Supporting Information for

Insights into isothiourea-catalyzed asymmetric [3 + 3] annulation of α,β-unsaturated aryl esters with 2-acylbenzazoles: Mechanism, origin of stereoselectivity and switchable chemoselectivity

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Table of Contents

Part 1: Computational details.

All of the computations were conducted by using density functional theory (DFT) method in Gaussian 09 program[1]. Fully optimized structures for all reactants, intermediates, transition states, products at the level of M06-2X[2]/6-31G(d, p) in THF solvent using integrated equation formalism polarizable continuum model (IEFPCM[3]). The harmonic vibrational frequencies were also calculated at the same level and were used to determine that the transition state has one and only one imaginary frequency, meanwhile the other optimized stationary states as true minima with no imaginary frequency. Thereafter, we used the IEFPCM solvation model to perform a single point energy calculations for all optimized structures in THF at the level of M06-2X-GD3/6-31++G (2df, 2dp). Finally, the energy we discussed is the Gibbs free energies obtained through the addition of single point energy at the M06-2X-GD3/6-31++G(2df, 2dp)//IEFPCM$_{THF}$ level to corresponding free energy correction obtained at the M06-2X/6-31G(d, p)//IEFPCM$_{THF}$ level. All 3D-structures in this work were drawn by CYLview[4].

In the distortion/interaction theory[5], the activation energy ($\Delta E^{\ddagger}$) is divided into two main components: the distortion ($\Delta E^{\ddagger}_{dist}$) and interaction ($\Delta E^{\ddagger}_{int}$) energies. The distortion energy involves geometric and electronic changes to deform the reactants to their transition state geometry. The interaction energy is obtained by the relationship: $\Delta E^{\ddagger}_{int} = \Delta E^{\ddagger} - \Delta E^{\ddagger}_{dist}$

Part 2: Different ways for the catalyst to attack the reactant R1.

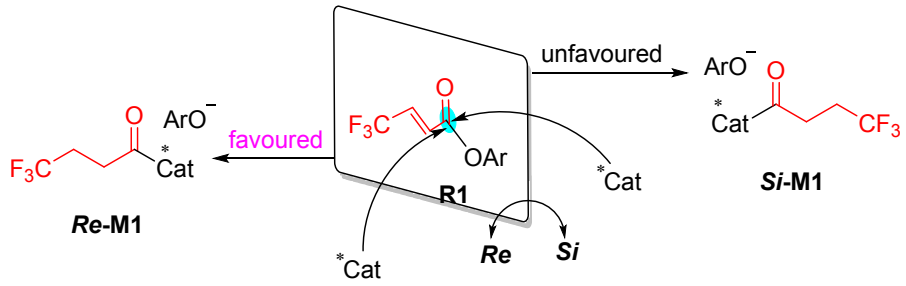

Fig. S1 Different ways for the catalyst to attack the reactant **R1**.

Part 3: The deprotonation of pre-R2 by with assistance of ArO^- or *i*-Pr_2NEt for generating R2.

After the end of the first step, intermediate **M1** undergoes the α-C-H deprotonation process of the reactant precursor **pre-R2** via transition state **TS1'** to form the real reactant **R2**. The corresponding barrier for this process was calculated to be 7.4 kcal/mol. As an alternative, we also attempted to carry out α-C-H deprotonation of the reactant precursor **pre-R2** by using the base ***i*-Pr_2NEt** via transition state **TS1"**. It is clear that its energy barrier is 14.7 kcal/mol higher than that of **TS1'** (Fig. S1). In summary, **ArO^-** assisted α-C-H deprotonation process is somewhat advantageous.

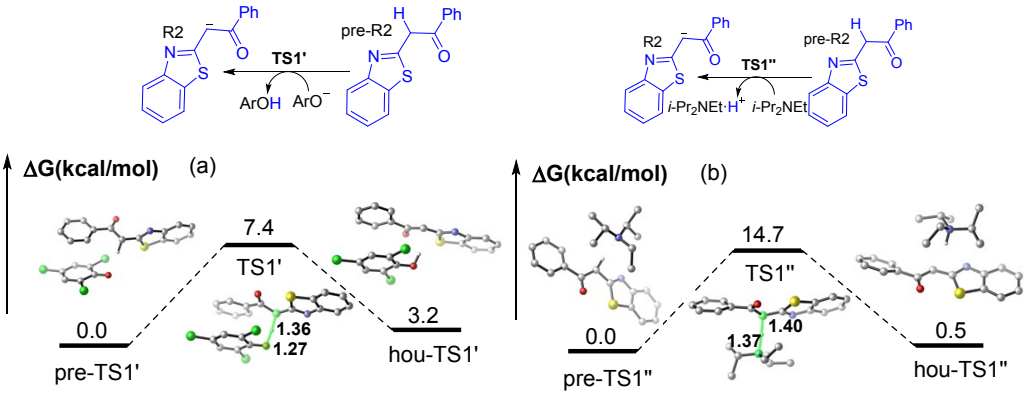

Fig. S2 (a) The relative Gibbs free energy profiles of the deprotonation of **pre-R2** generating **R2** via **ArO^-** assistance. (b) The relative Gibbs free energy profiles of the deprotonation of **pre-R2** generating **R2** via ***i*-Pr_2NEt** assistance.

Part 4: Local nucleophilic (P_k^-) and electrophilic (P_k^+) Parr function analysis on the reactant R2.

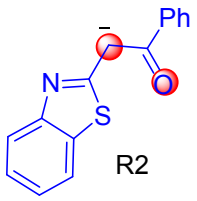

Table S1 Local nucleophilic (P_k^-) and electrophilic (P_k^+) Parr function analysis on the reactant **R2**.

	C		O	
SP	P_k^+	P_k^-	P_k^+	P_k^-
R2	-0.13	0.61	0.12	0.23

Part 5: The role of isothiourea.

In order to understand the actual role of isothiourea catalyst, we analyzed global reaction index (GRI). For the global reactivity index (GRI[6]) analysis, the relevant parameters of GRI, *i.e.*, global electrophilicity index ω, which is calculated from the electronic chemical potential μ and the chemical hardness η with the equation $\omega = (\mu^2/2\eta)$. Both quantities may be approached in terms of the one-electron energies of the frontier molecular orbital HOMO and LUMO, E_H and E_L, respectively, as $\mu \approx (E_H + E_L)/2$ and $\eta \approx (E_L - E_H)$. According to the HOMO energies obtained within the Kohn−Sham scheme[7], Domingo and co-workers provided nucleophilicity index N[6d,8], de fined as $N = E_{HOMO(SR)} - E_{HOMO(TCE)}$, to handle a nucleophilicity scale.

As shown in Table S2, the electrophilicity (ω) of the reactant **R1** is 1.82 eV, the nucleophilicity (N) of the reactant **R2** is 5.03 eV, the electrophilicity (ω) of the reactant **M1** is 2.55 eV. Herein, the electrophilicity (ω) of the reactant **R1** is enhanced in intermediate **M1** after being connected with the catalyst, which makes it easier to react with the nucleophilic reactant **R2**.

Table S2. GRI analysis of **R1**, **R2** and **M1.**

SR	E_{HOMO} (a.u.)	E_{LUMO} (a.u.)	μ (a.u.)	η (a.u.)	ω (eV)	N (eV)
R1	-0.31995	-0.05584	-0.188	0.264	**1.82**	1.85
R2	-0.20316	-0.00150	-0.102	0.202	0.71	**5.03**
M1	-0.32808	-0.09244	-0.210	0.236	**2.55**	1.63

Part 6: Different conformations and configurations of TS2s.

The reactant **R2** acts as a nucleophile in this experiment and attacks on intermediate **M1**, we considered and studied that when the formation of stable C-C bond through transition state **TS2**, each reaction mode will have a different conformation. Therefore, based on the transition states **TS2*SS*, TS2*RS*, TS2*RR*, TS2*SR***, each transition state **TS2** is rotated 90° each time based on the dihedral angle *Φ1* (C1–C2–C3–C4), and rotated four times for a total of 360°, so there should be sixteen (4 × 4) possible conformations obtained in theory. Actually, we have only obtained fifteen conformations: **TS2*SS*, TS2*RS*, TS2*RR*, TS2*SR*** & **TS2'*SS*, TS2'*RS*, TS2'*RR*, TS2'*SR*** & **TS2''*SS*, TS2''*RS*, TS2''*RR*, TS2''*SR*** & **TS2'''*RS*, TS2'''*RR*, TS2'''*SR*** in the Table S3. The relative energy of each conformation is shown in **Table S2**, in which we found that all **TS2*SS*, TS2*RS*, TS2*RR*, TS2*SR*** are relatively lower in relative energy than the corresponding three other isomers. More importantly, the relative energies of **TS2*RS***, **TS2*RS'***, **TS2*RS''***, **TS2*RS'''*** are 12.0, 16.4, 18.0, 15.0 kcal/mol, respectively. This indicates that the transition state **TS2*RS*** is the most advantageous structure in the searched configurations.

