475893
C	1.233992	-1.297255	2.986224
C	0.767883	-3.403139	1.939513
H	-1.077975	-3.576824	0.914922
C	1.620335	-2.598853	2.695841
H	1.865396	-0.657453	3.593262
H	1.040134	-4.430223	1.717878
H	2.562046	-2.984255	3.072978
Br	-0.475009	0.933656	3.113123

Vibrational frequencies

-240.7757	19.5502	21.6318
26.5589	30.0339	38.4279
40.1901	45.2266	49.0722
54.2460	60.3618	66.8604
70.6696	72.6696	75.8272
80.1635	88.5474	94.3946
105.3516	110.5994	113.8070
115.9828	131.9137	139.6361
143.9885	146.4757	157.5132
175.6839	186.1800	189.4528
194.5641	202.7740	209.7516
218.7528	223.7017	229.2219
230.8817	244.3259	250.2954
261.5474	268.3067	277.5563
287.4249	291.0867	314.8324
322.8985	329.6853	334.6615
356.2489	364.7931	381.1944
389.5131	398.4260	403.6247
409.6651	422.5871	436.2021

447.1215	450.3855	451.5592
458.7103	479.3944	497.7947
508.5333	511.1316	516.0499
528.5411	536.9571	537.8181
543.8755	546.9975	556.2483
562.2926	582.9635	587.6730
592.1533	604.9317	612.4207
619.5077	625.4580	640.3986
642.9422	649.3083	683.7074
686.2891	707.1566	714.3501
716.1331	717.3109	727.7252
741.8834	746.1793	746.8935
757.6481	763.1922	768.5313
775.7855	782.7459	784.7315
785.6500	797.6243	803.8503
811.4429	820.5017	840.4833
848.7923	862.0373	867.1394
883.6534	885.1473	888.0144
894.1199	899.4277	916.1444
918.7333	922.9809	924.9034
949.2089	952.8682	969.5140
972.8284	982.3779	984.3260
992.6226	997.3131	1002.3930
1014.9589	1017.6266	1018.5247
1020.5236	1025.8819	1028.3247
1039.9377	1046.2197	1047.6484
1049.5930	1052.5563	1055.6690
1061.7490	1065.6201	1066.6565
1068.7420	1072.3365	1074.5385
1074.9414	1077.0053	1080.4142

1090.9204	1119.9895	1120.6512
1127.8408	1135.0965	1143.6930
1160.5412	1168.1696	1179.8147
1182.0384	1185.9190	1186.5969
1196.3627	1196.8905	1204.5552
1210.0654	1214.1968	1227.1349
1235.4271	1247.7675	1252.3370
1266.3780	1287.6953	1292.0270
1292.6884	1294.6128	1300.7212
1314.4098	1318.9494	1332.5940
1333.1875	1336.7015	1342.5175
1344.0716	1347.0158	1355.6887
1362.9133	1371.1595	1374.0844
1377.0939	1386.2319	1393.5869
1404.1327	1423.8629	1426.5787
1427.4619	1432.5911	1440.1572
1457.9574	1469.2829	1474.7392
1476.9101	1486.4387	1486.7280
1490.6370	1492.0209	1495.6572
1496.2514	1497.4644	1497.7811
1503.0119	1513.3426	1515.6797
1517.3043	1523.0012	1528.3192
1536.0871	1539.2273	1547.4202
1551.4942	1574.3143	1597.1219
1630.5278	1642.3489	1660.2444
1670.6973	1672.3593	1673.8704
1674.8556	1679.5416	1685.2835
1688.1947	1693.6749	1699.2841
1746.7613	2979.4264	3069.0053
3069.8948	3070.5814	3077.6520

3091.8027	3141.4509	3143.9596
3144.5735	3145.7687	3167.6467
3169.7650	3169.8315	3173.3583
3176.8375	3191.5728	3211.8483
3211.9103	3214.7498	3215.1562
3215.6888	3216.0492	3218.0809
3221.7282	3223.5158	3224.3388
3226.2050	3227.9807	3232.1984
3235.4088	3235.5691	3241.2442
3241.6866	3248.3552	3253.4228
3262.2060	3268.2476	3284.0087

TS4RR(Φ= -156°)

Zero-point correction= 0.729632

Thermal correction to Energy= 0.775826

Thermal correction to Enthalpy= 0.776770

Thermal correction to Gibbs Free Energy= 0.647751

Sum of electronic and zero-point Energies= -5135.061044

Sum of electronic and thermal Energies= -5135.014849

Sum of electronic and thermal Enthalpies= -5135.013905

Sum of electronic and thermal Free Energies= -5135.142924

Cartesian coordinates

C	1.505441	0.120908	-1.266853
C	0.535363	0.970172	-0.706949
H	1.115277	-0.663273	-1.907504
C	-0.816447	0.570583	-0.725496
O	-1.242307	-0.575908	-1.018149
C	2.855666	0.603185	-1.599119
C	3.561305	0.008737	-2.660748
C	3.493759	1.617211	-0.858055

C	4.862010	0.405129	-2.966703
H	3.084224	-0.777456	-3.238009
C	4.792014	2.012487	-1.166032
H	2.975743	2.087696	-0.027881
C	5.484723	1.405474	-2.218926
H	5.391776	-0.075165	-3.784524
H	5.269758	2.792155	-0.579038
H	6.500742	1.711077	-2.452011
C	-1.876317	1.620608	-0.504890
C	-3.842004	2.615577	-0.547575
C	-3.889443	0.326597	-1.490287
H	-3.149525	-0.233028	-2.057279
N	-3.040683	3.494306	-0.009955
N	-1.817764	2.862908	0.014360
N	-3.175235	1.463602	-0.871601
C	-5.269444	2.739681	-0.962127
H	-5.569514	3.788208	-0.976903
H	-5.927972	2.191469	-0.274852
C	-5.062559	0.839804	-2.417377
O	-5.340144	2.238566	-2.295000
C	-5.915595	-0.730534	-0.764240
C	-4.568277	-0.536673	-0.450036
C	-3.996934	-1.101296	0.689758
C	-4.810839	-1.862005	1.532250
C	-6.163987	-2.057854	1.226683
C	-6.723900	-1.498854	0.075020
C	-6.286248	-0.040629	-2.052115
H	-2.944043	-0.956886	0.907552
H	-6.784301	-2.651272	1.892568
H	-7.773539	-1.653092	-0.159743

H	-7.183680	0.580856	-1.968563
H	-6.475508	-0.770197	-2.847846
C	-0.701388	3.563637	0.593479
C	0.104956	4.347218	-0.243085
C	-0.495248	3.436241	1.972202
C	1.193117	4.993144	0.350001
C	0.605724	4.102501	2.514719
C	1.462547	4.873564	1.719868
H	1.846370	5.598376	-0.272757
H	0.806235	3.998823	3.576177
C	-1.423579	2.600716	2.811944
H	-1.391723	1.552499	2.501337
H	-2.458924	2.945256	2.712651
H	-1.139713	2.642713	3.863640
C	2.673244	5.535268	2.329488
H	3.469990	4.799804	2.496489
H	2.438420	5.979853	3.301952
H	3.075239	6.318426	1.680547
C	-0.165158	4.437987	-1.722043
H	-1.207227	4.706334	-1.924876
H	0.024275	3.473225	-2.207336
H	0.480309	5.184432	-2.190312
H	-4.776274	0.719433	-3.462461
H	-4.387205	-2.303948	2.427484
H	0.809113	1.944175	-0.334388
C	-1.022036	-3.366459	1.001297
C	-0.470325	-4.459717	0.292167
C	-1.126722	-5.686861	0.185554
C	-2.369905	-5.830830	0.802682
C	-2.937670	-4.759904	1.510420

C	-2.277410	-3.538439	1.616838
C	-0.153983	-2.201920	0.981119
C	1.054987	-2.420591	0.287135
H	-0.680645	-6.510977	-0.362731
H	-2.896256	-6.778245	0.733410
H	-3.904666	-4.887046	1.988882
H	-2.701761	-2.715402	2.175948
S	1.113664	-4.072008	-0.369633
C	-0.441114	-0.968859	1.680821
O	-1.429453	-0.766489	2.395790
H	0.310812	-0.167188	1.565905
C	2.128431	-1.493725	0.169253
H	2.151392	-0.777458	0.978601
C	3.451247	-1.814966	-0.369028
C	4.645109	-1.351517	0.228311
C	3.605824	-2.510171	-1.591123
C	5.902942	-1.602318	-0.316880
C	4.854828	-2.773250	-2.143952
H	2.712649	-2.807553	-2.130543
C	6.013255	-2.325709	-1.504044
H	6.789153	-1.229527	0.184677
H	4.922114	-3.312676	-3.084040
H	6.993672	-2.522292	-1.926700
Br	4.594795	-0.310434	1.844740

Vibrational frequencies

-208.4712	12.3533	15.5716
25.7476	31.2357	36.0742
38.9353	43.3858	45.6665
49.0167	53.0701	60.1046
65.9028	69.3479	74.2338

80.9014	86.1605	89.7997
94.2784	104.7530	111.8474
123.1257	132.4763	136.0614
142.1808	146.6741	155.1901
156.1016	166.8213	184.4289
190.3323	198.7156	207.3432
214.2347	219.7081	228.9541
237.8209	242.3138	244.8777
251.4898	262.0551	281.1620
289.2122	293.2424	298.9356
317.1074	321.9802	338.3769
352.9727	365.1348	379.5869
387.7554	394.8334	403.8347
416.8073	425.0893	431.5293
446.3680	448.7096	450.2528
459.0370	474.0542	491.9508
502.8251	510.6432	515.0915
525.7786	528.5518	533.0460
539.4535	542.2291	546.3143
569.4488	581.6274	584.1235
593.8291	600.8926	606.1971
615.7412	617.5036	631.1695
633.1128	641.5175	667.7693
684.2557	698.0839	701.9906
708.5458	710.7353	715.7935
731.7656	736.4076	743.2846
752.2536	754.2961	759.6688
765.4402	766.8630	770.0360
774.7041	785.7582	789.4175
801.6853	812.0792	828.0516

846.1580	865.0100	868.8701
871.0297	872.3680	878.7759
882.6378	886.8982	902.1987
905.8908	909.5029	928.5141
943.3534	948.2570	950.6204
954.4387	959.0205	976.2974
978.8577	985.1724	988.9195
992.0617	993.1580	1007.7426
1008.0156	1010.4287	1013.3495
1016.3800	1033.2165	1037.2643
1040.5824	1047.6241	1050.4366
1052.2465	1053.7676	1057.1522
1058.4114	1061.3919	1064.6418
1067.3714	1069.3916	1070.5137
1080.6212	1085.6666	1099.1163
1110.3563	1112.8942	1116.2761
1141.5721	1154.5037	1156.3352
1180.9569	1184.0949	1186.5932
1186.9083	1192.9453	1193.1948
1202.2388	1213.6224	1214.6268
1218.1539	1223.6103	1234.8494
1244.1337	1272.9329	1273.9313
1278.5053	1288.9818	1291.3018
1296.9663	1301.1264	1309.4597
1321.3927	1327.7819	1329.5249
1332.1652	1337.7676	1343.9877
1350.5510	1362.1545	1368.1339
1369.0945	1375.9164	1380.6343
1382.7816	1402.9792	1406.6096
1415.8835	1421.4404	1426.1430

1438.4181	1447.7323	1450.0784
1458.9884	1468.8655	1469.2085
1471.8233	1478.2842	1480.9989
1481.8651	1484.2883	1487.6676
1490.0845	1494.2153	1496.6509
1496.9096	1503.5297	1504.3693
1507.8074	1520.4757	1528.2190
1533.2702	1536.2396	1558.8454
1602.3989	1606.3026	1613.2516
1629.2259	1635.5560	1636.8408
1639.1513	1639.8519	1640.7820
1652.8111	1653.1123	1656.9409
1702.3797	2952.0394	3041.3236
3046.5049	3048.2611	3048.9185
3059.4297	3100.6152	3101.6475
3106.9062	3113.5564	3128.9716
3132.4101	3142.2330	3143.6950
3152.0319	3155.4733	3178.9408
3182.2832	3182.3001	3183.1596
3185.6131	3189.5564	3190.0811
3193.7079	3193.8854	3194.9949
3198.9868	3205.0731	3205.5341
3206.6926	3207.3932	3213.0499
3219.5944	3219.9724	3224.1151
3241.0830	3244.5122	3254.7340

TS4RR' (Φ=147°)

Zero-point correction= 0.730663

Thermal correction to Energy= 0.776296

Thermal correction to Enthalpy= 0.777240

Thermal correction to Gibbs Free Energy= 0.650607

Sum of electronic and zero-point Energies= -5135.056220

Sum of electronic and thermal Energies= -5135.010587

Sum of electronic and thermal Enthalpies= -5135.009643

Sum of electronic and thermal Free Energies= -5135.136276

Cartesian coordinates

C	1.059184	-1.514092	-0.121124
C	-0.128371	-0.969825	-0.631883
H	1.114318	-1.540902	0.961567
C	-0.970001	-0.250151	0.237817
O	-0.712600	0.142379	1.399742
C	1.834995	-2.549639	-0.815187
C	2.664380	-3.403125	-0.062816
C	1.815002	-2.704384	-2.215714
C	3.458926	-4.362591	-0.685515
H	2.690115	-3.296432	1.016974
C	2.608777	-3.665955	-2.836127
H	1.183453	-2.063626	-2.823112
C	3.438065	-4.496563	-2.075267
H	4.099330	-5.002507	-0.085304
H	2.583769	-3.766603	-3.917705
H	4.060213	-5.241428	-2.563128
C	-2.401279	-0.069227	-0.215120
C	-4.481041	-0.483438	-0.791926
C	-3.020413	-2.503257	-0.751950
H	-1.997651	-2.648233	-1.095605
N	-4.465984	0.784654	-0.480558
N	-3.161862	1.023660	-0.102795
N	-3.236825	-1.044148	-0.646651
C	-5.581063	-1.351022	-1.308897
H	-6.348492	-0.748449	-1.797110

H	-6.044213	-1.911211	-0.484799
C	-4.051475	-3.142893	-1.765034
O	-5.003549	-2.212122	-2.286026
C	-4.214229	-4.227363	0.413792
C	-3.275707	-3.204124	0.565717
C	-2.680702	-2.939217	1.800951
C	-3.047977	-3.720564	2.898066
C	-3.988492	-4.749019	2.753385
C	-4.575889	-5.008850	1.513059
C	-4.708209	-4.327893	-1.006118
H	-1.959347	-2.135494	1.915553
H	-4.264859	-5.349138	3.615589
H	-5.307029	-5.805246	1.405585
H	-5.799315	-4.264535	-1.079664
H	-4.415941	-5.278803	-1.463973
C	-2.789038	2.346017	0.331999
C	-2.432332	3.288445	-0.638698
C	-2.885567	2.640102	1.700989
C	-2.145672	4.582154	-0.189906
C	-2.577282	3.943218	2.093138
C	-2.203103	4.923295	1.164148
H	-1.862068	5.334514	-0.917030
H	-2.636862	4.201320	3.147382
C	-3.306512	1.592213	2.696951
H	-2.562701	0.790071	2.724549
H	-4.269749	1.146480	2.423724
H	-3.400915	2.021464	3.697231
C	-1.864747	6.317423	1.628969
H	-1.815210	7.020027	0.793020
H	-0.891808	6.332191	2.133706

H	-2.605892	6.686791	2.345922
C	-2.361661	2.933236	-2.101715
H	-3.235267	2.353066	-2.416467
H	-1.467103	2.343529	-2.330968
H	-2.318299	3.837904	-2.712041
H	-3.512644	-3.486339	-2.647917
H	-2.599789	-3.530038	3.868588
H	-0.449335	-1.139944	-1.653339
C	1.272406	3.340188	-1.198280
C	1.595847	3.852083	0.079807
C	1.465453	5.205519	0.393974
C	1.027346	6.079254	-0.601216
C	0.717499	5.596367	-1.881993
C	0.825126	4.240911	-2.183192
C	1.542952	1.917478	-1.307645
C	2.149007	1.373310	-0.155523
H	1.717926	5.573693	1.383752
H	0.930196	7.137821	-0.379839
H	0.382486	6.288470	-2.649536
H	0.582574	3.862218	-3.167600
S	2.233670	2.596589	1.139991
C	1.272723	1.128755	-2.485776
O	0.637456	1.510463	-3.479342
H	1.694036	0.108144	-2.478421
C	2.711145	0.075480	-0.026168
H	3.101410	-0.311363	-0.957933
C	3.416082	-0.388710	1.168141
C	4.650201	-1.071533	1.114142
C	2.830993	-0.267712	2.450983
C	5.280255	-1.572410	2.251981

C	3.454080	-0.751403	3.596673
H	1.840803	0.173095	2.519188
C	4.686133	-1.404552	3.503029
H	6.230291	-2.086936	2.158386
H	2.967436	-0.636978	4.560837
H	5.178526	-1.792660	4.389315
Br	5.538178	-1.349997	-0.570678