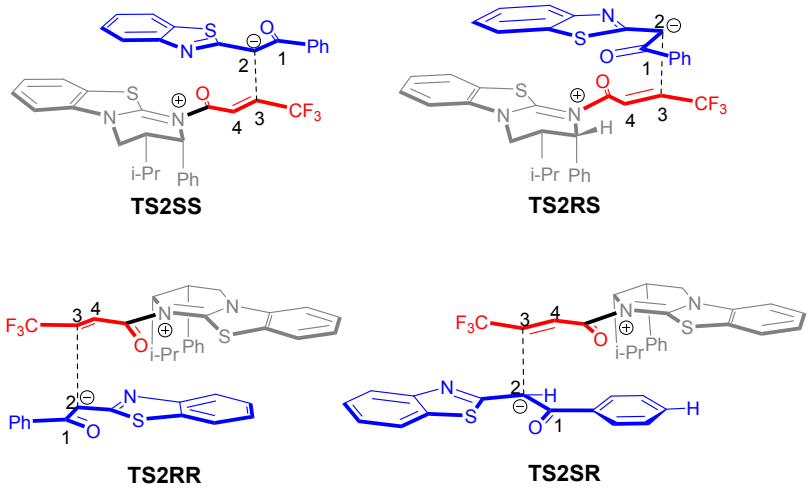

Table S3 The relative Gibbs free energies (Δ*G*) for different conformations of **TS2*SS*, TS2*RS*, TS2*RR*, TS2*SR*** & **TS2'*SS*, TS2'*RS*, TS2'*RR*, TS2'*SR*** & **TS2''*SS*, TS2''*RS*, TS2''*RR*, TS2''*SR*** & **TS2'''*RS*, TS2'''*RR*, TS2'''*SR*** with the energy of **R1+Cat** as 0.0 kcal/mol (unit: kcal/mol)

SP	$\Phi 1$(Optimized)	Energy
TS2(SS)	-174.75	14.0
TS2'(SS)	-90.49	16.3
TS2''(SS)	68.93	16.4
TS2(RS)	58.74	12.0
TS2'(RS)	1.59	16.4
TS2''(RS)	-28.24	18.0
TS2'''(RS)	-64.95	15.0
TS2(RR)	176.97	15.6
TS2'(RR)	124.23	30.0
TS2''(RR)	50.62	24.6
TS2'''(RR)	-83.38	28.3
TS2(SR)	155.96	15.5
TS2'(SR)	175.96	19.8
TS2''(SR)	68.71	20.0
TS2'''(SR)	-55.41	15.6

Part 7: The relative Gibbs free energy profiles of the deprotonation of M2*RS* generating M3 via TS3' with assistance of *i*-$Pr_2NEt•H^+$.

After the addition reaction (C-C bond formation), intermediate **M2*RS*** undergoes a proton transfer process. The second path is to assist the intermolecular proton transfer with ***i*-$Pr_2NEt•H^+$**. The energy barrier through transition state **TS3'** is 23.2 kcal/mol (Fig. S2).

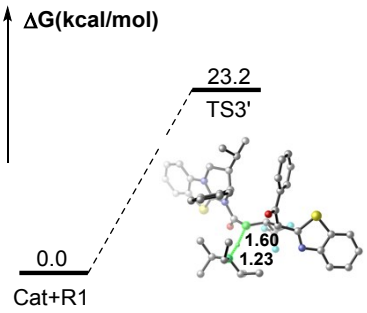

Fig. S3 The relative Gibbs free energy profiles of the deprotonation of **M2*RS*** generating **M3** via **TS3'** with assistance of ***i*-$Pr_2NEt•H^+$**.

Part 8: The relative Gibbs free energy profiles via TS4-A'and TS4-B'.

When the **X** atom is oxygen atom, the nitrogen atom nucleophilic attacks on carbonyl carbon atom of intermediate **M3'** through transition state **TS4-A'** (11.3 kcal/mol) to produce product **PA'**, and the oxygen atom nucleophilic attacks on carbonyl carbon atom via the transition state **TS4-B'** (4.5 kcal/mol) to produce product **PB'**. The relative energy of product **PB'** (-12.8 kcal/mol) is higher than that of product **PA'** (-19.7 kcal/mol) (Fig. S3), **PA'** should be the kinetically-unfavoured but thermodynamically-favoured product, which is consistent with that the main product is changed to **PA'** under the heating condition.

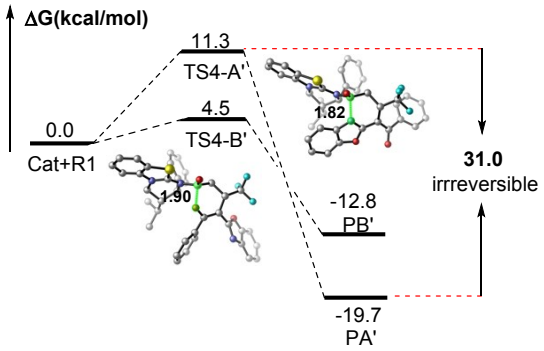

Fig. S4 The relative Gibbs free energy profiles of **TS4-A'** and **TS4-B'**.

Part 9: Prediction of chemoselectivity.

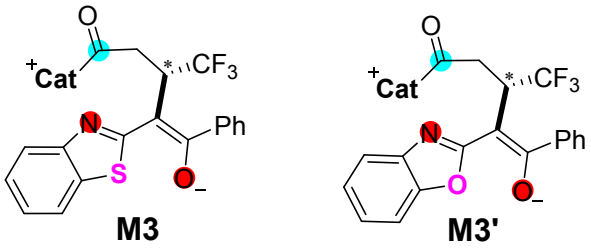

Table S4. Local nucleophilic Parr function (P_k^-) and nucleophilic atom energy (E_a^-, kcal/mol) of N and O atoms in intermediates **M3** and **M3'**, global nucleophilic index (N, eV), and the energy barriers of the fourth step in the reactions.

		N			O		
SP	N (eV)	P_k^-	E_a^-	$\Delta G_{TS4}^{\neq}$	P_k^-	E_a^-	$\Delta G_{TS4}^{\neq}$
M3	4.55	0.24	25.2	4.2_A	0.22	23.1	$4.3_{A'}$
M3'	4.69	0.17	18.4	11.3_B	0.26	28.2	$4.5_{B'}$

Part 10: Optimized geometries of some stationary points.

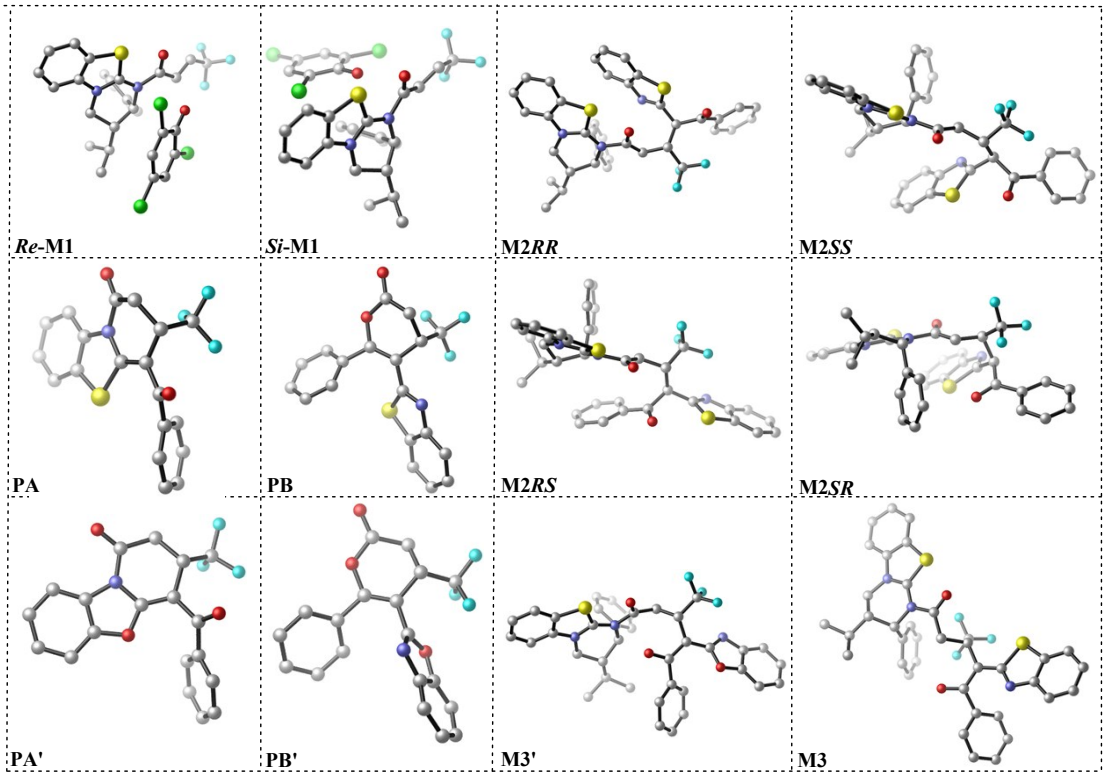

Fig. S5 Optimized geometries of the intermediates for the catalytic cycle. Hydrogen atoms that are not involved in the reaction have been omitted.

Part 11: Test results of the different computational methods.

We have compared the energies of the ***Re/Si*-TS1** and ***Re/Si*-M1** calculated at the M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCM_{THF}//M06-2X/6-31G(d, p)/IEF-PCM_{THF} (L1), M06-2X-D3/6-311++G(2df, 2pd)/SMD_{THF}//M06-2X/6-31G(d, p)/SMD_{THF} (L2), ωb97X-D/6-311++G(2df, 2pd)/IEF-PCM_{THF}//ωb97X-D/6-31G(d,p)/IEF-PCM_{THF} (L3) levels. As shown in Table S5, there are little differences between the results calculated by those methods and the results calculated by the aforementioned method and the various levels lead to the same conclusion. Thus the level of theory used is reliable for the systems studied in this work.

Table S5. Comparisons of relative Gibbs free energies for selected stationary points with different levels L1~L3 (Unit: kcal/mol)

Method	***Re*-M1**	***Si*-M1**	***Re*-TS1**	***Si*-TS1**
L1	-0.2	2.8	13.0	14.4
L2	-0.5	2.4	13.5	15.2
L3	-1.3	5.7	15.1	17.6

Part 12: Cartesian Coordinates and Vibrational frequencies of All the Optimized Structures.

Cat

Zero-point correction= 0.353199

Thermal correction to Energy= 0.371653

Thermal correction to Enthalpy= 0.372597

Thermal correction to Gibbs Free Energy= 0.306695

Sum of electronic and zero-point Energies= -1243.057263

Sum of electronic and thermal Energies= -1243.038809

Sum of electronic and thermal Enthalpies= -1243.037865

Sum of electronic and thermal Free Energies= -1243.103767

Cartesian coordinates

C	-4.242906	0.972649	1.719364
C	-5.066781	0.036669	1.098096
C	-4.563348	-0.790542	0.092104
C	-3.234023	-0.655880	-0.276435
C	-2.406669	0.293833	0.342338
C	-2.904278	1.110985	1.352836
H	-4.642577	1.605786	2.504290
H	-6.104898	-0.056360	1.397019
H	-5.197788	-1.525436	-0.392016
H	-2.265189	1.833291	1.848453
C	-0.851523	-0.656852	-1.134354
C	1.406907	-0.107940	-1.326282
C	0.991290	1.299780	-0.830390
C	-0.050050	1.183318	0.281388
H	-0.487090	2.164520	0.494613
S	-2.345226	-1.567902	-1.495755
N	-1.113204	0.292922	-0.162954
N	0.247119	-0.912155	-1.721815
C	2.170065	2.224908	-0.450840
C	2.616253	2.125738	1.013300
C	1.829039	3.680768	-0.783095
H	3.020074	1.930892	-1.081564
H	2.811766	1.097590	1.328368
H	3.534142	2.703285	1.156045
H	1.859063	2.551951	1.681179
H	1.611157	3.806830	-1.847421
H	0.951616	4.013676	-0.216661
H	2.659961	4.343110	-0.523433
H	0.479105	1.756031	-1.688577
H	2.007656	0.045634	-2.231126
C	2.278290	-0.859177	-0.335635
C	3.668461	-0.829972	-0.471024

C	1.723923	-1.542589	0.750664
C	4.490662	-1.433764	0.476743
H	4.110895	-0.324732	-1.325954
C	2.543389	-2.146080	1.701272
H	0.643654	-1.610606	0.853109
C	3.929537	-2.087170	1.571462
H	5.568959	-1.397654	0.357428
H	2.097276	-2.667752	2.542194
H	4.567661	-2.558210	2.312208
H	0.391338	0.797122	1.208251

Vibrational frequencies

29.3573	59.5164	65.4025
74.5989	88.3820	107.5033
130.8332	169.6509	200.8616
228.2453	243.7722	246.2478
269.2996	279.9200	296.0366
300.8438	318.1516	320.3684
420.0793	421.5243	426.9519
433.6154	473.6009	489.8586
500.7710	519.6992	552.1767
566.9978	594.8314	616.6787
628.2279	650.4440	691.7804
709.4615	725.8710	728.1155
734.5346	763.5061	788.1055
818.8392	862.1701	872.5905
879.8707	903.9922	930.4333
948.9696	952.7711	971.2496
993.8403	1000.1333	1004.1347
1008.0150	1016.3695	1025.2682
1034.5034	1057.2979	1064.9280
1070.8733	1076.9354	1089.3993
1112.9471	1130.4500	1151.8176
1158.7578	1175.7628	1176.8067
1184.2825	1210.1603	1212.7835
1238.4259	1244.5758	1269.2657
1297.7757	1311.7036	1324.3816
1342.6362	1351.3621	1361.4335
1363.9829	1374.9998	1380.6296
1401.1832	1409.9716	1413.4101
1428.9627	1435.1768	1495.1182
1501.2699	1503.5229	1511.2448
1512.7381	1516.8066	1518.9663
1536.7272	1552.7224	1674.8455
1676.2720	1683.6535	1698.5786

1731.3504	3054.1742	3056.7122
3057.4820	3062.0086	3077.5403
3078.8125	3127.1621	3131.7784
3135.0149	3145.0446	3157.9948
3193.3249	3200.0483	3207.9284
3208.2107	3215.7642	3218.3599
3224.5240	3227.2225	3231.3718

Cat+R1

Zero-point correction= 0.481267

Zero-point correction= 0.517563

Thermal correction to Enthalpy= 0.518508

Thermal correction to Gibbs Free Energy= 0.411741

Sum of electronic and zero-point Energies= -3456.581590

Sum of electronic and thermal Energies= -3456.545294

Sum of electronic and thermal Enthalpies= -3456.544350

Sum of electronic and thermal Free Energies= -3456.651116

Cartesian coordinates

C	-6.428631	0.362879	0.273258
C	-6.592231	-0.368212	-0.901834
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C	-4.215628	-0.526271	-1.128374
C	-4.051439	0.217794	0.049362
C	-5.158640	0.662896	0.764844
H	-7.300500	0.703783	0.821322
H	-7.588155	-0.590848	-1.268267
H	-5.600133	-1.394714	-2.526660
H	-5.037764	1.221354	1.686569
C	-1.804252	-0.156990	-0.485149
C	0.054166	0.530577	0.750595
C	-0.833443	1.711288	1.205982
C	-2.247553	1.215008	1.504347
H	-2.928905	2.061499	1.639676
S	-2.654634	-0.974278	-1.817092
N	-2.715463	0.425765	0.370961
N	-0.532232	-0.153313	-0.401971
C	-0.228182	2.563165	2.342781
C	-0.600978	2.094471	3.754127
C	-0.610021	4.034931	2.165463
H	0.864365	2.492714	2.240233
H	-0.405771	1.030166	3.910143
H	-0.022842	2.656434	4.493069
H	-1.660800	2.284067	3.958809
H	-0.249631	4.424702	1.208193

H	-1.698123	4.163179	2.195785
H	-0.180185	4.646938	2.963735
H	-0.910398	2.353241	0.315802
H	0.997482	0.971868	0.411258
C	0.421488	-0.431232	1.864172
C	1.631262	-0.248664	2.540816
C	-0.428224	-1.463676	2.266638
C	1.963347	-1.043521	3.633490
H	2.314190	0.530402	2.207014
C	-0.094745	-2.264912	3.356726
H	-1.350738	-1.648837	1.721275
C	1.093561	-2.048742	4.050211
H	2.903122	-0.884382	4.152730
H	-0.761662	-3.066193	3.658872
H	1.349521	-2.673071	4.900168
C	1.395043	-1.993748	-1.138168
H	1.815168	-1.324346	-0.397854
C	1.189887	-3.279728	-0.879021
H	0.754392	-3.949775	-1.613233
C	1.531662	-3.886719	0.441471
F	0.431420	-4.329210	1.071197
F	2.339348	-4.949807	0.283223
F	2.153528	-3.030122	1.257166
O	0.421161	-2.129440	-3.301714
C	1.040448	-1.493661	-2.495254
H	-2.274234	0.603295	2.414234
O	1.543131	-0.281242	-2.914205
C	1.897156	0.742674	-2.083373
C	3.111583	0.774488	-1.395424
C	1.075315	1.876628	-2.036529
C	3.459570	1.859932	-0.594363
C	1.413547	2.980402	-1.265328
C	2.595273	2.944844	-0.531136
H	4.395746	1.857201	-0.049322
H	0.765689	3.848857	-1.239648
Cl	-0.385324	1.898505	-2.957960
Cl	3.004593	4.300373	0.477238
Cl	4.227262	-0.541734	-1.566067