Vibrational frequencies

-194.3346	15.9034	18.3854
26.1273	35.2918	37.6370
39.4461	40.8024	50.3061
52.7368	56.1165	57.5320
67.2331	79.2608	81.2717
86.7682	96.6748	102.5677
105.8502	108.3225	112.8431
125.6722	132.9786	140.4483
147.0063	161.3547	178.7471
189.7495	193.2495	199.2662
205.4140	212.6100	213.3804
217.2302	221.6791	228.9337
231.5752	249.1807	259.1467
264.0356	270.2761	281.2297
292.5148	304.3290	310.9257
317.2340	320.2137	329.2923
346.5273	376.3547	383.9493
388.6506	395.9899	401.3884
422.1284	436.7395	438.1381
440.6545	450.1348	452.7066
473.4029	487.0542	496.7851
500.0616	504.4240	513.9786

519.8772 526.0091 529.8883

531.7759 543.0737 544.3318

561.2689 581.1097 583.4607

590.6912 596.5674 611.1593

613.9734 620.8362 623.0251

627.1358 632.4038 666.9006

687.3989 695.1228 702.7002

707.5450 711.5846 716.7008

738.8450 745.5569 746.5337

754.3610 764.3601 766.7114

770.6659 772.5862 773.4172

777.6285 790.1820 797.9473

811.1573 820.0598 828.5120

852.1924 861.9599 865.2548

872.1866 876.9590 880.5773

883.7605 896.4057 905.4668

907.9335 911.1313 912.2157

932.4320 951.3874 953.9714

961.7077 972.9367 976.1165

979.5595 981.7438 993.4192

993.9645 999.2199 1004.3560

1006.5821 1010.0165 1019.7298

1025.6273 1033.6385 1039.5705

1040.5484 1042.4906 1049.0160

1050.3888 1056.1469 1057.0957

1059.6842 1063.0931 1065.1938

1066.6008 1069.0820 1075.0688

1076.6069 1089.2213 1107.9082

1112.0612 1113.9878 1120.9065

1143.1657 1154.6476 1168.2340

1183.7125	1185.7959	1187.4056
1188.0377	1191.1711	1197.5090
1203.7098	1213.4396	1217.6898
1220.2792	1229.4598	1231.6520
1245.7000	1266.8662	1281.5105
1285.1334	1292.1510	1292.6656
1297.8228	1301.9048	1315.2104
1317.8805	1323.1078	1324.9451
1329.7251	1340.5117	1341.9839
1351.2502	1359.1714	1368.0517
1368.4385	1369.7226	1379.1653
1386.6383	1400.8223	1411.6746
1412.7291	1417.0662	1427.1800
1432.9531	1446.5141	1450.3124
1464.8741	1465.3358	1470.1761
1472.3430	1477.5312	1482.1044
1487.4468	1489.3191	1489.8774
1496.3431	1497.0712	1497.5938
1498.0449	1505.4360	1511.5337
1517.1952	1525.2972	1527.8441
1534.4678	1535.1766	1564.8674
1601.2320	1606.6294	1620.3877
1631.5570	1632.7246	1633.7292
1636.3257	1641.1426	1643.5911
1653.3674	1654.7310	1658.3431
1682.8702	2991.2317	3041.3883
3043.4062	3045.6745	3048.1416
3060.0654	3097.3426	3102.6837
3112.1523	3113.7431	3132.0750
3135.5139	3137.6628	3141.1043

3151.9164	3153.3771	3180.0291
3181.0265	3182.9029	3184.9328
3186.7600	3187.5564	3192.9146
3193.6177	3193.9518	3197.0509
3197.8662	3200.8508	3203.5213
3207.0090	3207.1182	3209.8088
3210.2752	3211.3530	3211.6488
3215.8648	3219.3257	3241.8501

TS4RR" (Φ= -169°)

Zero-point correction= 0.729933

Thermal correction to Energy= 0.775929

Thermal correction to Enthalpy= 0.776873

Thermal correction to Gibbs Free Energy= 0.647314

Sum of electronic and zero-point Energies= -5135.046135

Sum of electronic and thermal Energies= -5135.000139

Sum of electronic and thermal Enthalpies= -5134.999195

Sum of electronic and thermal Free Energies= -5135.128754

Cartesian coordinates

C	-0.951121	-0.991476	0.546492
C	0.360472	-0.529082	0.832459
H	-1.085869	-1.303439	-0.484537
C	1.161955	-0.089136	-0.225218
O	0.816406	0.113089	-1.419207
C	-1.760081	-1.740347	1.515846
C	-2.844884	-2.514399	1.054447
C	-1.530409	-1.683713	2.904162
C	-3.668884	-3.198725	1.944174
H	-3.039905	-2.572203	-0.011859
C	-2.348905	-2.379032	3.793738
H	-0.717994	-1.080644	3.294744

C	-3.423613	-3.135071	3.320034
H	-4.502033	-3.783406	1.564759
H	-2.153301	-2.320160	4.860746
H	-4.064915	-3.669479	4.014978
H	0.764765	-0.520414	1.838320
C	-5.319771	-0.651160	-1.501588
C	-4.439927	-1.097427	-2.515393
C	-4.869762	-1.874859	-3.591974
C	-6.217017	-2.228115	-3.657327
C	-7.109419	-1.799510	-2.662326
C	-6.676858	-1.017291	-1.594739
C	-4.652663	0.174222	-0.504816
C	-3.260995	0.266185	-0.700258
H	-4.171382	-2.200290	-4.357209
H	-6.573092	-2.839090	-4.481528
H	-8.156268	-2.083540	-2.723898
H	-7.364485	-0.683420	-0.828810
S	-2.796829	-0.539602	-2.225945
C	-5.389065	1.007673	0.429133
O	-6.592919	0.906794	0.678416
H	-4.806946	1.820311	0.894683
C	-2.162891	0.769506	0.072309
H	-1.343487	1.119314	-0.547816
C	-2.241973	1.436292	1.379925
C	-1.390068	2.510615	1.714016
C	-3.054377	0.953298	2.432526
C	-1.358304	3.082421	2.985852
C	-3.041303	1.517181	3.703265
H	-3.700386	0.106183	2.238721
C	-2.191038	2.588119	3.988656

H	-0.690364	3.913504	3.184398
H	-3.687178	1.107740	4.474149
H	-2.171937	3.036542	4.977270
Br	-0.220621	3.287526	0.394583
C	2.647293	0.016960	0.044415
C	4.738438	-0.548298	0.428089
C	3.101742	-2.366981	0.879808
H	2.110084	-2.345371	1.330356
N	4.804559	0.660255	-0.060707
N	3.489614	0.993455	-0.313028
N	3.438345	-0.976440	0.515233
C	5.805326	-1.457146	0.943716
H	6.689428	-0.885361	1.229695
H	6.090552	-2.188570	0.174985
C	4.167878	-2.946463	1.891272
O	5.285236	-2.080779	2.114876
C	3.974635	-4.391169	-0.063465
C	3.155176	-3.289727	-0.319641
C	2.492497	-3.139867	-1.539301
C	2.667579	-4.123421	-2.514903
C	3.485641	-5.233224	-2.264994
C	4.142898	-5.374510	-1.040361
C	4.574770	-4.330532	1.317820
H	1.867539	-2.272742	-1.734889
H	3.612165	-5.990583	-3.033350
H	4.779580	-6.234541	-0.852303
H	5.665394	-4.429964	1.313785
H	4.184700	-5.131916	1.954732
C	3.193750	2.298430	-0.847447
C	3.056389	3.359909	0.055179

C	3.126472	2.452082	-2.238028
C	2.810714	4.626496	-0.482071
C	2.874839	3.738874	-2.722586
C	2.708360	4.831831	-1.863472
H	2.687836	5.467248	0.194989
H	2.810579	3.889170	-3.796907
C	3.308663	1.277620	-3.161123
H	2.492138	0.564158	-3.010991
H	4.249529	0.753465	-2.958469
H	3.313477	1.599049	-4.205263
C	2.397748	6.202403	-2.411325
H	1.314481	6.376364	-2.423917
H	2.759412	6.317221	-3.437272
H	2.845067	6.990001	-1.797135
C	3.118787	3.129534	1.541828
H	4.029387	2.595305	1.831941
H	2.259537	2.533057	1.866897
H	3.088426	4.078142	2.082582
H	3.711856	-3.041898	2.876770
H	2.165033	-4.027096	-3.472618

Vibrational frequencies

-225.0793	10.1319	16.0233
21.1147	26.4684	30.1765
34.1031	37.2958	38.9654
49.3322	50.6093	54.2850
59.5035	68.0004	77.7888
79.8845	88.5153	93.9354
104.5598	107.4285	111.0271
119.8749	125.2861	129.9755
139.1935	157.0036	175.0111

185.4336	191.4069	193.4953
201.8533	207.6705	213.4544
217.2780	219.1151	219.4387
227.2758	252.6221	253.0669
260.7327	278.1038	288.6077
298.9354	302.4024	305.3913
317.8078	321.5190	328.7205
341.1388	364.8086	381.9730
385.7900	399.0727	405.4746
414.8006	431.8049	436.9647
445.7098	452.2200	456.0702
479.7303	484.2080	496.4991
498.4155	503.0817	512.1701
518.1779	526.2504	531.0378
536.8407	542.6887	547.5125
570.0607	582.5525	583.6984
590.6201	596.6459	608.5084
612.5763	618.9613	624.5115
627.6492	632.1980	670.4099
688.5497	697.1823	701.3446
708.1945	710.1086	718.1834
738.3067	746.1428	746.4661
749.4264	754.7388	767.0935
770.5711	771.0347	772.4553
775.0505	784.0509	790.9990
801.3957	823.6277	830.1177
848.2235	852.7843	870.2622
875.5128	880.5449	880.8220
887.0911	893.9302	903.8499
907.5011	909.2526	925.7584

951.8485	953.0631	955.7394
963.1906	970.2565	975.0966
976.3778	981.9300	992.5638
996.7751	1000.7330	1007.3678
1011.6236	1013.2693	1023.7747
1024.6812	1037.4817	1042.3747
1044.4308	1045.4842	1046.4708
1053.5064	1056.1625	1057.8459
1058.8707	1065.5992	1068.1096
1070.7196	1071.9965	1078.3894
1080.5930	1089.1089	1093.6503
1104.6339	1109.3619	1121.5383
1144.9407	1150.1734	1164.5480
1183.1349	1183.6476	1186.3325
1188.4073	1191.1570	1198.2016
1198.5225	1203.6479	1208.4207
1216.9678	1220.5941	1230.0410
1247.6328	1251.9978	1263.5542
1275.2479	1291.4474	1293.9940
1294.4322	1301.8769	1311.8557
1317.3352	1323.0013	1327.3327
1331.9487	1342.6829	1344.9135
1347.0038	1358.1845	1364.1905
1366.4862	1368.8870	1377.8533
1379.1238	1407.0722	1412.5171
1423.1057	1427.8911	1430.0847
1431.8661	1448.5131	1449.4483
1462.1696	1466.7857	1469.8605
1474.0513	1477.7125	1483.6026
1485.4920	1487.0105	1492.4557

1494.0833	1494.4736	1496.5067
1498.6214	1502.5591	1511.1895
1514.2069	1518.3660	1528.2654
1530.4243	1533.0824	1549.1873
1603.3963	1606.0783	1616.2970
1627.9500	1634.1315	1635.7006
1636.3283	1641.2046	1643.4541
1651.6938	1654.0472	1657.8337
1703.4322	3001.3282	3039.2901
3040.2163	3046.0004	3050.0425
3060.0802	3099.3207	3102.4383
3112.5034	3114.1158	3129.2563
3130.1550	3140.4574	3141.1028
3143.7764	3151.2609	3167.6781
3171.1482	3181.3513	3184.3581
3184.9208	3185.3112	3187.1452
3188.6586	3190.5311	3192.7643
3194.2275	3198.6262	3200.2266
3202.2301	3204.0822	3206.9288
3208.2242	3210.7348	3213.9974
3217.6454	3229.1815	3244.6135

TS4RR''' (Φ=78°)

Zero-point correction= 0.729725

Thermal correction to Energy= 0.775792

Thermal correction to Enthalpy= 0.776736

Thermal correction to Gibbs Free Energy= 0.648129

Sum of electronic and zero-point Energies= -5135.058191

Sum of electronic and thermal Energies= -5135.012124

Sum of electronic and thermal Enthalpies= -5135.011179

Sum of electronic and thermal Free Energies= -5135.139787

Cartesian coordinates

C	-1.091662	-0.873902	0.695506
C	0.241785	-0.490119	0.930424
H	-1.294950	-1.289950	-0.286220
C	1.111402	-0.244915	-0.142530
O	0.842475	-0.150833	-1.365097
C	-1.982278	-1.329256	1.762635
C	-3.055092	-2.189702	1.450439
C	-1.820817	-0.926128	3.104085
C	-3.928704	-2.633987	2.439840
H	-3.196698	-2.503731	0.421275
C	-2.695768	-1.373314	4.092352
H	-1.020320	-0.243853	3.368954
C	-3.752079	-2.229374	3.766262
H	-4.749571	-3.294052	2.174666
H	-2.556139	-1.049287	5.119907
H	-4.432334	-2.576064	4.538815
C	2.589173	-0.243873	0.193924
C	4.613835	-0.979021	0.626350
C	2.824505	-2.704096	0.856503
H	1.818241	-2.615006	1.268875
N	4.778017	0.270119	0.283194
N	3.500178	0.711851	-0.000422
N	3.288187	-1.329458	0.592259
C	5.582907	-1.996648	1.131828
H	6.486383	-1.512281	1.504958
H	5.860853	-2.697882	0.333324
C	3.794497	-3.424064	1.877839
O	4.947177	-2.651856	2.227604
C	3.582154	-4.737348	-0.165379

C	2.852113	-3.567237	-0.386285
C	2.234500	-3.313377	-1.612378
C	2.363831	-4.261035	-2.629705
C	3.091742	-5.438901	-2.415236
C	3.704818	-5.684141	-1.184251
C	4.151030	-4.788199	1.229004
H	1.676865	-2.395957	-1.779091
H	3.181850	-6.167952	-3.215469
H	4.271421	-6.596949	-1.022582
H	5.236373	-4.936013	1.237735
H	3.715598	-5.608945	1.808905
C	3.303113	2.085287	-0.386798
C	3.083136	3.030910	0.621673
C	3.402223	2.409201	-1.745049
C	2.976720	4.366808	0.228122
C	3.275799	3.758158	-2.086066
C	3.062716	4.745252	-1.116267
H	2.807376	5.124957	0.987872
H	3.336009	4.041792	-3.133463
C	3.596028	1.334127	-2.780548
H	2.750721	0.637267	-2.751293
H	4.507567	0.755726	-2.591540
H	3.664592	1.763476	-3.782625
C	2.849896	6.180932	-1.520950
H	1.784089	6.356811	-1.715377
H	3.395177	6.429743	-2.436187
H	3.157621	6.874308	-0.732674
C	2.938670	2.615455	2.062360
H	3.801898	2.033166	2.402878
H	2.047711	1.991249	2.195459

H	2.837264	3.487928	2.711208
H	3.274083	-3.558579	2.826071
H	1.892947	-4.084174	-3.592106
H	0.634695	-0.412515	1.938817
C	-5.088740	-0.925748	-1.602044
C	-5.872434	-0.355432	-0.571576
C	-7.230234	-0.636618	-0.419332
C	-7.830004	-1.515727	-1.321513
C	-7.074187	-2.094369	-2.352861
C	-5.719054	-1.809359	-2.500407
C	-3.705660	-0.487910	-1.556018
C	-3.441238	0.409816	-0.491637
H	-7.806158	-0.184100	0.382465
H	-8.885553	-1.750900	-1.221888
H	-7.553250	-2.777356	-3.049004
H	-5.132366	-2.254119	-3.293611
S	-4.914389	0.715417	0.447958
C	-2.690214	-0.927486	-2.487164
O	-2.865894	-1.738195	-3.406542
H	-1.681956	-0.492391	-2.346587
C	-2.180173	0.959775	-0.155726
H	-1.475105	0.936331	-0.976338
C	-1.885592	1.995862	0.826315
C	-0.869403	2.953773	0.586268
C	-2.489494	2.054394	2.104546
C	-0.475981	3.888881	1.541098
C	-2.110982	2.989400	3.063860
H	-3.243406	1.321998	2.362165
C	-1.095815	3.908620	2.790971
H	0.306140	4.599819	1.299944

H	-2.603136	2.988043	4.032077
H	-0.790115	4.638274	3.534598
Br	-0.016996	3.065766	-1.130859

Vibrational frequencies

-178.2398	13.0210	20.7639
20.8211	29.0135	34.3658
38.3585	41.1685	47.1737
48.8403	54.9670	61.5774
64.8015	74.6677	77.9489
78.4387	83.0475	93.6202
94.7098	105.2853	113.2515
119.1854	131.8498	134.5267
136.8207	160.6539	175.1148
181.6716	187.7279	189.6372
195.7817	200.9902	209.2876
216.0842	222.1039	225.9516
230.2886	231.8462	247.9568
251.3339	263.8813	274.6286
288.7911	294.9277	296.0253
318.9098	322.6789	327.7882
344.4178	367.9370	381.5239
381.7701	391.3491	397.1792
425.6586	431.6415	436.4675
448.2441	451.0375	454.7276
471.6179	484.2456	495.9721
499.1422	501.0628	511.5422
518.8754	524.3951	534.4897
535.1202	538.7194	545.1404
564.0482	580.2465	584.9394
590.2563	596.0621	612.4871