Vibrational frequencies

18.9668	27.1262	34.1893
37.3057	44.1425	48.7053
60.4953	62.8502	68.0581
71.9105	81.4886	85.1495
89.4086	97.7053	106.3546

111.3265	118.6393	123.5735
134.6180	150.6642	171.5369
174.5580	187.5596	198.0594
202.1479	228.3898	233.4513
248.0033	252.6532	257.1507
270.0496	274.4112	283.0823
288.2697	295.8086	299.3449
327.3947	334.7600	339.9186
344.4958	388.7731	405.7777
419.5175	424.1597	430.7432
433.2486	434.1810	438.6368
475.8274	496.9145	505.6484
510.6653	527.6539	536.1509
553.3288	562.6245	566.3848
574.1961	577.0457	588.0750
598.0358	618.5549	620.0992
630.5618	652.5486	670.4787
696.6867	710.7680	720.6374
722.9482	728.1137	740.6464
753.7224	761.8924	784.4004
796.3597	826.4621	829.5296
866.2645	869.5125	870.8342
872.7982	883.7489	902.7083
907.2175	910.0879	916.9752
936.8593	941.5355	953.4784
972.3111	986.5176	991.9332
996.8551	1000.5780	1008.4724
1015.2769	1018.0530	1018.9833
1038.2810	1060.7209	1065.4443
1073.2795	1080.2150	1092.6025
1115.4033	1119.4226	1132.0471
1154.6193	1161.3922	1165.7007
1181.9072	1182.7320	1183.4590
1185.5591	1208.9253	1214.9567
1216.3883	1229.8729	1235.7760
1239.1898	1252.5434	1274.2141
1303.8000	1305.8148	1315.3169
1322.9638	1328.0105	1330.5385
1343.6781	1352.9885	1356.9499
1364.5841	1367.0193	1369.5610
1380.6705	1387.7239	1406.9354
1412.0286	1416.0925	1431.1665
1435.6442	1442.6108	1493.7428
1500.3767	1506.8441	1509.2715

1511.2755	1515.5266	1518.5201
1521.0529	1536.8518	1554.9796
1648.1592	1660.8110	1676.2594
1680.2359	1683.6783	1698.3520
1729.8047	1786.8316	1892.2924
3046.3309	3054.1662	3057.8260
3061.9063	3075.3887	3124.5767
3129.3849	3133.2993	3136.1102
3146.7050	3156.1329	3179.2633
3190.9445	3209.2685	3210.5978
3213.6801	3216.9560	3224.4638
3233.8917	3234.2978	3243.1250
3247.6066	3253.3407	3272.2630

R1

Zero-point correction= 0.125865

Thermal correction to Energy= 0.142509

Thermal correction to Enthalpy= 0.143454

Thermal correction to Gibbs Free Energy= 0.077141

Sum of electronic and zero-point Energies= -2213.514168

Sum of electronic and thermal Energies= -2213.497523

Sum of electronic and thermal Enthalpies= -2213.496579

Sum of electronic and thermal Free Energies= -2213.562892

Cartesian coordinates

C	-2.435036	0.102587	0.246403
H	-2.570781	0.316213	1.300317
C	-3.451558	-0.084586	-0.586209
H	-3.296084	-0.300922	-1.639077
O	-0.152524	0.188628	0.734947
C	1.177580	0.090665	0.401259
C	1.939966	1.242450	0.223236
C	1.792037	-1.155070	0.286687
C	3.300918	1.164250	-0.046402
C	3.149415	-1.260692	0.013916
C	3.885055	-0.092423	-0.147084
H	3.885821	2.066462	-0.177382
H	3.617533	-2.233389	-0.073010
Cl	0.837529	-2.586053	0.494709
Cl	5.587288	-0.207286	-0.484319
Cl	1.169823	2.788507	0.344264
C	-4.875202	-0.012637	-0.131123
F	-4.981604	0.280003	1.169582
F	-5.546378	0.923933	-0.815718
F	-5.501498	-1.179310	-0.338401

O	-0.731223	-0.191041	-1.418244
C	-1.051520	0.010698	-0.279475

Vibrational frequencies

16.2199	24.9349	31.5938
45.0404	90.1641	110.7403
115.7273	144.2304	150.5606
187.3682	196.9360	208.3594
238.2324	276.6924	315.8817
374.4504	388.7312	399.6853
411.3241	435.8776	481.7589
529.7567	556.4552	575.7119
577.0576	590.6937	646.1296
700.8723	729.1656	753.2025
818.1962	833.5864	875.9743
883.6192	899.5655	909.5745
918.5674	1002.3433	1020.9208
1111.8067	1169.9459	1175.3788
1225.2344	1228.8458	1248.0665
1300.2676	1322.5560	1324.2423
1343.3535	1364.4772	1447.7373
1518.5551	1659.3740	1673.2832
1793.5544	1890.5919	3232.9226
3243.9140	3249.5527	3258.6106

pre-R2

Zero-point correction= 0.223769

Thermal correction to Energy= 0.237959

Thermal correction to Enthalpy= 0.238903

Thermal correction to Gibbs Free Energy= 0.180293

Sum of electronic and zero-point Energies= -1105.870035

Sum of electronic and thermal Energies= -1105.855845

Sum of electronic and thermal Enthalpies= -1105.854900

Sum of electronic and thermal Free Energies= -1105.913511

Cartesian coordinates

C	2.935381	0.824648	0.117597
C	3.059702	-0.553617	-0.132635
C	4.306652	-1.183113	-0.126509
C	5.427680	-0.405172	0.122243
C	5.314166	0.973088	0.370912
C	4.077060	1.594763	0.372368
C	0.791637	0.368342	-0.164233
H	4.396919	-2.247553	-0.314249
H	6.407965	-0.870217	0.125948
H	6.208851	1.554776	0.566030

H	3.971536	2.657156	0.564574
N	1.637282	1.312953	0.085154
S	1.477737	-1.241991	-0.374894
C	-0.663770	0.677132	-0.355224
H	-0.831298	0.947901	-1.407460
C	-1.649663	-0.427776	-0.020837
O	-1.277392	-1.568763	0.175012
C	-3.101674	-0.076200	0.024902
C	-4.003573	-1.078637	0.397849
C	-3.578409	1.197700	-0.299933
C	-5.364723	-0.810103	0.451764
H	-3.615006	-2.061354	0.643066
C	-4.943726	1.462699	-0.251956
H	-2.897778	1.988100	-0.598759
C	-5.835702	0.461842	0.125637
H	-6.059996	-1.589159	0.746162
H	-5.310190	2.450798	-0.508796
H	-6.899569	0.672518	0.165392
H	-0.883281	1.574747	0.228558

Vibrational frequencies

20.3118	30.3044	60.4232
71.4641	135.8417	153.7347
175.9503	202.5146	231.9256
303.2043	324.7283	400.1018
409.3784	421.5059	441.4800
466.1799	514.2911	519.1421
541.7777	576.6446	616.1719
626.3482	659.3449	677.4611
707.1741	713.7733	727.4543
750.8137	775.9797	781.2557
844.6933	873.4367	887.8850
895.1993	938.4204	975.2861
980.0981	1008.6974	1010.5472
1012.8287	1031.0835	1036.0591
1056.3860	1069.7033	1094.6612
1123.1348	1153.8170	1180.5909
1181.4749	1191.9474	1205.5015
1246.2501	1246.9642	1283.0412
1317.0163	1345.4021	1368.4112
1371.0027	1393.2609	1443.7283
1493.3617	1501.9496	1515.9016
1550.1245	1623.7349	1652.2552
1676.5554	1693.9575	1695.1499
1826.6997	3064.1174	3145.6829

3203.8187	3206.1697	3212.4597
3218.2442	3220.2545	3225.1079
3228.6312	3232.6297	3233.2306

R2

Zero-point correction= 0.210803

Thermal correction to Energy= 0.224562

Thermal correction to Enthalpy= 0.225506

Thermal correction to Gibbs Free Energy= 0.168953

Sum of electronic and zero-point Energies= -1105.396559

Sum of electronic and thermal Energies= -1105.382800

Sum of electronic and thermal Enthalpies= -1105.381856

Sum of electronic and thermal Free Energies= -1105.438409

Cartesian coordinates

C	2.922297	0.848334	0.104894
C	3.017423	-0.553075	-0.057529
C	4.250264	-1.194666	-0.132824
C	5.411881	-0.430567	-0.045185
C	5.332748	0.958765	0.116219
C	4.103973	1.600920	0.191448
C	0.733822	0.420376	0.049177
H	4.306408	-2.272048	-0.258543
H	6.381024	-0.915495	-0.104030
H	6.246238	1.542496	0.181585
H	4.036441	2.677394	0.314921
N	1.650570	1.364491	0.162341
S	1.408813	-1.239439	-0.134795
C	-0.657454	0.637924	0.064912
H	-0.969217	1.664369	0.206909
C	-1.594797	-0.401747	-0.048719
O	-1.299184	-1.618822	-0.148677
C	-3.065381	-0.045790	-0.022231
C	-3.974743	-1.055833	0.305056
C	-3.559521	1.226087	-0.329756
C	-5.341422	-0.800273	0.350069
H	-3.577695	-2.042457	0.520008
C	-4.927631	1.483538	-0.293912
H	-2.875775	2.016637	-0.622250
C	-5.823217	0.473284	0.051419
H	-6.033126	-1.594466	0.615263
H	-5.295833	2.474245	-0.543131
H	-6.889440	0.675835	0.080793

Vibrational frequencies

35.6386	46.2069	70.6758

97.9937	146.6101	167.2044
207.6180	221.2050	242.5409
318.2698	339.2577	404.0333
418.1179	435.6111	446.7312
487.2982	512.9235	548.5135
565.1386	628.2378	630.3049
636.0190	666.0520	709.0728
712.0419	717.6143	722.9554
743.3937	746.5639	772.2903
814.9934	873.6623	876.0587
877.0584	917.0602	951.5286
957.6677	991.7588	1002.0393
1017.8908	1020.3282	1057.1641
1067.4375	1086.7093	1103.6782
1125.7004	1151.0784	1173.4079
1174.1655	1197.5850	1236.8431
1258.7143	1283.4178	1323.2817
1337.4501	1359.9302	1365.4999
1469.6998	1485.6558	1496.4090
1503.5890	1538.0022	1557.5073
1643.0409	1648.7890	1682.6052
1687.3504	1695.2714	3190.8414
3195.3151	3197.8499	3203.9375
3209.8622	3215.3256	3218.3156
3223.1435	3230.4374	3240.6735

AROH

Zero-point correction= 0.075893

Thermal correction to Energy= 0.084613

Thermal correction to Enthalpy= 0.085558

Thermal correction to Gibbs Free Energy= 0.040697

Sum of electronic and zero-point Energies= -1685.965744

Sum of electronic and thermal Energies= -1685.957024

Sum of electronic and thermal Enthalpies= -1685.956080

Sum of electronic and thermal Free Energies= -1686.000941

Cartesian coordinates

C	-0.005210	0.935967	1.213771
C	0.006939	-0.453180	1.196223
C	0.015233	-1.177629	0.000000
C	0.006939	-0.453180	-1.196223
C	-0.005210	0.935967	-1.213771
C	-0.009664	1.611343	0.000000
H	-0.010525	1.474698	2.153408
H	-0.010525	1.474698	-2.153408

Cl	0.006939	-1.328136	-2.694944
Cl	0.006939	-1.328136	2.694944
Cl	-0.020117	3.353628	0.000000
O	0.106226	-2.533810	0.000000
H	-0.776865	-2.929673	0.000000

Vibrational frequencies

-246.1569	105.7230	137.1456
189.1882	192.0540	211.8858
297.3978	349.7906	382.7544
390.4475	435.7230	529.2256
580.8512	585.0729	711.1331
747.0498	820.6922	880.2231
884.7559	896.2184	1109.7435
1173.7225	1218.1347	1223.5438
1312.1854	1332.1264	1447.0608
1528.8009	1651.2378	1674.5534
3243.4553	3243.6368	3827.7354

OAr^-

Zero-point correction= 0.063775

Thermal correction to Energy= 0.071899

Thermal correction to Enthalpy= 0.072844

Thermal correction to Gibbs Free Energy= 0.029294

Sum of electronic and zero-point Energies= -1685.501523

Sum of electronic and thermal Energies= -1685.493399

Sum of electronic and thermal Enthalpies= -1685.492455

Sum of electronic and thermal Free Energies= -1685.536005

Cartesian coordinates

C	1.586307	0.000000	0.000027
C	0.894745	-1.206991	0.000006
C	-0.487941	-1.188086	0.000018
C	-1.307801	0.000000	0.000110
C	-0.487941	1.188086	0.000022
C	0.894745	1.206991	0.000009
H	1.429071	-2.150960	-0.000025
H	1.429071	2.150959	-0.000021
O	-2.559773	0.000000	0.000140
Cl	-1.346915	2.719089	-0.000079
Cl	-1.346915	-2.719089	-0.000087
Cl	3.344852	0.000000	0.000035

Vibrational frequencies

-49.8873	136.7942	179.7411
180.7273	219.3374	276.0527
321.2478	366.6464	380.2823

430.4879	487.6850	554.7676
613.6232	747.6914	754.6189
794.4772	880.8588	882.8081
884.9817	1087.2769	1156.4611
1184.6489	1279.1516	1388.6474
1476.8669	1584.6201	1625.9991
1677.8762	3219.7114	3219.9651

***i*-Pr_2NEt**

Zero-point correction= 0.264657

Thermal correction to Energy= 0.276213

Thermal correction to Enthalpy= 0.277157

Thermal correction to Gibbs Free Energy= 0.228953

Sum of electronic and zero-point Energies= -370.600045

Sum of electronic and thermal Energies= -370.588489

Sum of electronic and thermal Enthalpies= -370.587545

Sum of electronic and thermal Free Energies= -370.635749

Cartesian coordinates

N	-0.044135	-0.137101	-0.142360
C	-1.310922	0.507062	0.240385
H	-1.310227	0.753703	1.320241
C	-2.474780	-0.452242	-0.019998
H	-3.419395	0.012348	0.276700
H	-2.521698	-0.691308	-1.087500
H	-2.377378	-1.388453	0.534630
C	-1.562749	1.799016	-0.535856
H	-2.578644	2.148904	-0.335019
H	-0.877032	2.603121	-0.259620
H	-1.470783	1.615636	-1.611806
C	1.107334	0.772402	-0.265044
H	0.806240	1.553610	-0.969522
C	1.517516	1.458320	1.045121
H	1.867070	0.730812	1.784937
H	2.331509	2.167175	0.866727
H	0.680726	2.010127	1.484616
C	2.293801	0.057165	-0.910872
H	1.988708	-0.412197	-1.849970
H	3.090097	0.776575	-1.121935
H	2.714417	-0.715838	-0.259785
C	0.241959	-1.323556	0.679137
H	1.227686	-1.232329	1.148037
H	-0.467274	-1.384319	1.514951
C	0.197881	-2.614080	-0.133672
H	-0.781921	-2.743627	-0.601209

H	0.945847	-2.583993	-0.931054
H	0.400749	-3.484763	0.497896

Vibrational frequencies

82.6925	107.8755	136.9491
188.7610	209.5340	232.6546
245.4975	260.7599	266.8461
312.4479	327.5831	361.4699
385.1871	416.5929	449.5646
482.9021	512.1000	581.4602
740.4295	778.7854	866.4507
904.6242	922.2394	932.9261
956.4047	966.4621	975.1580
1028.2815	1086.4033	1114.5049
1139.5757	1141.7308	1165.1956
1188.0671	1206.0862	1253.5981
1262.2796	1350.9628	1368.0733
1370.3421	1376.8923	1397.4301
1404.2720	1409.8552	1418.7751
1422.2808	1429.4043	1433.9675
1487.9613	1489.2208	1496.3281
1497.2655	1500.0055	1504.9301
1509.4426	1512.1005	1516.5627
1527.6420	1537.1144	2956.8794
3054.7439	3060.5933	3061.9269
3064.0347	3065.8368	3066.4510
3101.2722	3107.8247	3138.8685
3141.0014	3143.4181	3144.7608
3145.5007	3148.3868	3152.1310
3153.0772	3153.5406	3159.7814