615.3821	617.1204	623.3359
631.6398	632.4502	669.1548
687.3015	694.5128	705.4395
708.1593	710.5268	715.7707
735.4244	744.9900	746.5361
749.5944	758.5978	764.1440
770.7737	772.1812	772.7159
777.4000	786.2915	796.0305
805.1446	808.2028	826.1597
852.1004	858.7073	861.5446
872.6998	875.7507	880.9640
882.0341	885.8772	902.8048
908.7852	912.0834	933.5549
940.0975	950.0523	953.5462
961.4826	964.9459	977.6482
980.0252	981.3700	992.3623
995.0620	995.3122	1002.6524
1009.2441	1010.4387	1012.5252
1026.3938	1033.2855	1038.0542
1041.4510	1044.6469	1046.1747
1049.9922	1053.7608	1056.4133
1057.8868	1063.0294	1063.5296
1067.6023	1075.0321	1076.0153
1078.3571	1084.2874	1104.4311
1107.9430	1110.2567	1121.1161
1142.2278	1153.7576	1163.9215
1183.7398	1185.4169	1185.6908
1188.3738	1190.4777	1198.3364
1203.7397	1210.3859	1219.7197
1222.0268	1230.6980	1231.6492

1246.8407	1264.6904	1274.4904
1274.9532	1290.3490	1293.8969
1297.0681	1302.6465	1317.2153
1320.8715	1326.8425	1330.0622
1333.1569	1343.0542	1347.9685
1348.7585	1359.9634	1365.3508
1365.5939	1369.0056	1378.8600
1379.8343	1403.3940	1407.4671
1419.3756	1422.0393	1427.0936
1436.9102	1450.5484	1457.1145
1466.9738	1468.7873	1470.6593
1473.1901	1481.0383	1482.0982
1485.0814	1486.1420	1489.3618
1492.9557	1495.2143	1496.9326
1497.9817	1504.4378	1510.2683
1520.0053	1527.7165	1530.8481
1533.1653	1543.0686	1560.6426
1601.2659	1606.3704	1616.9206
1627.2949	1633.6642	1634.8107
1635.0288	1641.2330	1644.5363
1651.5668	1654.2408	1658.4968
1688.4652	2952.6101	3036.5678
3042.2088	3042.9807	3045.0862
3059.6532	3097.0630	3101.1789
3102.4954	3106.2604	3122.3544
3130.4801	3135.4034	3139.5815
3141.7402	3151.9655	3180.9916
3182.1175	3182.8417	3182.8777
3185.5203	3185.5346	3188.5622
3190.2673	3192.8093	3192.8169

3197.9282	3200.5143	3201.6809
3203.6218	3206.2078	3209.7036
3210.0415	3210.3934	3213.7241
3221.6726	3234.6147	3243.0073

TS4RS (Φ=21°)

Zero-point correction= 0.729640

Thermal correction to Energy= 0.775720

Thermal correction to Enthalpy= 0.776664

Thermal correction to Gibbs Free Energy= 0.648864

Sum of electronic and zero-point Energies= -5135.060256

Sum of electronic and thermal Energies= -5135.014176

Sum of electronic and thermal Enthalpies= -5135.013232

Sum of electronic and thermal Free Energies= -5135.141032

Cartesian coordinates

C	1.398079	0.590294	-0.915956
C	0.048353	0.885403	-0.725213
H	1.624456	-0.395660	-1.304628
C	-0.932002	-0.127773	-0.800222
O	-0.720213	-1.364764	-0.873042
C	2.396560	1.628773	-1.193402
C	3.539985	1.294843	-1.944286
C	2.249004	2.962728	-0.760497
C	4.491454	2.260595	-2.270438
H	3.672893	0.269223	-2.275460
C	3.203708	3.923220	-1.081555
H	1.398410	3.238626	-0.148608
C	4.326740	3.579751	-1.843106
H	5.362647	1.980943	-2.855920
H	3.073284	4.945245	-0.736352
H	5.067470	4.333231	-2.094732

C	-2.375732	0.292433	-0.904473
C	-4.547805	0.184130	-1.257144
C	-3.410343	-2.019141	-1.456575
H	-2.444321	-2.260813	-1.891613
N	-4.317603	1.444263	-1.006674
N	-2.962801	1.501921	-0.782288
N	-3.395653	-0.555728	-1.209156
C	-5.806398	-0.482892	-1.697532
H	-6.521363	0.259183	-2.055164
H	-6.262346	-1.045346	-0.871460
C	-4.598103	-2.412841	-2.427293
O	-5.449974	-1.323568	-2.791313
C	-4.764931	-3.657431	-0.338361
C	-3.666947	-2.806299	-0.189659
C	-2.939136	-2.762193	0.999876
C	-3.343965	-3.578188	2.057874
C	-4.450902	-4.425872	1.920647
C	-5.164161	-4.474936	0.720800
C	-5.364887	-3.560570	-1.716345
H	-2.069689	-2.121640	1.092828
H	-4.753474	-5.054689	2.753237
H	-6.017914	-5.138229	0.612846
H	-6.438447	-3.342931	-1.699575
H	-5.241033	-4.498263	-2.268945
C	-2.388538	2.785747	-0.468715
C	-1.896876	3.573255	-1.520836
C	-2.366438	3.186297	0.870537
C	-1.331224	4.803133	-1.182200
C	-1.794482	4.430561	1.155530
C	-1.266008	5.243776	0.147732

H	-0.925636	5.428778	-1.972874
H	-1.752058	4.761935	2.189171
C	-2.915303	2.290830	1.947984
H	-2.410372	1.320499	1.942298
H	-3.984126	2.102677	1.796741
H	-2.779558	2.738430	2.934210
C	-0.597865	6.554597	0.479567
H	-0.850146	7.328286	-0.252529
H	0.493612	6.443185	0.467992
H	-0.883092	6.912496	1.472703
C	-1.919422	3.071791	-2.939747
H	-2.917968	2.728966	-3.230553
H	-1.235167	2.222497	-3.053104
H	-1.606499	3.854100	-3.634550
H	-4.176593	-2.744279	-3.376323
H	-2.789692	-3.559328	2.990440
H	-0.257808	1.904978	-0.565186
C	4.773652	-2.617082	-0.566110
C	5.765248	-1.684790	-0.173615
C	7.115477	-1.851471	-0.487189
C	7.492715	-2.982966	-1.208850
C	6.528173	-3.920931	-1.610778
C	5.182286	-3.748265	-1.299992
C	3.435634	-2.218270	-0.159346
C	3.417602	-1.015758	0.574442
H	7.853420	-1.118359	-0.175405
H	8.538195	-3.135968	-1.459988
H	6.836272	-4.797080	-2.174538
H	4.435244	-4.465889	-1.613051
S	5.056663	-0.350785	0.726214

C	2.224751	-2.881415	-0.612471
O	2.196188	-3.940994	-1.249676
H	1.279257	-2.363307	-0.382157
C	2.369909	-0.224389	1.132979
H	2.676459	0.783857	1.393250
C	1.271679	-0.708746	1.957120
C	0.368276	0.186346	2.582713
C	1.082093	-2.075143	2.284640
C	-0.644506	-0.234885	3.445368
C	0.071799	-2.509654	3.129444
H	1.777343	-2.803621	1.885377
C	-0.809064	-1.591207	3.712889
H	-1.290311	0.499134	3.913526
H	-0.021271	-3.569351	3.347501
H	-1.599166	-1.919648	4.380310
Br	0.571658	2.093135	2.382586

Vibrational frequencies

-118.6718	20.7338	24.8197
25.6552	28.6827	35.8550
38.0595	45.7290	47.5293
49.1991	54.3490	61.5773
63.4537	71.1424	77.1457
83.5250	84.7155	87.6446
97.9962	104.2413	118.2816
122.8600	125.8662	141.6085
141.7645	152.2275	154.1553
158.5384	178.8342	185.3630
193.7447	199.1519	209.0227
214.4779	218.0379	218.8017
239.3537	244.7380	257.4138

264.0514	279.4398	286.7929
289.3956	296.9223	310.8244
320.3758	323.9084	339.2756
356.3478	367.5755	381.6853
387.8100	389.7662	392.3995
410.5457	417.3436	435.0274
445.6087	449.4309	453.2823
462.6181	476.9879	492.4936
500.0238	508.7197	514.9375
522.6648	527.1303	530.4862
531.3779	537.5070	555.3021
555.3469	569.8566	583.4582
588.0658	598.9240	605.1041
609.9985	620.6238	631.6145
635.3790	645.4598	661.0121
671.9487	683.6975	694.7100
703.4964	708.6411	713.8613
729.7053	735.9681	746.7015
750.2320	752.6230	761.5269
764.8833	767.8660	772.4992
772.7791	781.8198	794.8147
801.0277	826.1684	831.2306
850.2887	851.8049	857.1328
870.6189	873.0815	879.4369
880.6883	882.3592	900.2147
903.2578	908.5753	918.4219
921.3524	948.9962	952.9565
960.3231	962.4445	972.3472
973.1496	977.1200	992.6980
996.9628	997.6017	999.4293

1003.3292	1007.5124	1013.6772
1021.6823	1037.2524	1039.4484
1041.5045	1045.1231	1047.0740
1053.5013	1054.5499	1055.1575
1057.0700	1058.2144	1060.2005
1065.4490	1067.8641	1075.2521
1076.6818	1090.9147	1102.5982
1107.1679	1112.5675	1121.6874
1144.7749	1150.9400	1153.3350
1180.9588	1183.7898	1185.5502
1185.8029	1192.4031	1195.6761
1199.8087	1201.6191	1212.2075
1213.6534	1223.3704	1239.9193
1243.1220	1254.3234	1274.7642
1286.4144	1288.4653	1291.0772
1295.3001	1305.0932	1310.8796
1317.1567	1326.9574	1328.2293
1331.0781	1337.5310	1344.0105
1347.6882	1357.5910	1366.9726
1367.1924	1369.8103	1379.1301
1382.5598	1408.5786	1415.5715
1419.2056	1425.1023	1426.3383
1436.6434	1447.4543	1448.8428
1455.2781	1469.2088	1471.5146
1472.1712	1475.2158	1481.0943
1482.8437	1486.8319	1488.3216
1492.4397	1493.4454	1494.6432
1496.3126	1498.8972	1507.7500
1510.2318	1513.8093	1520.5918
1526.2099	1533.6522	1570.0199

1593.9875	1604.2718	1608.3527
1628.1144	1633.5016	1635.6009
1638.0356	1640.5177	1641.6640
1651.8555	1654.1201	1657.7457
1692.8628	3019.9613	3040.6556
3043.5648	3044.4588	3051.6470
3058.1872	3095.2991	3101.8199
3105.9039	3115.2192	3131.4513
3131.9794	3142.5224	3149.6223
3155.4919	3171.7788	3173.5647
3180.3159	3183.2067	3184.0055
3184.8983	3188.1440	3191.4465
3192.1824	3193.2916	3198.1016
3198.4620	3205.9064	3206.4779
3207.6041	3212.3427	3214.2885
3219.5819	3220.4311	3225.3239
3226.6464	3243.9319	3295.0148

TS4RS' (Φ=171°)

Zero-point correction= 0.730070

Thermal correction to Energy= 0.776052

Thermal correction to Enthalpy= 0.776996

Thermal correction to Gibbs Free Energy= 0.648046

Sum of electronic and zero-point Energies= -5135.049122

Sum of electronic and thermal Energies= -5135.003140

Sum of electronic and thermal Enthalpies= -5135.002196

Sum of electronic and thermal Free Energies= -5135.131146

Cartesian coordinates

C	0.755465	-1.457843	-0.518092
C	-0.225203	-0.464473	-0.777985
H	0.514788	-2.107055	0.312604

C	-1.076589	-0.050153	0.246471
O	-1.035603	-0.356135	1.469011
C	1.549506	-2.087940	-1.573456
C	2.173762	-3.324808	-1.308255
C	1.743515	-1.499680	-2.838330
C	2.967216	-3.945133	-2.268222
H	2.032884	-3.783147	-0.333947
C	2.529671	-2.129441	-3.802992
H	1.290519	-0.540816	-3.066010
C	3.148825	-3.348867	-3.522056
H	3.444871	-4.894168	-2.041874
H	2.673689	-1.656233	-4.769901
H	3.769053	-3.832011	-4.271361
C	-2.289236	0.763832	-0.159250
C	-4.312434	1.247762	-0.872912
C	-3.514373	-1.032593	-1.502237
H	-2.526231	-1.369987	-1.819248
N	-3.945626	2.291316	-0.179135
N	-2.682026	1.966108	0.274928
N	-3.325454	0.294543	-0.888046
C	-5.535180	0.980851	-1.687215
H	-6.036358	1.914036	-1.948391
H	-6.238382	0.346499	-1.130465
C	-4.507431	-0.931910	-2.728344
O	-5.091232	0.364135	-2.894264
C	-5.311051	-2.574749	-1.115933
C	-4.168727	-2.007453	-0.546309
C	-3.744422	-2.353414	0.738398
C	-4.493523	-3.289773	1.453929
C	-5.638634	-3.866465	0.888601

C	-6.053624	-3.514182	-0.397905
C	-5.562227	-2.048919	-2.505648
H	-2.860816	-1.897997	1.177765
H	-6.210493	-4.593940	1.457637
H	-6.944146	-3.960511	-0.831746
H	-6.571727	-1.642796	-2.631010
H	-5.442571	-2.837521	-3.256638
C	-1.956316	2.907669	1.089088
C	-1.242071	3.928963	0.447592
C	-2.055334	2.792497	2.482831
C	-0.579992	4.850711	1.263693
C	-1.356232	3.728779	3.250291
C	-0.611579	4.756892	2.660608
H	-0.034458	5.666751	0.798661
H	-1.405264	3.658011	4.333596
C	-2.889482	1.710914	3.116797
H	-2.481856	0.727971	2.861049
H	-3.922368	1.747481	2.751840
H	-2.906305	1.819563	4.203694
C	0.158453	5.735401	3.511119
H	0.247132	6.709777	3.021298
H	1.176170	5.367888	3.692864
H	-0.315257	5.879519	4.486635
C	-1.177241	4.019548	-1.055165
H	-2.169030	3.925538	-1.508155
H	-0.549400	3.220942	-1.466027
H	-0.747091	4.972725	-1.368774
H	-3.950826	-1.086897	-3.652590
H	-4.184919	-3.573323	2.455836
H	-0.316632	0.002597	-1.752294

C	3.470987	2.181670	-1.503185
C	2.551690	2.986225	-0.786526
C	2.349749	4.335702	-1.084889
C	3.076870	4.902300	-2.129169
C	3.989237	4.123267	-2.859433
C	4.191492	2.780276	-2.557280
C	3.504652	0.807629	-1.027901
C	2.649271	0.589775	0.071270
H	1.645863	4.927826	-0.512158
H	2.937574	5.951205	-2.374077
H	4.550632	4.576962	-3.671548
H	4.895523	2.178212	-3.116124
S	1.751956	2.059570	0.474258
C	4.272861	-0.237492	-1.686871
O	5.061330	-0.056485	-2.619184
H	4.112403	-1.257960	-1.307083
C	2.280689	-0.567137	0.837212
H	1.473137	-0.380837	1.543124
C	3.240193	-1.566356	1.346421
C	2.847101	-2.673300	2.136966
C	4.638571	-1.439584	1.169873
C	3.747704	-3.617487	2.628464
C	5.551929	-2.366129	1.658590
H	5.018150	-0.562779	0.660812
C	5.110834	-3.478918	2.376562
H	3.378665	-4.452646	3.213327
H	6.612418	-2.209228	1.484961
H	5.810853	-4.217981	2.753299
Br	1.005664	-2.934384	2.645093

Vibrational frequencies

-215.8201	12.8668	16.5916
18.9921	24.6676	28.5538
36.6305	38.5312	46.4142
52.1601	52.7299	62.4164
67.2043	71.9303	77.2874
86.7296	89.3231	91.4169
103.6948	109.6943	116.5035
120.3556	129.5823	136.5925
145.5861	151.5479	160.5854
160.9312	169.8658	191.1978
193.9997	204.1496	210.9493
216.3415	218.3015	223.3491
231.1786	239.1071	252.8594
261.1022	277.7409	286.9188
292.2400	298.5296	314.1915
321.9552	327.3682	333.0426
354.8713	367.5992	380.4986
390.3289	395.9531	414.3918
421.5001	434.5125	438.8086
446.9757	453.2968	459.6263
476.6669	485.1635	497.6501
499.0245	502.5969	511.3575
518.1666	524.8292	528.0941
534.5088	539.0582	541.8929
567.2341	580.5784	583.1639
591.2447	595.6632	611.8063
612.7935	615.0371	623.0297
632.1781	644.9377	667.6286
673.8719	696.8367	703.4387
710.2565	710.4822	715.5597