***i*-$Pr_2NEt•H^+$**

Zero-point correction= 0.280418

Thermal correction to Energy= 0.292092

Thermal correction to Enthalpy= 0.293036

Thermal correction to Gibbs Free Energy= 0.244379

Sum of electronic and zero-point Energies= -371.040867

Sum of electronic and thermal Energies= -371.029193

Sum of electronic and thermal Enthalpies= -371.028249

Sum of electronic and thermal Free Energies= -371.076906

Cartesian coordinates

N	-0.032407	-0.139669	-0.156274
C	-1.374077	0.472713	0.244044
H	-1.281756	0.679661	1.313836
C	-2.471883	-0.556109	-0.004076

H	-3.424057	-0.130144	0.316201
H	-2.550056	-0.786348	-1.071655
H	-2.325927	-1.485115	0.549232
C	-1.653042	1.755910	-0.526138
H	-2.672290	2.070485	-0.294362
H	-0.986997	2.575445	-0.254106
H	-1.596370	1.589586	-1.606649
C	1.118002	0.858949	-0.262923
H	0.760001	1.609196	-0.968822
C	1.405155	1.516868	1.077541
H	1.764035	0.802034	1.821807
H	2.193111	2.257191	0.925954
H	0.534459	2.038499	1.480985
C	2.334038	0.178649	-0.877076
H	2.092789	-0.288594	-1.836413
H	3.090257	0.943741	-1.063076
H	2.778401	-0.569593	-0.216264
C	0.313798	-1.345318	0.702068
H	1.282906	-1.157287	1.159915
H	-0.421064	-1.396768	1.505079
C	0.343096	-2.620555	-0.120432
H	-0.623852	-2.819968	-0.589678
H	1.109952	-2.569545	-0.897752
H	0.581959	-3.460716	0.533595
H	-0.169173	-0.490720	-1.111959

Vibrational frequencies

73.8397	91.5733	124.9820
200.5587	205.7639	223.7733
238.4251	263.8136	273.0681
308.9819	329.8826	365.7965
375.0786	407.4076	444.2690
467.5529	492.5630	589.4422
783.8008	796.1677	863.8351
902.5451	943.4906	947.7949
952.8606	963.0237	972.6818
981.6545	1051.0227	1090.7431
1119.1489	1143.9783	1163.2463
1192.0002	1206.8097	1216.6543
1219.3487	1319.7969	1343.3313
1346.7265	1375.5590	1399.4062
1404.9699	1426.0766	1427.7841
1439.4519	1444.1547	1444.4606
1447.2988	1460.5440	1483.3766
1491.5757	1498.8269	1502.1611

1503.2570	1511.4018	1512.8159
1516.0104	1521.0810	1528.8421
1544.5545	3075.1879	3077.5712
3077.9098	3083.6775	3090.2943
3127.8352	3151.1494	3155.4615
3161.6344	3164.6256	3165.0384
3166.2319	3174.8366	3176.6068
3179.1874	3180.1847	3181.7793
3183.1155	3211.5523	3424.2515

R2'

Zero-point correction= 0.227656

Thermal correction to Energy= 0.241240

Thermal correction to Enthalpy= 0.242184

Thermal correction to Gibbs Free Energy= 0.185042

Sum of electronic and zero-point Energies= -782.902371

Sum of electronic and thermal Energies= -782.888787

Sum of electronic and thermal Enthalpies= -782.887843

Sum of electronic and thermal Free Energies= -782.944985

Cartesian coordinates

C	-2.974148	0.652036	-0.429587
C	-2.807011	-0.316818	0.561044
C	-3.828585	-1.125720	1.032009
C	-5.074305	-0.917970	0.445843
C	-5.269530	0.050830	-0.553422
C	-4.227513	0.850994	-1.007717
C	-0.940686	0.686242	0.165221
H	-3.665524	-1.869929	1.802117
H	-5.916352	-1.520740	0.768714
H	-6.259549	0.173896	-0.979332
H	-4.373594	1.599459	-1.778304
N	-1.743378	1.275934	-0.652278
C	0.511139	0.936302	0.351921
H	0.740298	1.048487	1.417221
C	1.353023	-0.200652	-0.227562
O	0.821157	-1.143854	-0.776419
C	2.836959	-0.104865	-0.096884
C	3.608650	-1.156983	-0.601357
C	3.465177	0.990612	0.503099
C	4.993024	-1.115987	-0.504466
H	3.101532	-1.996210	-1.065364
C	4.853058	1.030546	0.597782
H	2.883109	1.817717	0.896646
C	5.615827	-0.021073	0.095775

H	5.589056	-1.934048	-0.895015
H	5.337965	1.881775	1.063344
H	6.697938	0.011922	0.171702
H	0.768091	1.874672	-0.146752
O	-1.494882	-0.286584	0.941517

Vibrational frequencies

25.6831	36.5359	44.4448
71.9956	143.3518	155.0845
178.3924	267.8891	269.9546
306.2741	355.6434	410.9964
421.0569	446.5326	461.2958
480.7773	535.3268	586.0926
594.7035	625.7910	637.7136
647.3337	698.9239	707.0762
747.6592	777.0815	777.8778
788.6512	849.4178	874.0513
889.6978	897.0184	898.1897
943.2495	977.6694	980.2904
1000.9186	1012.1042	1014.7938
1019.9253	1032.3791	1036.9338
1045.9759	1069.6152	1122.9422
1141.1191	1175.0069	1180.1311
1193.0546	1206.3514	1228.5746
1252.2047	1305.5192	1321.0840
1338.0057	1352.2652	1367.5952
1380.9084	1406.5234	1452.9478
1502.6155	1513.8027	1539.0281
1550.2207	1676.5960	1678.9427
1694.1157	1704.6022	1721.9398
1837.8547	3092.0243	3152.4166
3208.6859	3213.0153	3222.9032
3225.3252	3235.1413	3238.4992
3242.0067	3253.5181	3259.4970

TCNE

Zero-point correction= 0.047687

Thermal correction to Energy= 0.056886

Thermal correction to Enthalpy= 0.057830

Thermal correction to Gibbs Free Energy= 0.012559

Sum of electronic and zero-point Energies= -447.316515

Sum of electronic and thermal Energies= -447.307317

Sum of electronic and thermal Enthalpies= -447.306373

Sum of electronic and thermal Free Energies= -447.351644

Cartesian coordinates

C	0.000004	0.678099	0.000000
C	-0.000005	-0.678097	0.000000
C	-1.227082	-1.422245	0.000002
C	1.227063	-1.422260	-0.000002
C	1.227083	1.422246	0.000002
C	-1.227064	1.422262	-0.000002
N	-2.212895	-2.025077	0.000002
N	-2.212871	2.025104	-0.000002
N	2.212898	2.025075	0.000002
N	2.212868	-2.025106	-0.000002

Vibrational frequencies

71.6136	95.7430	111.0875
141.6228	151.1276	250.1761
260.7921	393.7135	444.7782
477.1911	519.8367	548.1641
597.2896	610.0123	612.3419
742.9304	981.4091	1186.7177
1323.2217	1679.0254	2425.8639
2430.4382	2432.9553	2444.2951

***Re*-TS1**

Zero-point correction= 0.481423

Thermal correction to Energy= 0.516560

Thermal correction to Enthalpy= 0.517505

Thermal correction to Gibbs Free Energy= 0.413329

Sum of electronic and zero-point Energies= -3456.562546

Sum of electronic and thermal Energies= -3456.527409

Sum of electronic and thermal Enthalpies= -3456.526465

Sum of electronic and thermal Free Energies= -3456.630640

Cartesian coordinates

C	-6.419737	-0.316659	0.227549
C	-6.557657	-0.590328	-1.134706
C	-5.435404	-0.734108	-1.946930
C	-4.179693	-0.587268	-1.370806
C	-4.047333	-0.302927	-0.012268
C	-5.162796	-0.172035	0.809446
H	-7.303414	-0.218827	0.848588
H	-7.546432	-0.698688	-1.566304
H	-5.536014	-0.955211	-3.004151
H	-5.062185	0.026318	1.870404
C	-1.804572	-0.387944	-0.627869
C	0.040700	-0.061076	0.862371
C	-0.920616	0.830936	1.674118
C	-2.300913	0.191488	1.722634