733.5142	741.5021	744.6716
747.2909	749.1840	765.6168
769.9607	771.0452	772.1422
773.0832	782.3167	790.2093
800.5666	824.3745	833.3916
850.4835	862.1090	867.9204
870.5854	881.3319	881.8822
884.3427	890.8207	899.4914
908.9459	916.0732	934.4965
954.5397	955.1524	960.4050
964.0064	973.4682	974.9141
981.5720	983.9964	990.3206
996.3029	1000.3601	1008.0474
1011.7875	1012.3698	1013.7495
1028.0233	1037.3915	1041.3825
1042.6592	1044.1269	1050.3254
1051.4949	1054.3395	1056.0091
1058.7158	1061.8368	1063.4564
1065.7648	1070.0452	1074.4742
1083.2509	1085.4595	1095.1658
1103.5144	1110.6687	1121.2679
1145.0978	1152.2677	1163.0389
1183.7257	1184.9801	1187.3032
1189.3190	1195.9969	1199.0978
1199.7117	1203.9221	1210.5311
1220.0261	1227.4895	1231.6170
1247.6823	1250.0764	1267.0344
1274.8045	1290.5112	1295.1036
1295.9474	1303.8365	1309.2683
1318.5523	1324.7486	1330.6039

1332.6678	1343.2615	1344.0153
1346.7602	1359.4605	1367.7152
1368.6762	1369.2345	1381.3127
1381.9783	1407.6889	1415.5622
1417.1163	1422.7375	1433.1795
1435.1671	1446.1736	1452.3515
1464.3857	1468.2916	1470.1826
1474.1433	1475.9993	1484.2967
1485.9557	1486.3996	1486.4798
1491.3401	1492.4273	1494.2142
1499.0833	1506.5009	1508.9919
1511.9334	1516.2048	1527.5162
1530.7862	1532.2177	1555.3702
1601.7347	1603.7805	1616.1562
1626.6172	1634.0064	1636.3312
1637.4681	1640.1145	1640.9833
1652.1689	1652.8130	1657.0019
1701.9247	3026.2299	3039.6364
3040.0302	3044.1499	3050.3334
3059.7868	3097.9690	3102.8984
3111.4846	3112.7821	3120.5539
3130.1932	3135.4445	3137.4779
3141.0510	3145.0421	3151.3921
3181.6826	3183.3792	3183.8922
3184.3726	3186.2913	3188.8721
3189.2432	3191.3064	3197.3601
3197.7799	3199.8547	3200.5236
3205.7975	3206.4910	3209.2937
3214.8540	3219.2363	3224.5619
3229.6166	3230.1833	3246.7426

TS4RS" (Φ= -163°)

TS4RS"

Zero-point correction= 0.731114

Thermal correction to Energy= 0.776648

Thermal correction to Enthalpy= 0.777592

Thermal correction to Gibbs Free Energy= 0.651940

Sum of electronic and zero-point Energies= -5135.055903

Sum of electronic and thermal Energies= -5135.010369

Sum of electronic and thermal Enthalpies= -5135.009425

Sum of electronic and thermal Free Energies= -5135.135077

Cartesian coordinates

C	1.511212	-0.711473	-1.300964
C	0.311597	0.030469	-1.261500
H	1.387612	-1.778797	-1.440995
C	-0.924468	-0.613801	-1.100085
O	-1.103319	-1.842856	-0.878605
C	2.739820	-0.145713	-1.882408
C	3.759674	-1.009128	-2.329283
C	2.937688	1.242345	-2.040584
C	4.937562	-0.509020	-2.881831
H	3.621796	-2.080074	-2.240181
C	4.114144	1.741161	-2.593898
H	2.172214	1.942252	-1.725657
C	5.123979	0.869067	-3.012709
H	5.709259	-1.198537	-3.212120
H	4.241653	2.815129	-2.697661
H	6.042132	1.260114	-3.441514
C	-2.172310	0.217525	-1.283851
C	-4.293532	0.744212	-1.580757
C	-3.921221	-1.687708	-1.198494

H	-3.135561	-2.334183	-1.580514
N	-3.661855	1.884245	-1.640167
N	-2.342706	1.548540	-1.446787
N	-3.429037	-0.297968	-1.368459
C	-5.734542	0.442411	-1.818858
H	-6.203445	1.256784	-2.373156
H	-6.269544	0.312046	-0.868150
C	-5.289101	-1.898868	-1.966258
O	-5.778775	-0.729685	-2.626307
C	-5.567215	-2.394486	0.405263
C	-4.242208	-1.981928	0.249988
C	-3.378831	-1.881265	1.341173
C	-3.872238	-2.181595	2.611863
C	-5.204303	-2.584405	2.778481
C	-6.056852	-2.699131	1.677471
C	-6.287931	-2.460049	-0.916125
H	-2.345336	-1.592970	1.191324
H	-5.575967	-2.815287	3.772822
H	-7.086968	-3.018711	1.809219
H	-7.214846	-1.876162	-0.925334
H	-6.563209	-3.489832	-1.167875
C	-1.372722	2.607697	-1.342716
C	-0.670281	3.001176	-2.487379
C	-1.152984	3.160548	-0.072917
C	0.337920	3.956499	-2.317609
C	-0.131759	4.104064	0.043866
C	0.637198	4.495684	-1.060834
H	0.918284	4.263298	-3.183575
H	0.081803	4.525036	1.021188
C	-1.980961	2.729382	1.107924

H	-1.887287	1.653696	1.284755
H	-3.042923	2.937762	0.936334
H	-1.667049	3.245910	2.015023
C	1.799534	5.436761	-0.875911
H	1.530444	6.287085	-0.240328
H	2.165088	5.821917	-1.831947
H	2.620843	4.907534	-0.378449
C	-0.928495	2.350533	-3.820176
H	-1.999091	2.294691	-4.041676
H	-0.537674	1.325679	-3.821684
H	-0.435479	2.900737	-4.624928
H	-5.126983	-2.609125	-2.777206
H	-3.217266	-2.110849	3.475659
H	0.346061	1.101357	-1.350912
C	0.896309	1.775246	2.876418
C	-0.118779	0.902323	3.332979
C	-1.084251	1.295918	4.262133
C	-1.028113	2.595919	4.759731
C	-0.026233	3.480523	4.325703
C	0.927455	3.085414	3.391961
C	1.770705	1.147600	1.897713
C	1.467221	-0.200362	1.664675
H	-1.857335	0.606861	4.588338
H	-1.763224	2.924461	5.488285
H	0.005155	4.490263	4.724794
H	1.696371	3.765968	3.051080
S	0.019048	-0.671880	2.568661
C	2.774683	1.870769	1.137461
O	3.014989	3.076203	1.248238
H	3.329337	1.270405	0.401559

C	2.037046	-1.234456	0.835214
H	1.374279	-2.091546	0.759188
C	3.445266	-1.636887	0.883663
C	3.885202	-2.862896	0.325593
C	4.462284	-0.879709	1.512970
C	5.214050	-3.277514	0.335929
C	5.793358	-1.278781	1.535731
H	4.190432	0.032782	2.027532
C	6.185191	-2.476795	0.934575
H	5.484494	-4.222566	-0.121815
H	6.526433	-0.651419	2.034330
H	7.223374	-2.793095	0.937930
Br	2.632879	-4.073292	-0.509456

Vibrational frequencies

-229.0817	20.1207	22.6782
27.9454	31.7966	37.2523
43.2028	46.1180	49.0417
57.1721	60.3633	67.4033
70.2457	72.7663	78.5622
84.1474	92.0948	103.2259
112.5384	115.0484	124.4497
127.5966	135.9095	144.1173
145.1227	152.5930	157.9144
187.7295	192.0274	197.0080
205.4233	208.3472	216.8551
219.3805	220.0063	222.8419
235.8974	251.0001	258.1508
264.9011	277.0894	290.9158
294.0972	303.2244	314.9719
321.4760	326.6575	350.3965

358.4646	370.7053	384.4298
388.6546	391.3961	402.0792
409.4268	434.5723	439.1322
444.5787	451.5710	460.6417
467.9260	479.6498	493.9423
504.0711	512.4486	515.2231
526.5395	532.0988	532.9855
534.1348	538.5471	558.3535
563.5472	570.7210	584.0389
585.8293	597.8157	607.1209
610.7304	623.3364	632.5364
641.1846	644.9884	663.0677
671.3717	675.9527	692.7810
710.8977	714.7250	716.2981
732.6367	739.9934	746.5210
749.1729	752.7315	762.7272
765.7044	768.9757	770.6176
772.1505	779.5488	792.0387
799.2061	825.2010	834.8294
854.5372	867.2228	872.6080
874.5246	875.5149	877.6821
880.5224	882.7579	902.7244
903.2641	908.4590	951.2104
952.0261	953.7013	959.5190
962.6577	967.6180	974.6421
978.0600	993.0768	993.2692
993.7317	996.6754	1001.4196
1007.5561	1013.1341	1018.7638
1026.0796	1037.0703	1040.3791
1042.3169	1043.2644	1049.6596

1051.3082	1054.3456	1056.3755
1058.9841	1064.0814	1065.3048
1069.6548	1071.3687	1075.0127
1081.9652	1097.1268	1104.1268
1108.5346	1115.6748	1121.9507
1144.6395	1152.1493	1152.7643
1181.0451	1185.6415	1185.9713
1186.7345	1193.7019	1195.9854
1200.0763	1200.5750	1214.5662
1218.6522	1223.0616	1238.0444
1241.2033	1250.0206	1272.6509
1273.8576	1286.8152	1293.0624
1298.8485	1305.0873	1310.5734
1314.4070	1323.6381	1326.8753
1327.5512	1334.9298	1342.9137
1348.8720	1360.1983	1368.8399
1371.5207	1375.0215	1377.1479
1381.4286	1409.9039	1417.1074
1420.0139	1422.2199	1428.1353
1433.5768	1444.8345	1446.6462
1452.4131	1469.1350	1469.6477
1474.5589	1476.3107	1483.7089
1485.4776	1486.5109	1488.0162
1490.4434	1494.6531	1495.9542
1497.1988	1498.3954	1508.0752
1509.4527	1520.4080	1523.1683
1527.5718	1535.9641	1560.8728
1599.2649	1604.7834	1607.8372
1627.0936	1635.7875	1637.8787
1639.7283	1640.1247	1641.8289

1652.5085	1653.3146	1658.0410
1701.1527	3036.9955	3038.5875
3042.2473	3043.0496	3051.9831
3059.5334	3095.9539	3106.2157
3107.0141	3110.6455	3129.4866
3131.8847	3141.1508	3152.0457
3161.6526	3166.0898	3170.5020
3181.0333	3181.9852	3186.4510
3186.8357	3190.2394	3191.0711
3192.2232	3196.3280	3200.7964
3204.1062	3204.3793	3206.4463
3208.6759	3208.9425	3219.4866
3219.5922	3225.8856	3234.5046
3236.2134	3245.6725	3307.3761

TS4RS''' (Φ=24°)

Zero-point correction= 0.730309

Thermal correction to Energy= 0.776091

Thermal correction to Enthalpy= 0.777035

Thermal correction to Gibbs Free Energy= 0.649832

Sum of electronic and zero-point Energies= -5135.051846

Sum of electronic and thermal Energies= -5135.006064

Sum of electronic and thermal Enthalpies= -5135.005120

Sum of electronic and thermal Free Energies= -5135.132323

Cartesian coordinates

C	1.177975	0.791390	0.702261
C	-0.166285	0.498494	0.863415
H	1.542608	0.859023	-0.315784
C	-0.990226	0.152834	-0.236078
O	-0.662871	-0.151099	-1.400000
C	1.995395	1.445549	1.720024

C	3.091262	2.230675	1.310928
C	1.717936	1.349234	3.099611
C	3.865549	2.919000	2.243576
H	3.325866	2.298695	0.252935
C	2.499583	2.028930	4.028518
H	0.913253	0.707021	3.439336
C	3.571385	2.824530	3.605347
H	4.703000	3.522640	1.905965
H	2.276708	1.937396	5.087886
H	4.176381	3.356435	4.333851
C	-2.475996	0.347344	0.013115
C	-4.412219	1.322667	0.367369
C	-2.459346	2.861634	0.530916
H	-1.468637	2.716749	0.962200
N	-4.709869	0.091524	0.051212
N	-3.486955	-0.502707	-0.186074
N	-3.054624	1.519317	0.361741
C	-5.276614	2.464788	0.788393
H	-6.230824	2.101721	1.172595
H	-5.469457	3.133857	-0.061625
C	-3.362810	3.748847	1.476588
O	-4.593537	3.123496	1.851660
C	-3.027273	4.859821	-0.667503
C	-2.406200	3.614223	-0.781363
C	-1.830120	3.191781	-1.980494
C	-1.885658	4.048116	-3.081765
C	-2.504310	5.300944	-2.975409
C	-3.075821	5.715284	-1.769907
C	-3.567250	5.089086	0.720329
H	-1.356986	2.217036	-2.061559

H	-2.540366	5.956677	-3.840598
H	-3.557400	6.685965	-1.692550
H	-4.626840	5.365935	0.725188
H	-3.026006	5.894590	1.228341
C	-3.461374	-1.896605	-0.553606
C	-3.543594	-2.849465	0.468299
C	-3.459748	-2.221273	-1.918722
C	-3.631466	-4.190899	0.081614
C	-3.528770	-3.576181	-2.246768
C	-3.621507	-4.570540	-1.263577
H	-3.696699	-4.953528	0.852755
H	-3.519118	-3.862395	-3.295227
C	-3.388795	-1.151029	-2.975665
H	-2.445148	-0.602636	-2.893201
H	-4.203611	-0.426480	-2.863412
H	-3.456476	-1.587351	-3.974737
C	-3.683977	-6.023326	-1.662824
H	-4.514227	-6.208478	-2.353584
H	-3.810601	-6.675420	-0.794530
H	-2.765162	-6.323532	-2.180191
C	-3.494638	-2.455050	1.921731
H	-4.182592	-1.633762	2.146095
H	-2.485734	-2.130826	2.202751
H	-3.756482	-3.302399	2.559839
H	-2.847137	3.899468	2.424943
H	-1.445984	3.740131	-4.025529
H	-0.648742	0.615259	1.826866
C	5.096828	0.113997	-1.735092
C	5.939903	0.150643	-0.596821
C	7.236902	0.662633	-0.641723

C	7.718381	1.147895	-1.858149
C	6.903250	1.122342	-3.000075
C	5.606538	0.615886	-2.949084
C	3.774495	-0.416202	-1.442133
C	3.631060	-0.835748	-0.096231
H	7.857838	0.681037	0.249122
H	8.727462	1.545141	-1.916989
H	7.288608	1.504209	-3.941567
H	4.972304	0.601713	-3.825901
S	5.128850	-0.519504	0.813895
C	2.660282	-0.331273	-2.361861
O	2.734923	0.035973	-3.542825
H	1.672775	-0.591327	-1.942855
C	2.556764	-1.369574	0.651092
H	2.679794	-1.308237	1.727671
C	1.606408	-2.382003	0.230872
C	0.572478	-2.840040	1.084501
C	1.701525	-3.068842	-1.007656
C	-0.299380	-3.870906	0.741005
C	0.832063	-4.085728	-1.369844
H	2.507951	-2.803487	-1.681263
C	-0.185884	-4.491608	-0.500051
H	-1.064177	-4.182884	1.441691
H	0.957469	-4.577017	-2.330555
H	-0.875641	-5.281942	-0.773877
Br	0.376065	-2.124413	2.870906

Vibrational frequencies

-12.4320	15.7366	19.2888
23.0818	30.8654	35.4981
36.2637	42.0580	45.4009

51.9284	58.7611	65.0776
71.6667	77.0263	79.4559
85.6605	93.6012	96.6085
113.6574	114.8288	118.5584
124.1282	125.4167	132.7319
144.6233	149.5176	159.2213
186.0268	195.0435	203.3283
208.6318	211.5447	214.2622
218.0182	225.2540	231.2521
240.7477	245.6411	254.6659
264.8419	279.1052	288.0410
291.3619	297.9243	309.1451
318.6819	320.5847	327.3265
348.7239	360.0572	380.9443
384.8427	395.7079	398.5574
419.7790	433.2533	434.2477
443.4226	452.0327	453.7695
464.8536	485.7857	486.9499
498.9634	501.2957	511.3292
518.8647	525.2066	528.2921
530.2078	538.2060	543.8025
556.5563	581.6531	583.3569
586.7505	595.4979	602.4741
611.4796	617.6787	624.0748
631.5945	632.3940	669.2860
679.6304	694.6341	700.9788
707.7625	708.6915	716.6694
733.5651	737.3359	747.0376
747.8499	765.1726	766.2344
769.1773	771.4600	772.1515

773.7608	791.2118	795.1558
802.3197	826.7240	838.2170
843.9834	849.6780	855.2018
871.3910	880.1436	880.4080
881.1052	882.9426	904.3005
908.4331	911.7034	913.4668
925.9277	947.0820	953.6361
962.0659	962.9009	977.4826
978.5854	980.5763	992.7737
994.0193	994.4951	998.2260
1003.6005	1009.3552	1012.1075
1016.4524	1037.0892	1039.2006
1042.8548	1045.4333	1051.1562
1054.6765	1056.6022	1056.9251
1057.9991	1058.5497	1065.2443
1071.2421	1075.0031	1077.3882
1078.4426	1084.3926	1093.5345
1105.2986	1113.4504	1121.1253
1144.5507	1149.9499	1155.6433
1182.6527	1184.2221	1186.6827
1187.7549	1192.8960	1197.6418
1204.5565	1206.0491	1211.2806
1219.1196	1230.3390	1237.3970
1246.1564	1255.8053	1271.1096
1292.4308	1294.8331	1296.7472
1297.3255	1302.0428	1317.3216
1318.5697	1328.7790	1330.0230
1330.9515	1341.5975	1342.5854
1350.2390	1356.3465	1368.0917
1368.5233	1368.8597	1374.6911

1379.2952	1406.6085	1418.4925
1422.2908	1430.5503	1433.6465
1436.4072	1452.0646	1459.5030
1464.9043	1471.2603	1471.7386
1475.7244	1479.3570	1479.7832
1486.7099	1488.7059	1492.8974
1494.5715	1496.6801	1498.1255
1499.8011	1506.2154	1514.7256
1515.8373	1522.4931	1527.0166
1533.8649	1536.0946	1576.7585
1594.6954	1604.2188	1622.4600
1633.1964	1635.0348	1635.6125
1640.2590	1642.5202	1644.2766
1652.8969	1655.1851	1658.0586
1685.4117	3001.0304	3040.4208
3043.9298	3046.0316	3046.9198
3062.1783	3098.7271	3101.0741
3110.0334	3113.2465	3129.9854
3130.6839	3137.8510	3139.5303
3143.6643	3155.8206	3174.8777
3181.4784	3183.6554	3184.8459
3185.0383	3189.9111	3190.2043
3191.1467	3191.6250	3192.4272
3200.0185	3201.8078	3205.0245
3208.6384	3210.1501	3210.5103
3215.2415	3219.2109	3221.2538
3224.7863	3229.0718	3239.3945

TS4SR (Φ= -29°)

Zero-point correction= 0.729078

Thermal correction to Energy= 0.775532

Thermal correction to Enthalpy= 0.776476

Thermal correction to Gibbs Free Energy= 0.646500

Sum of electronic and zero-point Energies= -5135.064743

Sum of electronic and thermal Energies= -5135.018289

Sum of electronic and thermal Enthalpies= -5135.017345

Sum of electronic and thermal Free Energies= -5135.147321

Cartesian coordinates

C	-1.374471	0.242145	-0.567843
C	-0.070459	0.725080	-0.306302
H	-1.411641	-0.633307	-1.211193
C	1.060980	-0.047459	-0.590776
O	1.114100	-1.224357	-1.041015
C	-2.499328	1.182827	-0.720404
C	-3.517996	0.908564	-1.649173
C	-2.606276	2.349907	0.061690
C	-4.592386	1.783670	-1.815476
H	-3.461699	0.001942	-2.244561
C	-3.678653	3.222164	-0.103564
H	-1.863680	2.547499	0.827396
C	-4.675175	2.945699	-1.047174
H	-5.369633	1.549346	-2.537047
H	-3.745891	4.113579	0.513782
H	-5.513764	3.624737	-1.170036
C	2.394373	0.608084	-0.342408
C	4.538635	0.864332	0.076638
C	3.775955	-1.496097	0.174104
H	2.826861	-1.940009	0.469878
N	4.105903	2.072512	-0.166538
N	2.765806	1.897617	-0.439929
N	3.529045	-0.057475	-0.029104

C	5.857421	0.383193	0.583341
H	6.438229	1.215597	0.982698
H	6.435624	-0.102753	-0.213230
C	4.879559	-1.707556	1.283370
O	5.564922	-0.506827	1.660281
C	5.509830	-2.864573	-0.761978
C	4.348183	-2.150452	-1.065234
C	3.839269	-2.103980	-2.362895
C	4.529110	-2.780310	-3.371464
C	5.698264	-3.494556	-3.077014
C	6.193066	-3.545530	-1.771109
C	5.838051	-2.781546	0.707170
H	2.919446	-1.564863	-2.562272
H	6.224712	-4.014984	-3.872126
H	7.098771	-4.101726	-1.545579
H	6.877865	-2.502491	0.905181
H	5.665162	-3.743941	1.202587
C	1.946333	3.031484	-0.779656
C	1.559426	3.897881	0.254312
C	1.530189	3.185493	-2.108325
C	0.689473	4.938633	-0.078257
C	0.658149	4.242813	-2.385314
C	0.214525	5.114200	-1.384558
H	0.360773	5.616400	0.705114
H	0.309396	4.378349	-3.405518
C	1.961505	2.226195	-3.187133
H	1.392416	1.291053	-3.125309
H	3.022674	1.970724	-3.103419
H	1.789070	2.655915	-4.176683
C	-0.791060	6.194636	-1.692300

H	-1.807366	5.832480	-1.491574
H	-0.751882	6.495752	-2.743047
H	-0.631930	7.081097	-1.070850
C	2.014471	3.674098	1.672955
H	3.105476	3.640919	1.748055
H	1.628630	2.723630	2.057076
H	1.647951	4.469677	2.325919
H	4.405004	-2.038695	2.206964
H	4.154589	-2.756190	-4.390662
H	0.057617	1.711516	0.109906
C	-5.394435	-1.952961	-0.271607
C	-4.703217	-3.020013	-0.889495
C	-5.334026	-3.935799	-1.732964
C	-6.697086	-3.775939	-1.977099
C	-7.405297	-2.720661	-1.379999
C	-6.771355	-1.814518	-0.534837
C	-4.528840	-1.149026	0.572466
C	-3.193887	-1.592105	0.590816
H	-4.777696	-4.748050	-2.190895
H	-7.209922	-4.471949	-2.634236
H	-8.467005	-2.608435	-1.580884
H	-7.314210	-0.998669	-0.075920
S	-2.997545	-3.016525	-0.451030
C	-4.991843	-0.003918	1.336050
O	-6.125628	0.476484	1.280200
H	-4.253447	0.444667	2.026252
C	-2.082969	-0.884272	1.157920
H	-2.406596	0.003444	1.685090
C	-0.871714	-1.455769	1.753150
C	-0.025828	-0.659670	2.563144

C	-0.432922	-2.785370	1.561647
C	1.157251	-1.134093	3.129518
C	0.740279	-3.277009	2.118622
H	-1.038849	-3.461728	0.973029
C	1.549989	-2.451185	2.904050
H	1.757982	-0.479332	3.750921
H	1.021284	-4.310860	1.942022
H	2.465397	-2.827190	3.349778
Br	-0.523480	1.143711	3.050100

Vibrational frequencies

-222.4169	12.4502	19.5133
25.2670	27.8998	31.6972
37.9942	43.8131	44.3278
49.7673	53.7133	56.8564
63.2406	66.6486	72.0944
75.9576	77.4647	83.6505
94.5022	103.7145	109.0850
125.5546	128.8235	132.6946
138.8823	147.5881	152.0086
155.8981	157.7786	166.6051
177.9965	193.3379	203.8578
213.3960	221.6703	223.5092
227.7584	230.4832	235.6516
254.9551	262.1841	278.8998
286.2440	293.2369	309.4579
319.4811	327.1002	331.2845
353.0714	366.9527	375.2918
389.4962	396.5405	403.9321
409.5478	417.5078	429.2377
442.2737	445.5403	449.0725

453.4591 479.9078 494.0215

501.7242 508.7848 513.0900

525.3894 529.3899 533.1532

536.8834 544.7156 547.7443

559.3308 577.8189 581.2701

588.3054 599.8222 606.9182

616.9897 619.8376 631.1834

640.0170 642.9765 669.4476

673.0015 696.4839 703.3488

706.8808 708.8646 717.5470

729.7980 730.7078 744.5665

746.1768 748.0216 757.9146

765.2733 769.8609 770.5310

772.3626 782.9204 790.1717

799.7088 809.1517 828.7658

846.8704 855.2283 868.0667

870.7781 875.7037 880.7263

882.4046 887.7870 905.1797

906.6455 912.7661 928.8738

949.0683 953.4553 954.1534

959.3428 960.1201 974.7850

977.1485 978.7205 990.7480

993.4151 995.2590 998.2522

999.1417 1005.8139 1012.7257

1020.3924 1036.0131 1039.6175

1042.8608 1044.2494 1049.3298

1052.1630 1053.1384 1055.5343

1057.2151 1060.4422 1063.1615

1066.2787 1067.3945 1069.8490

1077.9470 1093.1132 1100.6855

1104.6624	1109.2284	1117.5868
1143.4549	1152.9223	1156.4750
1184.1394	1184.6762	1184.9446
1186.2428	1192.6987	1193.1695
1202.5532	1210.9422	1214.0093
1216.5841	1224.9341	1233.8118
1243.9477	1268.0165	1273.7081
1273.9834	1290.5104	1291.1125
1293.5519	1303.3529	1309.7814
1316.3416	1321.8128	1323.2563
1331.2675	1339.2215	1342.5005
1348.9619	1360.1629	1366.6371
1369.4154	1373.7752	1377.6083
1382.5626	1399.9832	1412.5920
1416.0865	1419.5694	1425.0504
1439.0726	1446.6863	1450.5654
1463.5786	1467.5382	1469.5720
1471.7150	1479.6596	1483.7719
1485.6612	1486.6526	1488.2643
1489.9109	1494.5377	1497.0901
1498.0371	1499.6602	1504.1693
1506.6651	1520.5739	1526.5433
1528.1613	1532.0225	1555.2905
1600.6879	1607.3483	1611.6731
1628.3083	1635.3686	1636.5339
1637.4392	1640.4241	1641.8130
1652.3979	1653.2197	1658.1844
1710.1442	2960.8815	3038.7868
3046.0659	3049.7036	3053.5158
3059.0275	3102.2251	3102.4568

3108.3487	3120.2770	3130.7423
3137.9904	3141.0419	3141.1375
3155.1652	3155.7180	3164.0467
3180.8465	3183.2951	3183.5146
3185.5534	3187.3173	3187.4171
3192.6881	3193.9508	3196.4686
3196.6894	3205.3749	3205.8207
3206.2564	3206.9340	3208.8986
3212.8330	3218.3848	3222.2347
3229.7673	3244.4323	3274.2918

TS4SR' (Φ= -97°)

Zero-point correction= 0.729754

Thermal correction to Energy= 0.775734

Thermal correction to Enthalpy= 0.776678

Thermal correction to Gibbs Free Energy= 0.649160

Sum of electronic and zero-point Energies= -5135.063362

Sum of electronic and thermal Energies= -5135.017382

Sum of electronic and thermal Enthalpies= -5135.016437

Sum of electronic and thermal Free Energies= -5135.143956

Cartesian coordinates

C	1.072841	-0.209559	1.589352
C	0.080583	0.659518	1.055897
H	0.693209	-1.052236	2.160019
C	-1.267707	0.290817	1.016760
O	-1.821584	-0.672738	1.617936
C	2.385962	0.286252	2.034100
C	2.870664	1.565142	1.700159
C	3.218256	-0.557933	2.795055
C	4.139168	1.978881	2.106507

H	2.256370	2.250622	1.127731
C	4.483857	-0.144446	3.202566
H	2.860720	-1.547809	3.064066
C	4.953069	1.126802	2.855190
H	4.491275	2.968996	1.831139
H	5.107724	-0.814243	3.787499
H	5.942397	1.448351	3.167405
C	-2.163603	1.080623	0.098452
C	-3.869756	1.571274	-1.209557
C	-4.036842	-0.672042	-0.161671
H	-3.262942	-1.388958	0.101143
N	-3.079610	2.606293	-1.301639
N	-2.023392	2.294715	-0.474319
N	-3.351357	0.619203	-0.369543
C	-5.089504	1.219886	-1.991727
H	-5.194947	1.887315	-2.848060
H	-5.994839	1.286334	-1.374102
C	-4.808463	-1.109222	-1.469482
O	-4.867379	-0.101134	-2.483826
C	-6.324890	-1.071023	0.437295
C	-5.101878	-0.586192	0.906065
C	-4.953012	-0.125391	2.213387
C	-6.069525	-0.132625	3.052259
C	-7.303841	-0.605197	2.585980
C	-7.438300	-1.082662	1.279443
C	-6.215569	-1.551077	-0.987962
H	-3.981461	0.210453	2.560380
H	-8.164440	-0.603900	3.248961
H	-8.395372	-1.454354	0.923875
H	-6.986128	-1.136117	-1.646017

H	-6.304686	-2.642067	-1.040778
C	-0.896719	3.185612	-0.397010
C	0.058794	3.111647	-1.423324
C	-0.747005	3.989713	0.738097
C	1.229346	3.853985	-1.260556
C	0.437097	4.726907	0.845416
C	1.440309	4.652639	-0.127958
H	2.018576	3.755301	-1.998962
H	0.590846	5.345341	1.725787
C	-1.782343	3.990285	1.832067
H	-1.757331	3.041184	2.380912
H	-2.794056	4.109939	1.431200
H	-1.595039	4.796510	2.544837
C	2.735587	5.408087	0.032618
H	2.931879	5.648793	1.081289
H	2.712922	6.352239	-0.525724
H	3.576504	4.823666	-0.353594
C	-0.144115	2.213591	-2.615508
H	-1.014070	2.524664	-3.204057
H	-0.320884	1.176758	-2.309884
H	0.734427	2.226750	-3.263929
H	-4.264429	-1.923482	-1.947715
H	-5.980086	0.224414	4.074089
H	0.406941	1.528376	0.510168
C	5.127149	-0.666498	-0.910862
C	5.420749	-1.952503	-0.401329
C	6.724386	-2.443694	-0.314872
C	7.767580	-1.624793	-0.744447
C	7.501363	-0.341872	-1.249776
C	6.199268	0.141459	-1.336939

C	3.706530	-0.376065	-0.888159
C	2.931225	-1.429943	-0.366891
H	6.921929	-3.435696	0.080095
H	8.790811	-1.983484	-0.684602
H	8.325742	0.285254	-1.577318
H	5.989273	1.130014	-1.723946
S	3.957732	-2.796631	0.093607
C	3.129179	0.874187	-1.340565
O	3.760126	1.824001	-1.815991
H	2.032206	0.956261	-1.247014
C	1.514580	-1.405723	-0.148651
H	1.033402	-0.694960	-0.803337
C	0.684548	-2.604695	0.076136
C	-0.524853	-2.827917	-0.615614
C	1.003204	-3.558695	1.066282
C	-1.340199	-3.930393	-0.376663
C	0.203524	-4.669356	1.318212
H	1.883205	-3.395010	1.678636
C	-0.972591	-4.863572	0.593644
H	-2.257258	-4.063012	-0.939741
H	0.493319	-5.372895	2.092725
H	-1.607240	-5.723739	0.781832
Br	-1.155416	-1.581351	-1.955361

Vibrational frequencies

-267.7363	19.9051	21.5411
24.9952	26.9711	37.7721
40.3088	44.8327	46.1275
49.1826	54.8580	59.4108
65.0007	68.2717	76.0793
80.7061	89.5476	94.7041

102.5500	105.5244	129.2006
130.1534	131.8883	133.8263
152.2090	154.9513	163.6358
172.3546	177.2854	190.9627
193.7268	205.3300	208.6731
214.3231	223.5440	227.1884
235.4683	241.2472	244.0755
253.8299	267.5073	282.9334
288.1004	294.2585	308.0495
314.1710	321.1779	329.1596
363.2479	371.4982	382.6352
384.3852	394.1245	406.5250
418.2838	422.8613	431.7279
441.0231	448.8186	449.0065
464.0368	467.4547	495.1538
501.0847	505.4318	512.2164
522.2228	523.6248	530.9855
537.8743	544.6667	547.1858
564.4374	572.5836	582.7645
591.0936	601.0356	608.8537
615.8345	617.8837	632.0055
633.0333	647.5680	662.4513
670.7373	689.7879	702.3193
705.8284	709.5030	716.3307
731.1370	741.7387	744.8522
747.6368	755.9072	760.3321
763.6601	769.7860	771.2744
771.5699	779.8901	792.5141
799.5160	809.3139	827.8005
847.7116	855.3261	870.0252

871.9271	877.5518	879.2545
886.6575	900.8532	902.6922
903.5943	909.9153	928.7534
949.4269	951.5265	958.9216
960.6601	962.5840	974.4217
975.6919	978.2728	989.3561
996.5251	997.5345	998.6986
1004.1244	1010.4639	1013.8408
1019.4609	1037.0325	1037.6509
1041.2122	1045.6041	1049.2078
1052.0329	1054.0139	1057.8943
1060.1151	1061.5239	1065.3136
1065.8421	1066.9204	1070.4200
1076.9427	1095.6812	1104.1126
1108.9308	1114.1827	1118.3060
1139.1436	1142.4220	1156.2214
1182.4389	1184.0974	1185.6370
1188.3569	1189.7138	1194.7528
1201.7618	1212.9006	1215.6198
1216.4631	1224.9046	1230.5136
1244.6925	1253.3951	1268.2754
1272.3464	1286.2916	1289.1261
1295.6894	1303.4291	1309.5538
1313.9700	1318.2867	1325.9724
1328.3867	1336.1544	1340.1199
1349.0169	1360.9228	1368.1197
1368.7570	1373.3655	1374.9971
1382.7981	1400.6480	1412.2543
1412.9065	1417.7156	1423.5802
1432.3024	1441.6673	1448.8101