H	-3.034606	0.904894	2.107889
S	-2.613683	-0.761688	-2.158072
N	-2.707727	-0.180598	0.367975
N	-0.514973	-0.298063	-0.480697
C	-0.378830	1.230356	3.065984
C	-0.744404	0.262646	4.197264
C	-0.846450	2.644622	3.420732
H	0.716310	1.255968	2.981877
H	-0.484414	-0.774210	3.969226
H	-0.213267	0.550672	5.108496
H	-1.816607	0.308942	4.418873
H	-0.489658	3.374813	2.687946
H	-1.940639	2.699758	3.450362
H	-0.473127	2.940593	4.404955
H	-1.020479	1.751626	1.085075
H	0.954717	0.527229	0.724650
C	0.426011	-1.352439	1.560348
C	1.633302	-1.413278	2.259612
C	-0.407528	-2.473285	1.547627
C	1.988781	-2.560296	2.963780
H	2.303799	-0.556558	2.246693
C	-0.053042	-3.621325	2.250899
H	-1.330578	-2.462831	0.973141
C	1.141325	-3.664950	2.967043
H	2.931530	-2.593671	3.500174
H	-0.708150	-4.486239	2.233353
H	1.417255	-4.562067	3.511389
C	1.694896	-1.275479	-1.207609
H	2.285215	-0.684762	-0.516691
C	1.981691	-2.551836	-1.412031
H	1.393468	-3.162978	-2.088562
C	3.098537	-3.228727	-0.693992
F	2.641375	-4.202918	0.110854
F	3.956132	-3.810161	-1.551344
F	3.811731	-2.385457	0.068193
O	-0.139508	-1.328995	-2.720964
C	0.507772	-0.665520	-1.913385
H	-2.318141	-0.701359	2.357067
O	0.798355	0.690900	-2.420616
C	1.247897	1.668519	-1.606298
C	2.612134	1.846476	-1.321811
C	0.365173	2.625296	-1.075354
C	3.059582	2.809805	-0.423839
C	0.784366	3.600858	-0.179525

C	2.129172	3.654734	0.165744
H	4.116345	2.902762	-0.204585
H	0.074346	4.312744	0.225097
Cl	-1.293348	2.634201	-1.586483
Cl	2.663614	4.842867	1.319642
Cl	3.794115	0.881330	-2.152914

Vibrational frequencies

-198.7095	15.5256	25.6649
30.0347	34.5992	42.9973
50.4126	58.8575	66.6333
70.9985	75.5990	85.8667
92.2278	102.5524	115.2448
126.1019	128.1279	134.3326
141.8600	153.5589	177.0556
182.4833	189.0724	197.4372
215.5364	216.6380	235.4085
249.4279	253.6465	269.5006
276.1500	280.6706	299.0529
303.7031	322.3742	325.9009
329.6092	339.4720	376.4454
386.8775	398.6393	415.3502
418.2121	430.2637	432.9928
436.4811	437.8613	452.1789
472.1500	495.9201	510.8702
518.0739	532.1058	538.8901
540.3611	548.5094	553.8338
577.2265	581.5344	593.5751
604.8934	619.2735	625.2981
628.5681	644.4621	658.6394
668.1036	699.6919	720.4769
723.2236	731.0788	755.3106
769.4305	771.0424	788.5852
794.5475	818.3258	826.3315
831.7001	866.7502	871.9726
880.4702	884.6773	897.9834
912.4277	913.6735	917.5733
920.2570	938.1045	945.7115
962.9659	975.6231	997.6584
1004.0093	1012.9964	1014.1159
1019.5663	1024.5569	1027.3591
1037.1915	1064.8577	1069.6932
1072.6704	1073.9570	1093.1486
1106.0371	1118.8855	1129.6647
1138.6305	1157.3273	1169.8740

1178.8379	1183.8307	1186.8172
1189.0018	1191.6564	1214.5652
1217.4613	1230.2484	1231.7677
1251.2817	1258.5829	1289.2464
1296.1216	1302.7967	1310.1860
1314.0717	1324.8456	1328.4941
1347.4550	1356.9802	1362.6220
1365.8687	1367.8147	1371.8684
1384.3969	1395.4567	1406.1643
1414.4005	1420.3692	1435.2500
1440.6822	1445.8236	1493.9151
1500.0515	1503.5831	1507.0070
1511.2934	1517.0514	1518.8394
1520.8896	1535.9682	1554.2686
1620.5058	1632.7170	1662.6798
1681.3793	1682.2601	1689.9676
1697.6559	1720.5276	1802.6302
3056.2905	3058.9938	3065.6792
3089.1467	3095.9613	3100.6875
3134.0847	3138.3671	3147.7258
3149.6321	3167.4284	3189.9413
3200.0428	3212.8713	3216.8175
3221.2852	3223.9215	3233.6965
3236.9131	3243.8967	3244.3945
3246.4479	3250.3889	3265.4685

***Si*-TS1**

Zero-point correction= 0.480460

Thermal correction to Energy= 0.515622

Thermal correction to Enthalpy= 0.516567

Thermal correction to Gibbs Free Energy= 0.412935

Sum of electronic and zero-point Energies= -3456.561897

Sum of electronic and thermal Energies= -3456.526734

Sum of electronic and thermal Enthalpies= -3456.525790

Sum of electronic and thermal Free Energies= -3456.629422

Cartesian coordinates

C	-4.656216	-3.932609	0.802066
C	-4.873768	-4.127705	-0.564935
C	-4.150806	-3.407433	-1.511218
C	-3.200536	-2.496976	-1.061684
C	-2.994764	-2.299784	0.303182
C	-3.714397	-3.015012	1.256546
H	-5.228463	-4.504537	1.524048
H	-5.612596	-4.849194	-0.895566

H	-4.317911	-3.554996	-2.572701
H	-3.544832	-2.867110	2.317131
C	-1.434642	-0.815852	-0.560958
C	0.136550	0.359075	0.788865
C	-1.034803	0.518391	1.785103
C	-1.745576	-0.821843	1.895493
H	-2.706320	-0.711867	2.407389
S	-2.167435	-1.453403	-2.029760
N	-2.021829	-1.328284	0.548903
N	-0.413703	0.010618	-0.535730
C	-0.662207	1.132075	3.154517
C	-0.328961	0.110461	4.246923
C	-1.791989	2.052242	3.627794
H	0.225697	1.757455	2.991613
H	0.440637	-0.601734	3.938895
H	0.031968	0.632072	5.137507
H	-1.222073	-0.452548	4.540708
H	-1.987766	2.845605	2.900629
H	-2.720050	1.485721	3.766727
H	-1.539149	2.515363	4.585582
H	-1.729413	1.213323	1.293976
H	0.618670	1.335903	0.674030
C	1.200082	-0.621503	1.259569
C	2.253673	-0.138929	2.040848
C	1.144935	-1.989670	0.979283
C	3.215901	-1.002639	2.555835
H	2.329045	0.928953	2.236591
C	2.110584	-2.855233	1.488722
H	0.364609	-2.388759	0.337055
C	3.144139	-2.366448	2.283437
H	4.030681	-0.606897	3.154077
H	2.056505	-3.913780	1.255540
H	3.897953	-3.041772	2.674699
C	-0.907164	2.387372	-1.080199
H	-0.224638	2.957330	-0.456498
C	-2.192604	2.704036	-1.157307
H	-2.879032	2.146594	-1.788241
C	-2.787187	3.776982	-0.310801
F	-3.534609	4.634743	-1.020240
F	-3.597781	3.241170	0.627115
F	-1.864602	4.495969	0.346348
O	-1.009057	0.749061	-2.807032
C	-0.385840	1.167633	-1.827342
H	-1.142417	-1.561185	2.432887

O	1.056509	1.427146	-2.043366
C	2.105119	0.749003	-1.550259
C	2.394317	-0.592266	-1.839316
C	3.046362	1.441390	-0.770191
C	3.538492	-1.216877	-1.355824
C	4.212262	0.854897	-0.302576
C	4.436934	-0.483644	-0.595728
H	3.721875	-2.260924	-1.579548
H	4.910126	1.422450	0.301324
Cl	2.706859	3.091532	-0.334419
Cl	5.871985	-1.261013	0.015186
Cl	1.308247	-1.513976	-2.824814

Vibrational frequencies

-108.9718	20.2787	25.8678
32.5008	39.7182	47.2001
53.2836	57.1374	66.2047
74.6424	79.1613	88.3013
96.2542	100.7731	107.0543
116.2828	134.4848	138.7398
141.6223	162.5234	170.1788
180.4896	191.2246	212.0779
214.1321	224.8346	236.2189
240.9346	250.9636	259.8154
263.6789	276.1427	289.7147
302.6914	315.4713	324.8074
326.3920	331.2654	367.5011
386.9640	391.4629	422.4125
424.5682	431.4671	434.6088
436.0737	438.5797	460.4223
474.9882	484.4974	501.3626
518.3445	527.0260	530.5699
548.9080	552.2765	566.0326
577.9464	578.9487	582.4017
609.8486	615.9754	623.0675
629.8381	643.1655	663.2245
674.2408	710.9140	724.8244
727.2303	730.0990	747.8137
769.0389	770.8536	772.9228
789.1010	824.0525	833.8219
836.0280	870.2159	876.0588
878.4519	880.7308	893.2688
896.3974	904.7801	917.7382
925.2424	935.8321	952.0215
967.7087	977.3830	995.6475