1453.0285	1466.1692	1467.2772
1469.6679	1478.6254	1484.2672
1485.7656	1486.6803	1487.7727
1489.5055	1496.3972	1498.3649
1498.6342	1502.8180	1504.5730
1507.7847	1522.0276	1525.6063
1529.0932	1534.0433	1550.6076
1604.9559	1607.6192	1610.6266
1628.6656	1636.3660	1637.2242
1637.7125	1640.8006	1641.1340
1652.5663	1652.8815	1659.2718
1695.6098	2998.9847	3040.8722
3042.9377	3044.3115	3051.3324
3055.3066	3097.9710	3103.7958
3105.0303	3109.8082	3131.7875
3133.3720	3139.7119	3146.1409
3152.1300	3162.5082	3178.9246
3181.4497	3182.8107	3184.3147
3184.3960	3188.3584	3193.1043
3193.9161	3193.9252	3196.7979
3204.1218	3205.0426	3206.3086
3206.8482	3207.2384	3212.5144
3215.8793	3217.0673	3220.7541
3231.3537	3243.8866	3283.9880

TS4SR"(Φ=63°)

Zero-point correction= 0.729786

Thermal correction to Energy= 0.775762

Thermal correction to Enthalpy= 0.776706

Thermal correction to Gibbs Free Energy= 0.649035

Sum of electronic and zero-point Energies= -5135.061183

Sum of electronic and thermal Energies= -5135.015207

Sum of electronic and thermal Enthalpies= -5135.014263

Sum of electronic and thermal Free Energies= -5135.141934

Cartesian coordinates

C	-1.548861	-0.375022	-1.168210
C	-0.723837	0.615715	-0.597358
H	-1.038874	-1.088264	-1.810928
C	0.675785	0.521340	-0.667742
O	1.369417	-0.370798	-1.221656
C	-2.954549	-0.113961	-1.518559
C	-3.548980	-0.850302	-2.560136
C	-3.744732	0.822652	-0.826044
C	-4.883762	-0.656179	-2.903104
H	-2.950098	-1.580634	-3.098295
C	-5.084484	1.005801	-1.161610
H	-3.317596	1.392217	-0.007704
C	-5.659970	0.269339	-2.199694
H	-5.322988	-1.232883	-3.712286
H	-5.683008	1.720715	-0.603871
H	-6.705239	0.413876	-2.457650
C	1.466508	1.620807	-0.007309
C	3.147214	2.680985	0.936117
C	3.595607	0.278655	0.504601
H	2.939700	-0.588875	0.487775
N	2.215970	3.589262	0.810456
N	1.174051	2.916620	0.207400
N	2.731835	1.470482	0.446321
C	4.459507	2.718097	1.646355
H	4.524093	3.603230	2.280414

H	5.294673	2.728682	0.933731
C	4.477504	0.305320	1.812531
O	4.483304	1.567915	2.492078
C	5.883809	-0.000720	-0.148133
C	4.593654	0.228730	-0.631433
C	4.337370	0.353510	-1.996135
C	5.411012	0.258476	-2.884246
C	6.709423	0.032976	-2.408011
C	6.953534	-0.103222	-1.038704
C	5.892426	-0.130715	1.354076
H	3.320556	0.499436	-2.343914
H	7.534405	-0.039441	-3.111131
H	7.961101	-0.281243	-0.672954
H	6.653700	0.486073	1.841957
H	6.077565	-1.168983	1.652350
C	-0.043855	3.613894	-0.114138
C	-0.957480	3.854922	0.922032
C	-0.285058	3.964361	-1.449495
C	-2.177330	4.441771	0.574635
C	-1.518551	4.552212	-1.741490
C	-2.480740	4.780578	-0.749985
H	-2.910530	4.624753	1.355300
H	-1.737167	4.825225	-2.770409
C	0.723362	3.676935	-2.531054
H	0.738282	2.607636	-2.773210
H	1.735804	3.958546	-2.224098
H	0.476888	4.222313	-3.444860
C	-3.832269	5.342242	-1.111828
H	-4.326597	5.793833	-0.247060
H	-4.485568	4.545092	-1.488366

H	-3.756067	6.097150	-1.900645
C	-0.649679	3.453774	2.341413
H	0.247956	3.958957	2.712504
H	-0.468834	2.376207	2.412280
H	-1.482829	3.701329	3.002493
H	4.061363	-0.385033	2.546876
H	5.237247	0.353191	-3.952161
H	-1.169651	1.457913	-0.091478
C	1.414295	-3.693875	-0.197615
C	1.866304	-3.042563	0.973406
C	3.173721	-3.169117	1.448484
C	4.068906	-3.950411	0.719982
C	3.646974	-4.600504	-0.451528
C	2.337748	-4.486579	-0.908823
C	0.023193	-3.411152	-0.486590
C	-0.564656	-2.515300	0.434907
H	3.484843	-2.669593	2.360974
H	5.093539	-4.057044	1.063423
H	4.355036	-5.205550	-1.010800
H	2.011165	-4.989578	-1.809687
S	0.588120	-2.086996	1.709445
C	-0.687303	-3.946201	-1.624695
O	-0.213765	-4.702278	-2.480132
H	-1.749038	-3.642853	-1.711793
C	-1.872065	-1.945109	0.349781
H	-2.530283	-2.519218	-0.289557
C	-2.584959	-1.223171	1.404445
C	-3.993796	-1.292958	1.537325
C	-1.945688	-0.307582	2.273926
C	-4.700337	-0.559665	2.487607

C	-2.639055	0.434739	3.225515
H	-0.881744	-0.145213	2.169874
C	-4.022921	0.306264	3.345634
H	-5.778025	-0.661206	2.548833
H	-2.094017	1.120964	3.866064
H	-4.574889	0.874684	4.087701
Br	-5.047916	-2.401899	0.372372

Vibrational frequencies

-236.9887	16.0398	22.7054
25.8406	27.3240	33.1811
36.9326	43.2392	45.6935
50.7518	57.4960	58.6378
70.5025	79.4627	79.8570
81.8409	89.9944	97.2585
103.8958	106.3817	109.4476
127.9065	139.4233	141.5867
153.2326	156.4853	164.8580
172.7166	177.9283	184.6109
188.6796	196.8213	202.2032
213.6448	222.7956	223.5765
229.1963	231.9943	243.8605
258.4295	261.6830	283.3127
289.6021	295.2001	309.4246
319.5001	327.8704	334.6247
361.8184	369.1826	381.9003
384.8164	397.9879	406.4148
411.5993	412.0426	432.1199
441.5497	445.6318	452.6715
466.0109	483.4060	493.7661
502.1493	509.9848	512.4281

526.3733	528.5900	530.8476
534.0629	544.6040	546.0497
570.4438	580.3245	582.0502
592.5468	600.6407	609.0001
617.6281	618.9755	631.0293
640.8734	643.7915	668.6251
676.3024	692.6987	701.0157
705.3267	710.4597	717.4206
729.8391	745.5639	748.0889
748.5626	756.8441	761.6670
762.6092	772.1610	772.6638
773.7857	788.7955	795.4309
797.9707	808.8833	828.8842
845.2580	854.8231	870.0352
873.1872	875.3906	876.0478
883.0820	885.9483	903.0839
905.9887	910.3221	923.5607
927.3863	949.1227	954.5771
957.0486	961.2097	972.6906
975.1388	976.7399	990.0361
990.4135	994.7837	995.1465
998.6715	1001.7001	1010.2751
1025.6522	1035.8050	1040.9473
1043.4128	1046.9927	1050.2640
1051.2487	1053.2958	1056.3232
1060.3526	1064.6940	1064.8305
1067.0220	1068.4688	1071.1457
1082.6390	1091.8142	1100.2144
1106.7947	1113.2446	1117.1156
1143.7193	1150.8310	1156.3059

1184.3677	1184.7650	1185.6705
1185.9041	1190.9815	1193.5266
1204.7366	1209.9996	1217.3522
1218.8277	1227.5141	1230.6384
1246.8647	1265.9657	1272.2524
1276.8250	1289.8578	1291.5856
1294.5903	1304.8883	1311.4940
1319.4351	1322.4303	1326.5995
1332.8875	1341.0124	1342.8899
1351.6623	1361.4807	1367.4597
1369.8898	1370.5175	1375.5317
1387.7928	1403.3579	1417.1758
1417.4206	1420.3138	1425.4892
1441.7512	1446.7021	1447.8147
1462.7102	1464.6336	1466.2299
1472.8178	1479.3119	1482.1989
1485.1675	1487.7177	1489.7221
1494.6050	1497.4922	1498.4794
1502.8112	1505.6050	1506.3971
1507.5057	1519.8132	1525.0460
1527.6596	1532.2933	1560.5064
1601.6271	1604.4803	1612.6292
1630.0310	1633.9162	1635.6215
1636.2611	1640.7290	1641.4887
1652.4666	1653.3933	1658.2082
1697.0595	2938.6159	3038.6546
3046.1241	3052.3507	3052.7361
3056.5633	3102.1482	3102.6930
3107.8938	3114.6571	3131.1331
3133.1943	3141.4357	3144.6262

3152.9386	3168.1679	3169.1448
3175.4179	3181.2976	3182.2510
3184.2684	3187.0328	3189.3738
3191.4012	3192.1518	3193.6591
3194.3286	3203.1893	3204.2294
3206.9236	3207.0884	3207.8874
3211.6908	3218.4435	3220.0979
3243.0034	3243.1298	3264.8141

TS4SR'"(Φ=77°)

Zero-point correction= 0.729711

Thermal correction to Energy= 0.775710

Thermal correction to Enthalpy= 0.776655

Thermal correction to Gibbs Free Energy= 0.649055

Sum of electronic and zero-point Energies= -5135.060889

Sum of electronic and thermal Energies= -5135.014890

Sum of electronic and thermal Enthalpies= -5135.013946

Sum of electronic and thermal Free Energies= -5135.141545

Cartesian coordinates

C	1.422085	-0.283452	1.385981
C	0.488296	0.591642	0.794885
H	0.998988	-1.130622	1.920519
C	-0.874925	0.256883	0.705597
O	-1.433390	-0.770567	1.169217
C	2.724243	0.197486	1.888661
C	3.480190	-0.625894	2.741793
C	3.267279	1.442627	1.517373
C	4.731238	-0.226863	3.205735
H	3.081238	-1.595063	3.029186
C	4.519542	1.841645	1.980207

H	2.717028	2.105401	0.859936
C	5.258499	1.010104	2.826177
H	5.298033	-0.884240	3.858679
H	4.918452	2.805932	1.677312
H	6.235517	1.322116	3.184111
C	-1.793825	1.226678	0.000759
C	-3.610209	2.061584	-0.926738
C	-3.944232	-0.218716	0.003832
H	-3.281587	-1.080345	0.000136
N	-2.715878	3.002558	-1.055081
N	-1.588481	2.476911	-0.466317
N	-3.095312	0.961708	-0.291333
C	-5.001136	1.989837	-1.459293
H	-5.141900	2.729732	-2.248525
H	-5.734175	2.177856	-0.663144
C	-5.090689	-0.369212	-1.075197
O	-5.145362	0.693534	-2.031428
C	-6.049376	-0.230465	1.160552
C	-4.671551	-0.066627	1.321931
C	-4.113813	0.191461	2.574477
C	-4.966222	0.300588	3.674981
C	-6.349985	0.143427	3.519619
C	-6.898778	-0.128184	2.263994
C	-6.410000	-0.522506	-0.272530
H	-3.038922	0.285396	2.681678
H	-7.001832	0.230903	4.384231
H	-7.971746	-0.253341	2.146571
H	-7.174114	0.155597	-0.667668
H	-6.801874	-1.539723	-0.382391
C	-0.382735	3.264080	-0.491353

C	0.353668	3.290357	-1.686425
C	0.005980	3.947836	0.666442
C	1.545184	4.016594	-1.684354
C	1.213505	4.652822	0.616458
C	1.998589	4.688854	-0.540847
H	2.141065	4.048367	-2.592262
H	1.550205	5.174724	1.507784
C	-0.803164	3.862298	1.932409
H	-0.704076	2.864652	2.376991
H	-1.867639	4.035512	1.744634
H	-0.457314	4.594069	2.665946
C	3.319918	5.415261	-0.567441
H	4.138920	4.717020	-0.776373
H	3.528703	5.908059	0.385791
H	3.337381	6.175478	-1.356431
C	-0.116316	2.546399	-2.909136
H	-1.033011	2.990232	-3.312515
H	-0.343292	1.500762	-2.676673
H	0.645256	2.563942	-3.691821
H	-4.884570	-1.252891	-1.676544
H	-4.553278	0.502846	4.658939
H	0.832415	1.513920	0.359987
C	-1.041845	-3.499871	-0.789110
C	-1.292258	-2.548025	-1.806395
C	-2.473318	-2.535280	-2.550719
C	-3.442646	-3.496413	-2.267052
C	-3.222837	-4.446751	-1.255314
C	-2.040009	-4.459246	-0.522996
C	0.252091	-3.317471	-0.166730
C	0.960060	-2.207302	-0.680202

H	-2.637106	-1.791649	-3.325036
H	-4.370269	-3.506825	-2.831518
H	-3.989329	-5.186550	-1.042489
H	-1.867579	-5.190665	0.255848
S	0.058030	-1.439608	-1.992921
C	0.775932	-4.173186	0.870487
O	0.178866	-5.120212	1.394990
H	1.811711	-3.950432	1.196192
C	2.169012	-1.653382	-0.168478
H	2.652349	-2.312016	0.541163
C	3.126583	-0.820258	-0.906678
C	4.522674	-1.007512	-0.778473
C	2.733021	0.290990	-1.684676
C	5.455000	-0.175330	-1.392159
C	3.652707	1.126973	-2.311753
H	1.681136	0.535025	-1.753672
C	5.021215	0.897468	-2.171342
H	6.514119	-0.368005	-1.263574
H	3.295687	1.968695	-2.896139
H	5.748247	1.543863	-2.653036
Br	5.238732	-2.466742	0.261887

Vibrational frequencies

-234.4533	15.9468	23.7911
25.3263	32.6400	34.6698
36.1569	45.4872	48.7171
50.1330	55.7564	62.6895
68.5657	71.0485	76.7503
78.2853	86.2029	90.3760
101.8825	109.1860	119.2097
125.4103	135.2885	141.5898

150.0855	159.2124	171.9438
175.5359	176.8565	178.5604
195.0966	198.8220	203.8995
211.8677	220.3704	225.4165
229.1982	233.3094	235.0289
253.7751	268.6960	282.1462
285.4502	297.8974	311.3333
316.9941	321.0878	339.1145
362.8131	372.2068	382.2343
387.5197	393.8279	406.2832
413.8943	416.0380	433.3301
442.2231	448.2953	449.7023
464.9307	477.7535	493.6935
503.4727	507.8131	515.2805
525.9602	529.6091	530.8736
534.7382	546.2526	553.5400
566.9941	575.0751	581.7570
592.9089	598.9476	607.9772
619.4456	620.1171	631.9088
640.9254	648.4437	661.7022
670.4229	690.8395	697.1880
701.7126	710.6181	712.8399
727.9489	741.7199	747.9615
749.7527	751.3313	760.1622
762.8800	767.7880	774.7198
774.8897	783.2845	788.4761
798.8395	808.3970	826.2142
850.2662	853.3565	869.4994
871.9327	874.1114	877.0672
881.4998	884.4260	899.1953

906.0886	908.9996	925.5577
929.7234	947.9005	957.8506
959.1584	960.9390	972.0516
973.9800	976.8084	993.3895
997.0594	997.7225	997.9943
998.2889	1004.4642	1011.2140
1023.3974	1038.4197	1039.0634
1040.4970	1048.2520	1049.9571
1051.8067	1053.2540	1054.9044
1058.3195	1063.6530	1064.7722
1067.5975	1069.9723	1072.6359
1082.7440	1100.6634	1105.6656
1106.5062	1113.9316	1119.7438
1143.7645	1149.4695	1156.1140
1181.0735	1182.1151	1184.9562
1187.5446	1194.8576	1195.1397
1202.2286	1211.8005	1214.4611
1219.7452	1223.8777	1231.9064
1243.7137	1266.7399	1271.9163
1278.3802	1289.1135	1292.7301
1294.0177	1304.8223	1313.6610
1319.4056	1322.9028	1324.2476
1329.0813	1335.1482	1346.0362
1349.6017	1361.8456	1365.4104
1369.0038	1370.6182	1375.9154
1384.4727	1402.0510	1414.2469
1418.1074	1420.3190	1425.6793
1426.8501	1444.0425	1450.2981
1455.5024	1467.8634	1469.0279
1472.4212	1479.9009	1480.0581

1480.2220	1483.0557	1488.4952
1493.1250	1495.2306	1497.1010
1497.3043	1500.3560	1505.5863
1509.2592	1520.8597	1526.4828
1529.3849	1534.4165	1562.8451
1603.0123	1604.6960	1614.5930
1631.0367	1635.6605	1637.3828
1638.7520	1640.2230	1643.4351
1653.1593	1654.5261	1658.2955
1697.6660	2931.1094	3040.0832
3040.9229	3041.7479	3049.6098
3057.8140	3095.9686	3101.1649
3105.3670	3109.4553	3131.6738
3140.5010	3142.9670	3150.8803
3157.5247	3165.3997	3167.9460
3177.9235	3181.3668	3183.3456
3183.5321	3186.3892	3189.0451
3191.6217	3192.9780	3193.6490
3197.1767	3203.4743	3205.8225
3206.1726	3211.9599	3212.3511
3216.4130	3220.9460	3223.3945
3242.8068	3243.4422	3292.2479

TS4SS(Φ= -111°)

Zero-point correction= 0.729731

Thermal correction to Energy= 0.775850

Thermal correction to Enthalpy= 0.776794

Thermal correction to Gibbs Free Energy= 0.647854

Sum of electronic and zero-point Energies= -5135.057418

Sum of electronic and thermal Energies= -5135.011299

Sum of electronic and thermal Enthalpies= -5135.010355

Sum of electronic and thermal Free Energies= -5135.144015

Cartesian coordinates

C	-1.581143	0.318498	-1.538333
C	-0.376877	0.741865	-0.954985
H	-1.516858	-0.515856	-2.228778
C	0.810892	-0.002942	-1.032784
O	1.010779	-1.102840	-1.618812
C	-2.705592	1.236813	-1.779266
C	-3.771489	0.812208	-2.598549
C	-2.769068	2.531870	-1.228526
C	-4.857815	1.643243	-2.855350
H	-3.740376	-0.186615	-3.026404
C	-3.859409	3.363385	-1.485820
H	-1.961912	2.902383	-0.607478
C	-4.908283	2.925720	-2.297564
H	-5.666176	1.293153	-3.491091
H	-3.886579	4.358233	-1.049869
H	-5.755047	3.575987	-2.497176
C	2.009915	0.592223	-0.345649
C	3.930481	0.776301	0.707109
C	3.333068	-1.564601	0.139971
H	2.376741	-2.077159	0.093505
N	3.522022	2.006995	0.552634
N	2.327936	1.881597	-0.122955
N	3.046026	-0.116413	0.158467
C	5.075702	0.225750	1.490869
H	5.442709	0.972275	2.196732
H	5.901878	-0.072158	0.831477
C	4.124285	-1.981752	1.439887

O	4.554973	-0.871770	2.237445
C	5.352919	-2.658241	-0.552130
C	4.244951	-1.939572	-1.008067
C	4.065193	-1.661445	-2.362948
C	5.032131	-2.104869	-3.267776
C	6.148763	-2.822398	-2.818357
C	6.313376	-3.107796	-1.460308
C	5.307793	-2.852859	0.942298
H	3.180651	-1.127234	-2.692861
H	6.892896	-3.162269	-3.533187
H	7.178708	-3.667300	-1.115730
H	6.234708	-2.555559	1.444036
H	5.132411	-3.904544	1.195498
C	1.615095	3.065965	-0.527282
C	0.982347	3.825815	0.466867
C	1.566808	3.392433	-1.891239
C	0.241398	4.935826	0.048928
C	0.813992	4.512185	-2.252070
C	0.133444	5.284261	-1.302195
H	-0.268956	5.534668	0.798413
H	0.751835	4.783228	-3.302602
C	2.263613	2.557781	-2.934838
H	1.700788	1.640010	-3.140901
H	3.269013	2.264156	-2.616804
H	2.349560	3.110783	-3.873193
C	-0.726985	6.442896	-1.738414
H	-1.686348	6.078884	-2.127041
H	-0.250189	7.015325	-2.540464
H	-0.941735	7.121719	-0.908400
C	1.079260	3.449839	1.920984

H	2.099504	3.582527	2.295590
H	0.814996	2.401290	2.083541
H	0.409708	4.064560	2.524649
H	3.449928	-2.531643	2.092905
H	4.915124	-1.897273	-4.327486
H	-0.369115	1.641437	-0.357891
C	-0.495759	-0.002376	2.899660
C	-1.474923	1.006423	3.062595
C	-1.381388	1.989258	4.048367
C	-0.268713	1.982322	4.889323
C	0.730226	1.009969	4.729972
C	0.626748	0.023800	3.751245
C	-0.816779	-0.928420	1.821867
C	-2.022985	-0.608968	1.154418
H	-2.152821	2.746295	4.152620
H	-0.174235	2.739346	5.662129
H	1.599698	1.022772	5.381184
H	1.399797	-0.722960	3.627529
S	-2.762526	0.838910	1.876916
C	-0.021184	-2.091213	1.518690
O	1.037147	-2.400534	2.086355
H	-0.411490	-2.748123	0.729191
C	-2.653975	-1.061048	-0.029798
H	-3.626627	-0.603140	-0.183009
C	-2.629020	-2.440386	-0.585725
C	-3.753698	-3.277744	-0.437050
C	-1.560528	-2.969906	-1.337959
C	-3.825441	-4.555731	-0.988980
C	-1.612086	-4.249354	-1.888587
H	-0.675237	-2.359392	-1.493696

C	-2.744980	-5.046436	-1.720741
H	-4.713264	-5.160279	-0.841045
H	-0.764450	-4.617362	-2.459244
H	-2.795359	-6.041023	-2.153336
Br	-5.272693	-2.686782	0.594301

Vibrational frequencies

-182.3997	13.9051	20.2968
20.8758	26.4845	30.2354
37.6701	39.1869	43.4106
49.0596	51.8313	58.4545
63.1879	68.7943	75.2378
81.8528	87.6955	94.1802
94.9404	104.0597	114.6282
128.8613	138.4134	144.8500
148.2635	152.4847	170.9264
175.6671	183.6931	187.2762
197.2923	202.8334	205.5948
211.1427	217.8023	221.3940
228.0608	232.2846	240.7115
252.6504	263.6149	273.4250
285.0612	290.8818	299.5042
319.9183	326.4909	330.1111
365.4318	371.0670	379.0708
393.2364	402.9642	407.6802
415.3266	420.9798	435.6586
441.4310	445.4146	452.3360
468.8114	475.1564	491.0179
499.9509	509.7561	512.4988
514.5471	527.9999	529.1155
532.9971	541.2700	543.6308

561.5727 578.1048 582.5476

588.8427 599.3843 607.7709

613.1021 619.8482 630.6478

638.4521 642.2700 647.5022

670.4603 672.1553 701.2655

705.0121 710.2324 712.8262

729.2255 747.2683 747.9309

749.6138 760.5598 762.9572

770.7352 773.6229 775.3651

780.1076 788.1226 798.8713

806.6289 827.5567 831.3823

844.9650 855.0246 868.9195

878.1190 880.0066 881.5386

887.7314 900.9255 906.2758

907.5129 912.6092 927.8501

942.8878 946.9431 952.3946

962.4625 973.6376 976.6817

978.0620 985.9097 989.9840

992.5665 998.7114 1001.4834

1003.5135 1012.0421 1013.1200

1023.9014 1037.0480 1040.4486

1042.4341 1046.0011 1047.8857

1048.6252 1050.7307 1052.1013

1055.6502 1059.8489 1061.2202

1066.1584 1068.1236 1070.4769

1077.2475 1095.6986 1097.6239

1101.8051 1112.3249 1116.6028

1144.3479 1149.9960 1152.6411

1183.2363 1183.7071 1184.3908

1186.1559 1192.1845 1195.4835

1199.2764	1199.6522	1210.6248
1213.0087	1221.2239	1235.0231
1241.0861	1245.7922	1271.7120
1272.7467	1286.0127	1291.6228
1297.3868	1303.9001	1309.8800
1316.8923	1330.5613	1331.4940
1332.7081	1336.7636	1342.8089
1349.1877	1357.3769	1367.7749
1368.2359	1373.9890	1378.3945
1379.3934	1414.3040	1418.8540
1420.3880	1425.4121	1428.1789
1438.7042	1447.1860	1454.0161
1463.7561	1466.0579	1467.9217
1470.3470	1480.2878	1482.4241
1484.5997	1485.5187	1489.4691
1490.9166	1493.7669	1495.9399
1497.4966	1500.1431	1505.7077
1508.4076	1518.5739	1520.4573
1525.1861	1532.2663	1574.7883
1603.2973	1605.9664	1607.8836
1626.8027	1634.5812	1634.8470
1637.1998	1639.5767	1641.2641
1650.9606	1652.5338	1657.0192
1680.7742	3039.2611	3040.9188
3048.1232	3052.5142	3056.5634
3059.6156	3096.9283	3101.8152
3111.4255	3123.8395	3131.3877
3139.0586	3151.2319	3153.9489
3163.1842	3166.9552	3168.3486
3178.1756	3182.4427	3182.9484

3184.3827	3184.5938	3186.9051
3187.0473	3191.2392	3192.2408
3193.9252	3193.9645	3196.2973
3204.4735	3205.1903	3206.6649
3207.5597	3218.1466	3218.6439
3221.7662	3244.9879	3249.2859

TS4SS' (Φ= -24°)

Zero-point correction= 0.729961

Thermal correction to Energy= 0.775906

Thermal correction to Enthalpy= 0.776850

Thermal correction to Gibbs Free Energy= 0.648931

Sum of electronic and zero-point Energies= -5135.057945

Sum of electronic and thermal Energies= -5135.012000

Sum of electronic and thermal Enthalpies= -5135.011056

Sum of electronic and thermal Free Energies= -5135.138975

Cartesian coordinates

C	1.026787	-0.439283	1.554150
C	0.076335	0.381405	0.896308
H	0.596508	-1.220796	2.174188
C	-1.304312	0.163991	0.971567
O	-1.947491	-0.594173	1.746658
C	2.299470	0.110137	2.060868
C	2.750653	1.402649	1.731794
C	3.105443	-0.674603	2.907018
C	3.970261	1.879579	2.211556
H	2.141811	2.050555	1.111119
C	4.321474	-0.197227	3.389769
H	2.772025	-1.673718	3.174508
C	4.764919	1.081367	3.037052

H	4.297272	2.878736	1.937022
H	4.927100	-0.824085	4.038297
H	5.715968	1.452252	3.408142
C	-2.126328	0.902872	-0.053252
C	-3.712299	1.334318	-1.517298
C	-4.086015	-0.755006	-0.217733
H	-3.386409	-1.495860	0.165994
N	-2.895310	2.347386	-1.613739
N	-1.916038	2.076510	-0.680253
N	-3.287763	0.436545	-0.570395
C	-4.899680	0.962994	-2.341012
H	-4.889962	1.506374	-3.286920
H	-5.835160	1.190839	-1.812987
C	-4.875651	-1.279805	-1.482904
O	-4.770052	-0.428444	-2.628156
C	-6.423251	-0.804620	0.336129
C	-5.162052	-0.413734	0.791053
C	-4.995855	0.210242	2.027822
C	-6.128618	0.456458	2.806325
C	-7.398583	0.073356	2.353873
C	-7.553344	-0.563097	1.119684
C	-6.342247	-1.470225	-1.013005
H	-4.000552	0.475249	2.368134
H	-8.271523	0.272817	2.969014
H	-8.538857	-0.860897	0.772401
H	-7.032081	-1.039883	-1.746527
H	-6.579239	-2.537709	-0.941564
C	-0.847438	3.018260	-0.474751
C	0.172303	3.082620	-1.436817
C	-0.840675	3.783618	0.700399

C	1.249637	3.932306	-1.174119
C	0.255919	4.625690	0.908373
C	1.311237	4.704539	-0.007744
H	2.075463	3.954130	-1.877303
H	0.291184	5.221453	1.816601
C	-1.938771	3.673509	1.726844
H	-1.823017	2.760450	2.322486
H	-2.928799	3.640858	1.261648
H	-1.911314	4.522613	2.413884
C	2.489923	5.611315	0.243086
H	3.417131	5.164357	-0.128937
H	2.612725	5.825250	1.308639
H	2.361620	6.570479	-0.274049
C	0.133216	2.245009	-2.688345
H	-0.531412	2.689672	-3.438135
H	-0.237009	1.236272	-2.488694
H	1.134538	2.161755	-3.115564
H	-4.437903	-2.218878	-1.817986
H	-6.024321	0.944073	3.771241
H	0.432719	1.158047	0.238124
C	5.164679	-0.587872	-0.961920
C	5.652632	-1.750757	-0.320017
C	7.016524	-2.035140	-0.222955
C	7.919088	-1.134376	-0.783843
C	7.458735	0.028045	-1.424063
C	6.098937	0.308037	-1.516416
C	3.714873	-0.490997	-0.906207
C	3.109896	-1.578257	-0.267376
H	7.364126	-2.934276	0.276568
H	8.984633	-1.335202	-0.723520

H	8.176029	0.721014	-1.854521
H	5.741864	1.204565	-2.006059
S	4.329355	-2.724872	0.301879
C	2.971187	0.682276	-1.333307
O	3.451063	1.652934	-1.923092
H	1.898894	0.671347	-1.086414
C	1.737054	-1.898793	0.074108
H	1.692087	-2.727421	0.776549
C	0.667301	-2.004105	-0.929458
C	-0.548636	-2.667838	-0.637857
C	0.757266	-1.475033	-2.235964
C	-1.588333	-2.784388	-1.559462
C	-0.283093	-1.557669	-3.156936
H	1.682493	-1.010837	-2.550677
C	-1.472641	-2.207136	-2.822086
H	-2.483938	-3.328613	-1.282881
H	-0.154383	-1.123077	-4.143628
H	-2.294337	-2.273148	-3.527697
Br	-0.840218	-3.498407	1.065123

Vibrational frequencies

-241.7861	15.9008	18.3223
24.0023	30.9678	33.4483
38.4621	41.8501	43.5519
46.7070	57.4346	61.5618
68.9080	69.0568	77.1250
90.2016	91.6659	96.3779
100.6535	107.3749	108.1867
121.3500	132.4680	138.5858
146.0533	157.8969	160.1375
164.8366	166.8474	181.9167

197.4377	210.6763	211.4564
217.1161	222.5454	228.0776
232.0724	232.9076	248.2870
261.3119	278.7864	290.8680
292.7345	303.3782	316.1457
318.0673	332.0899	345.8705
354.9721	372.7163	384.2761
390.9646	400.3819	407.6282
418.5959	423.5300	436.0855
443.1399	449.6559	455.0190
467.3709	472.8808	493.3895
502.7809	505.5965	512.7876
516.3403	526.7308	529.7735
531.8317	538.1039	543.6335
565.1623	576.8493	582.1695
592.0279	599.8940	608.7575
610.5085	615.7050	633.1428
639.5674	641.3759	663.2816
675.9730	684.9635	700.3504
709.7298	710.9005	714.7448
728.9282	737.3283	742.5726
745.7820	752.2610	762.7250
765.8941	769.2173	772.3624
773.2166	783.5460	792.2690
800.4283	828.0202	836.4741
849.6052	860.4537	861.5209
870.1644	877.0546	879.3723
884.0129	885.3251	896.9949
903.4924	908.5128	931.6659
950.0633	955.5578	960.5124

963.4954 973.3908 974.7566

979.4930 980.1358 990.2025

993.3085 997.2544 999.1344

1006.5798 1009.8734 1017.1830

1032.9217 1037.5242 1038.8242

1040.8770 1042.6334 1044.9277

1050.5300 1052.8523 1055.1482

1056.7625 1059.4669 1062.0106

1063.0398 1066.9344 1069.2725

1081.5058 1092.9725 1094.7848

1102.8094 1112.3369 1118.6353

1137.6220 1145.3405 1152.8292

1183.4614 1183.6181 1184.3194

1187.0437 1193.3151 1196.9121

1197.7641 1203.5125 1211.2653

1218.4573 1225.9891 1227.5105

1244.4183 1247.2148 1268.0589

1274.3898 1292.7910 1295.6567

1296.6759 1303.6691 1306.8320

1313.1595 1320.3898 1327.0862

1331.3364 1337.8082 1342.9699

1351.7845 1359.3709 1365.0000

1369.2590 1373.9991 1375.3572

1380.4623 1409.2855 1413.3683

1416.3360 1421.9828 1435.0425

1438.6303 1440.8651 1447.1038

1459.0165 1467.2759 1468.5649

1472.1196 1473.8076 1484.6781

1485.4042 1486.6985 1487.4464

1494.0435 1497.3761 1498.2007

1499.5722	1501.3124	1506.5991
1509.5794	1520.1964	1522.0472
1526.2427	1532.5078	1552.2185
1603.1409	1606.8349	1616.0375
1629.2197	1635.9092	1638.2189
1639.3622	1640.6230	1641.7987
1652.3618	1652.7178	1657.7101
1706.9441	3035.6706	3039.3113
3045.9623	3046.8143	3049.7019
3059.2193	3099.2273	3101.7845
3109.6454	3119.9869	3129.0239
3138.3035	3147.0822	3147.4515
3152.9424	3154.0988	3155.6956
3177.5154	3182.3480	3183.8095
3185.0080	3185.0998	3185.8988
3192.0725	3193.6218	3193.6992
3196.5183	3204.8954	3205.6400
3207.2418	3207.8242	3208.8720
3213.2364	3219.5818	3222.2616
3236.2073	3246.0653	3259.5380

TS4SS"(Φ= 59°)

Zero-point correction= 0.730615

Thermal correction to Energy= 0.776433

Thermal correction to Enthalpy= 0.777377

Thermal correction to Gibbs Free Energy= 0.648955

Sum of electronic and zero-point Energies= -5135.051285

Sum of electronic and thermal Energies= -5135.005467

Sum of electronic and thermal Enthalpies= -5135.004523

Sum of electronic and thermal Free Energies= -5135.132945

Cartesian coordinates

C	-1.286256	0.329417	-1.043394
C	0.019992	0.773753	-0.772189
H	-1.358964	-0.651003	-1.504259
C	1.083872	-0.140164	-0.803438
O	1.012149	-1.372161	-1.057617
C	-2.362733	1.262701	-1.377153
C	-2.443484	2.553015	-0.813921
C	-3.350897	0.870003	-2.300323
C	-3.479658	3.414530	-1.166523
H	-1.703637	2.874218	-0.088696
C	-4.378815	1.740451	-2.661391
H	-3.302237	-0.123376	-2.736611
C	-4.450270	3.013450	-2.092073
H	-3.534170	4.401325	-0.715281
H	-5.131487	1.418376	-3.374878
H	-5.256794	3.688357	-2.363151
C	2.444882	0.366662	-0.420712
C	4.507117	0.389656	0.347377
C	3.480118	-1.878017	0.303742
H	2.451615	-2.183805	0.486444
N	4.243697	1.639210	0.075451
N	2.955752	1.611750	-0.411630
N	3.440014	-0.420924	0.055463
C	5.678014	-0.223999	1.038155
H	6.276337	0.543659	1.530277
H	6.313289	-0.770919	0.328997
C	4.415200	-2.203585	1.539332
O	5.134097	-1.075741	2.045304
C	5.144546	-3.446101	-0.426029

C	4.091716	-2.634868	-0.854548
C	3.705537	-2.590861	-2.194348
C	4.409067	-3.369407	-3.115472
C	5.471468	-4.180694	-2.694614
C	5.842093	-4.228364	-1.348473
C	5.354299	-3.343224	1.062387
H	2.865173	-1.975158	-2.495652
H	6.010612	-4.780712	-3.422276
H	6.663924	-4.861007	-1.024650
H	6.389749	-3.112816	1.334427
H	5.094556	-4.281674	1.564424
C	2.308771	2.846854	-0.767589
C	1.869757	3.672513	0.278368
C	2.097553	3.139404	-2.121472
C	1.165624	4.827426	-0.073225
C	1.388945	4.306935	-2.416667
C	0.904922	5.152035	-1.410341
H	0.801059	5.478688	0.716615
H	1.200179	4.555154	-3.457698
C	2.560398	2.207558	-3.210232
H	1.892908	1.340204	-3.279909
H	3.570522	1.831370	-3.020674
H	2.556210	2.712064	-4.179094
C	0.079118	6.363630	-1.762237
H	-0.970619	6.079072	-1.908636
H	0.422938	6.826185	-2.692422
H	0.108759	7.115704	-0.968647
C	2.117056	3.308358	1.719478
H	3.169480	3.451558	1.988476
H	1.877127	2.259057	1.912403

H	1.506547	3.924696	2.382349
H	3.798887	-2.520044	2.381679
H	4.128107	-3.349755	-4.164391
H	0.193482	1.800620	-0.493030
C	-5.197212	-2.395223	-0.124376
C	-4.350473	-3.527110	-0.182703
C	-4.810874	-4.795766	-0.540468
C	-6.162378	-4.947829	-0.843747
C	-7.025704	-3.842554	-0.790737
C	-6.559371	-2.579065	-0.438201
C	-4.485868	-1.169392	0.227315
C	-3.122589	-1.385880	0.512507
H	-4.132276	-5.642533	-0.579348
H	-6.544657	-5.925848	-1.120798
H	-8.077796	-3.973102	-1.028126
H	-7.225842	-1.728399	-0.399328
S	-2.705145	-3.101376	0.251715
C	-5.126101	0.134486	0.127631
O	-6.334053	0.320116	-0.044526
H	-4.454958	1.001109	0.174701
C	-1.982431	-0.600803	0.903172
H	-1.079626	-1.203687	0.901693
C	-1.899390	0.453229	1.915597
C	-0.681614	0.734136	2.593750
C	-2.980234	1.274094	2.313198
C	-0.536802	1.774027	3.508442
C	-2.856006	2.314528	3.227542
H	-3.958507	1.070873	1.909420
C	-1.622771	2.593572	3.814523
H	0.418430	1.930178	3.995952

H	-3.732101	2.904672	3.479490
H	-1.505752	3.408783	4.521390
Br	0.875408	-0.419975	2.451588

Vibrational frequencies

-215.9136	12.4157	16.3416
22.1651	23.3781	28.2563
37.8569	43.7793	47.9162
49.2928	53.2318	59.5911
64.8855	76.2171	83.9846
86.7724	92.9022	97.9759
99.6630	102.8517	105.6187
118.9883	130.6594	135.0600
135.4800	149.7686	161.4020
177.9465	193.8759	195.9460
202.0225	205.4769	208.4777
216.4523	225.4169	229.2178
234.3931	241.0522	253.0129
265.2275	282.5039	295.5705
303.3700	309.1157	314.9063
325.6315	338.2456	345.9846
353.2419	373.5232	379.2990
400.8486	402.5647	408.6139
417.7599	422.5978	432.5170
444.9975	450.6148	454.6065
472.0239	478.7962	494.0934
500.3935	511.5231	515.5153
526.2476	530.6576	531.5166
534.9164	540.3341	548.3075
566.2830	577.0903	582.6873
589.8786	600.5783	609.4837

615.0267	621.7474	631.2526
636.4228	649.1914	665.7930
669.9703	675.3365	700.8003
706.8479	710.3928	715.0099
730.6166	732.3428	744.7878
752.3260	758.2216	765.0863
766.2593	768.7239	773.2896
775.8693	791.2239	797.1845
803.8188	823.6882	829.0304
848.8191	856.3902	866.1190
871.1515	878.6641	879.4694
882.5273	886.7866	903.7018
908.2616	909.7496	928.1997
951.4136	952.7990	953.5214
959.4722	964.7132	974.7027
977.0399	977.1803	989.4441
991.3769	996.2861	999.9397
1003.0007	1009.9094	1011.5823
1035.0004	1035.0841	1043.1366
1044.9161	1049.6757	1050.9704
1052.8506	1053.7791	1057.9056
1058.8884	1060.7587	1062.2759
1068.5242	1069.9282	1073.0313
1082.4967	1092.9399	1097.9723
1104.0665	1108.7372	1119.0381
1142.6141	1150.5171	1155.8937
1182.8071	1184.4018	1185.0291
1186.0269	1192.7639	1195.4569
1195.5666	1202.6785	1207.0236
1217.4197	1228.5770	1233.7694

1245.5316	1255.6382	1270.7008
1275.3438	1291.1336	1292.9911
1295.4217	1305.3941	1310.2590
1313.7323	1321.9414	1327.1894
1332.4707	1337.9325	1343.6940
1349.6225	1357.7851	1359.7905
1365.1419	1369.3465	1378.3935
1380.9308	1406.1413	1416.8745
1423.6200	1427.3441	1428.4875
1438.4593	1447.9786	1454.1745
1457.0284	1466.8658	1469.6992
1472.6642	1483.2385	1484.1004
1485.1860	1487.0092	1490.7971
1492.2411	1497.5908	1498.9459
1503.1825	1505.7608	1509.1457
1511.9442	1519.6614	1521.6155
1527.5274	1530.8625	1559.7312
1600.6891	1605.6628	1608.3971
1626.3175	1634.7153	1636.2038
1637.7975	1641.1267	1643.0381
1650.1823	1653.5091	1657.9495
1698.2515	3040.1138	3042.6534
3052.2550	3053.1311	3060.5803
3061.9865	3099.9964	3103.2531
3107.2399	3118.0261	3122.7539
3133.1838	3140.6557	3148.3816
3157.2959	3158.5442	3161.6595
3182.2885	3183.7383	3183.9749
3184.4503	3185.3174	3187.6853
3189.0399	3193.1668	3194.3337

3195.2660	3198.2438	3205.7285
3207.2794	3208.0237	3208.0925
3212.8326	3220.2172	3222.7557
3249.6415	3275.2147	3284.9435

TS4SS''' (Φ=175°)

Zero-point correction= 0.729789

Thermal correction to Energy= 0.775713

Thermal correction to Enthalpy= 0.776657

Thermal correction to Gibbs Free Energy= 0.649244

Sum of electronic and zero-point Energies= -5135.050378

Sum of electronic and thermal Energies= -5135.004454

Sum of electronic and thermal Enthalpies= -5135.003510

Sum of electronic and thermal Free Energies= -5135.130923

Cartesian coordinates

C	1.683881	0.065568	0.828601
C	0.628885	0.746178	0.191793
H	1.392566	-0.608637	1.625843
C	-0.718663	0.526995	0.516760
O	-1.229649	-0.305651	1.307640
C	3.015807	0.665439	0.980339
C	3.384840	1.865075	0.336544
C	3.957231	0.053387	1.829208
C	4.652550	2.407175	0.512454
H	2.677401	2.383556	-0.299810
C	5.230800	0.593575	1.997924
H	3.686640	-0.862366	2.345553
C	5.587902	1.767773	1.333827
H	4.915733	3.329485	0.001881
H	5.944854	0.093022	2.645659

H	6.581028	2.188872	1.462128
C	-1.708846	1.470176	-0.120375
C	-3.598072	2.297350	-0.879975
C	-3.710699	-0.123507	-0.347806
H	-2.965072	-0.917360	-0.376239
N	-2.775813	3.312616	-0.870325
N	-1.599616	2.784442	-0.381128
N	-2.987753	1.157788	-0.422104
C	-4.976850	2.159793	-1.432852
H	-5.217117	3.010430	-2.072210
H	-5.721217	2.098765	-0.627900
C	-4.715619	-0.245655	-1.559032
O	-4.959018	0.988790	-2.248167
C	-5.878578	-0.631471	0.537501
C	-4.586687	-0.226924	0.884181
C	-4.227417	0.001815	2.211718
C	-5.199213	-0.166531	3.201044
C	-6.498077	-0.567057	2.861703
C	-6.844685	-0.806808	1.529166
C	-6.004497	-0.847511	-0.948939
H	-3.209272	0.283543	2.455741
H	-7.242950	-0.694198	3.642271
H	-7.851879	-1.120130	1.268520
H	-6.888782	-0.376277	-1.389089
H	-6.054614	-1.918052	-1.178915
C	-0.465332	3.648840	-0.173154
C	0.297434	4.016894	-1.289305
C	-0.170632	4.067164	1.132718
C	1.415510	4.825941	-1.061716
C	0.959167	4.869732	1.304212

C	1.766603	5.250558	0.224754
H	2.030717	5.118250	-1.908369
H	1.218628	5.199768	2.306652
C	-1.016929	3.644476	2.305508
H	-0.861354	2.584892	2.539703
H	-2.084029	3.782910	2.102502
H	-0.759690	4.223167	3.195523
C	3.009719	6.070158	0.462479
H	3.766382	5.471644	0.983758
H	2.798789	6.941199	1.092082
H	3.447190	6.422202	-0.475625
C	-0.052504	3.522487	-2.669055
H	-1.061681	3.831095	-2.960943
H	-0.026190	2.427025	-2.710626
H	0.653156	3.906226	-3.409080
H	-4.289021	-0.893826	-2.322820
H	-4.943480	0.008004	4.242110
H	0.850396	1.502483	-0.547572
C	-1.333974	-3.282115	-0.260258
C	-1.467908	-2.843656	-1.600555
C	-2.636761	-3.037860	-2.339641
C	-3.714727	-3.667556	-1.718851
C	-3.618645	-4.080264	-0.379669
C	-2.447086	-3.895193	0.348404
C	-0.033405	-2.966929	0.304327
C	0.819225	-2.320246	-0.599231
H	-2.705808	-2.704858	-3.370872
H	-4.631933	-3.834818	-2.275379
H	-4.472308	-4.554329	0.096005
H	-2.371673	-4.211864	1.380198

S	0.000598	-2.048136	-2.146621
C	0.249484	-3.064500	1.725528
O	-0.464446	-3.619219	2.561430
H	1.183929	-2.574090	2.053345
C	2.150274	-1.779096	-0.509634
H	2.394123	-1.133365	-1.346885
C	3.319238	-2.510262	-0.026649
C	4.639874	-2.091567	-0.340232
C	3.247171	-3.696262	0.746724
C	5.777082	-2.741899	0.134847
C	4.371988	-4.357217	1.223342
H	2.275859	-4.126797	0.950767
C	5.651633	-3.872396	0.939428
H	6.757572	-2.362496	-0.131164
H	4.246397	-5.260933	1.812697
H	6.537900	-4.371649	1.318245
Br	4.960384	-0.602572	-1.517506

Vibrational frequencies

-208.8042	12.2666	15.2328
30.0475	33.3140	38.0966
40.0795	44.9837	54.0622
58.5104	62.1486	63.1067
72.8046	75.9784	81.9858
84.4752	89.5819	93.6673
106.3819	109.8766	115.8707
120.7879	128.0349	132.5444
144.2906	149.3127	158.4663
166.6437	168.6646	184.8827
194.0652	207.1163	208.9779
216.7664	219.5283	222.9801

225.1304	239.3149	254.1542
267.4835	277.2872	285.8842
288.9643	301.1020	312.3279
322.3409	325.1062	331.4122
354.0275	373.6779	383.4350
394.1661	397.7907	407.2225
410.4606	415.5983	438.4019
443.7111	451.8251	457.7813
462.6216	465.6100	491.5772
502.4583	506.8207	512.1280
518.6868	528.8464	530.4419
532.3595	535.7671	540.5641
558.5920	580.5197	583.0366
588.5546	600.4648	607.0201
608.7253	618.8404	629.8498
637.7404	641.5369	671.6016
676.6578	685.9076	695.3393
707.6227	711.2962	721.4651
732.9408	734.9303	747.9165
753.1118	758.0636	762.6413
764.7598	769.3562	773.3163
776.8965	789.9562	790.8004
797.3105	828.9700	837.2018
844.7686	851.0874	870.7919
874.6277	876.6475	879.9710
885.6113	886.5683	900.7660
908.8598	910.2639	925.0891
932.4580	946.9440	956.3876
959.5176	960.0139	972.9589
976.5536	980.4657	988.8014

990.7450	991.6797	1000.0275
1005.6902	1007.4028	1013.0525
1022.1398	1035.4268	1038.5654
1040.7987	1042.6821	1046.8132
1049.6851	1053.1918	1055.7958
1058.1860	1059.9207	1063.6952
1066.2015	1068.1833	1071.1967
1078.3894	1090.1699	1092.2477
1100.1226	1112.2065	1117.2281
1143.4185	1146.6643	1152.1684
1183.5962	1185.1442	1185.2718
1186.8440	1191.6351	1192.6338
1198.9297	1205.9471	1212.0572
1218.1505	1227.9345	1236.5754
1248.5824	1250.6291	1263.4089
1274.3688	1290.4467	1292.3604
1296.8727	1302.4264	1309.4308
1311.3905	1321.4585	1325.3562
1331.8097	1340.8413	1343.8462
1349.0215	1359.7704	1367.6438
1369.7173	1370.1836	1378.5328
1385.0012	1412.5820	1416.5744
1419.2365	1425.8132	1436.2810
1441.5253	1446.6073	1448.5376
1463.5306	1465.9609	1469.3004
1472.5219	1477.4669	1481.7738
1483.2408	1487.9442	1488.2842
1491.6078	1494.8688	1498.7271
1501.2042	1504.4576	1505.7257
1507.4072	1517.4333	1520.6108

1528.0131	1533.1997	1561.1453
1596.4736	1603.3216	1614.5144
1628.3800	1633.3152	1636.2114
1638.9250	1640.7122	1642.0733
1652.5559	1653.3139	1658.8925
1716.0371	2970.9395	3041.5995
3043.6904	3044.6224	3048.2051
3059.2346	3102.6177	3104.6068
3105.2366	3105.6503	3129.8021
3140.4121	3143.3143	3147.8824
3154.6278	3155.5223	3174.4705
3177.6572	3183.3770	3184.6141
3186.4843	3186.9206	3187.0198
3189.8042	3193.5178	3196.0226
3196.0591	3203.6869	3205.6629
3205.9407	3209.1804	3213.3188
3216.6213	3216.9166	3226.1145
3237.4950	3242.3885	3247.3442