999.7457	1010.7462	1014.1203
1015.6358	1018.1500	1022.0281
1024.4397	1040.5213	1064.3285
1067.7929	1073.3682	1083.5372
1105.8725	1114.4310	1125.6435
1136.0102	1156.2303	1165.0398
1171.9043	1177.8520	1180.7207
1183.7048	1187.4268	1211.5600
1215.8802	1226.1781	1226.6878
1238.2833	1247.9140	1288.4480
1295.6673	1302.0296	1305.0478
1310.0072	1318.6709	1324.8765
1329.3431	1344.2415	1360.8300
1363.5832	1365.8117	1368.9097
1378.6432	1395.0707	1407.5782
1414.8582	1418.6277	1434.7095
1443.2849	1445.5455	1495.7869
1500.2051	1504.8469	1508.1907
1508.5449	1516.2524	1520.7003
1523.5588	1534.2442	1551.9630
1580.6101	1641.0099	1660.0253
1677.2195	1678.7923	1686.5174
1689.7563	1696.9552	1788.1012
3055.6432	3062.0099	3066.6598
3077.8593	3091.5197	3120.9466
3133.2876	3140.4871	3146.3120
3151.6882	3156.5835	3183.8191
3202.0658	3208.9300	3217.2304
3217.8167	3221.3385	3226.3959
3226.6598	3233.7618	3235.4947
3240.2796	3243.7197	3254.1446

pre-TS1'

Zero-point correction= 0.289117

Thermal correction to Energy= 0.313816

Thermal correction to Enthalpy= 0.314760

Thermal correction to Gibbs Free Energy= 0.231250

Sum of electronic and zero-point Energies= -2791.389221

Sum of electronic and thermal Energies= -2791.364522

Sum of electronic and thermal Enthalpies= -2791.363578

Sum of electronic and thermal Free Energies= -2791.447087

Cartesian coordinates

C	-4.223041	-0.391258	-0.932845
C	-3.050514	-0.022867	-1.583804

C	-1.863986	-0.627338	-1.213554
C	-1.721286	-1.604668	-0.167340
C	-2.992308	-1.925573	0.422902
C	-4.201326	-1.352038	0.071127
H	-3.061532	0.731171	-2.363468
H	-5.112348	-1.636865	0.586309
O	-0.620941	-2.092541	0.206438
Cl	-2.970593	-3.088238	1.738358
Cl	-0.388772	-0.133940	-2.025058
Cl	-5.741006	0.378443	-1.371775
C	4.936263	-0.030011	0.706521
C	4.776563	-0.339724	-0.658115
C	5.876589	-0.597225	-1.478167
C	7.141832	-0.540004	-0.910741
C	7.312559	-0.232650	0.448586
C	6.220060	0.022180	1.261594
C	2.732409	0.081404	0.629591
H	5.746100	-0.835572	-2.528234
H	8.011468	-0.738389	-1.528609
H	8.313441	-0.194741	0.865607
H	6.335375	0.260548	2.313592
N	3.757796	0.202736	1.403359
S	3.079602	-0.337206	-1.049097
C	1.319265	0.267740	1.069585
H	1.304136	0.273555	2.165150
C	0.727633	1.580059	0.569784
O	1.403709	2.390769	-0.034445
C	-0.717454	1.837006	0.855158
C	-1.293866	2.997950	0.329351
C	-1.502829	0.948057	1.594641
C	-2.639984	3.267896	0.537938
H	-0.668439	3.669125	-0.250085
C	-2.849852	1.225611	1.811444
H	-1.081794	0.022481	1.976609
C	-3.418660	2.380894	1.282598
H	-3.085092	4.165356	0.120534
H	-3.457781	0.525568	2.375395
H	-4.472665	2.586866	1.442382
H	0.686696	-0.567939	0.727471

Vibrational frequencies

22.4428	25.1550	31.8299
39.4055	41.0695	49.7109
53.0284	78.2485	95.6333
110.7601	132.7905	146.3850

151.9678	168.8542	177.0383
184.5750	196.4973	198.4958
232.1370	282.5290	307.3018
309.3276	342.0753	348.3955
376.7466	386.2082	409.8367
417.8152	430.6896	431.4903
442.3477	459.5398	493.9121
513.9715	530.0707	544.7366
554.8770	585.1365	611.2555
616.3836	625.8066	656.2332
677.1858	709.3356	721.1187
726.5664	748.5898	749.6499
757.0324	773.9937	782.0862
797.9793	841.0114	868.4468
876.0316	881.1612	885.0771
885.1845	885.5884	950.0751
972.3695	986.3946	1003.8037
1010.4516	1012.7188	1026.8059
1031.7980	1056.5431	1071.3991
1089.7892	1091.0987	1124.3709
1153.0420	1156.5949	1174.6473
1181.0139	1183.1894	1186.1613
1210.5501	1233.1319	1273.1827
1278.1967	1286.6957	1320.8150
1351.0271	1365.9088	1371.5306
1387.2126	1388.4576	1470.0610
1472.9527	1492.4649	1503.5046
1515.1461	1552.7954	1587.2062
1606.1673	1641.1351	1651.6353
1666.5727	1677.3727	1695.5918
1696.2396	1821.4907	3011.7406
3110.9387	3203.7390	3206.0171
3213.1707	3214.8556	3220.2680
3222.6656	3223.0989	3224.7218
3229.8748	3231.5447	3236.8865

TS1'

Zero-point correction= 0.283712

Thermal correction to Energy= 0.307693

Thermal correction to Enthalpy= 0.308637

Thermal correction to Gibbs Free Energy= 0.227204

Sum of electronic and zero-point Energies= -2791.381039

Sum of electronic and thermal Energies= -2791.357057

Sum of electronic and thermal Enthalpies= -2791.356113

Sum of electronic and thermal Free Energies= -2791.437546

Cartesian coordinates

C	-4.586077	0.731369	0.299203
C	-4.623187	-0.468882	-0.437298
C	-5.810011	-1.183474	-0.602130
C	-6.967134	-0.687692	-0.014409
C	-6.941660	0.505950	0.722843
C	-5.762796	1.218391	0.883555
C	-2.437889	0.661031	-0.260208
H	-5.828715	-2.105495	-1.174388
H	-7.900436	-1.229630	-0.127998
H	-7.857727	0.875426	1.172796
H	-5.731005	2.141796	1.452611
N	-3.346239	1.338610	0.381886
S	-3.030143	-0.819684	-1.053596
C	-1.029981	1.044748	-0.278884
H	-0.465945	0.603332	0.874864
C	-0.147934	0.484626	-1.300097
O	-0.441507	-0.511873	-1.963283
C	1.229091	1.083322	-1.466100
C	2.192535	0.312597	-2.125799
C	1.586139	2.344061	-0.979089
C	3.490166	0.783858	-2.284429
H	1.901008	-0.665118	-2.494984
C	2.883815	2.820194	-1.144674
H	0.861887	2.962864	-0.460864
C	3.839442	2.040581	-1.791693
H	4.232599	0.168899	-2.784084
H	3.149946	3.799297	-0.758967
H	4.852869	2.411271	-1.911478
H	-0.926688	2.112472	-0.094514
C	2.469192	-2.097673	0.359372
C	1.320665	-1.518329	0.881397
C	1.298567	-0.248333	1.507374
C	2.566558	0.377905	1.602067
C	3.732268	-0.166888	1.090772
C	3.666331	-1.404293	0.460998
H	2.421984	-3.065205	-0.126938
H	4.669879	0.371718	1.164120
O	0.200813	0.323150	1.915455
Cl	2.635069	1.945053	2.364574
Cl	-0.189536	-2.379832	0.753053
Cl	5.121717	-2.090254	-0.229382

Vibrational frequencies

-1229.0203	16.5069	19.3618
32.6347	47.3434	52.8676
62.3111	72.9852	78.2535
106.3684	130.3404	143.4825
169.8076	173.2847	186.7830
198.5558	203.2121	207.9091
219.0285	235.1960	296.5121
316.3381	331.4259	361.4220
382.7270	389.7661	401.9724
411.7892	433.9050	442.7472
447.4904	459.3683	507.2699
510.9120	516.8487	547.3723
558.7321	572.5310	606.0190
625.5159	628.0118	650.3860
670.8762	687.6148	701.4452
719.9506	725.2503	749.4495
753.2310	754.1358	777.5897
796.9121	812.2075	857.7601
859.7948	870.6452	882.6893
884.9611	887.9719	895.2142
927.9359	946.4280	965.7759
998.2004	1002.2414	1015.8830
1019.3120	1057.9074	1062.7436
1069.4953	1094.9467	1106.5937
1113.3478	1154.9248	1166.8434
1172.8842	1180.7062	1192.6359
1214.3977	1228.1353	1245.7900
1285.2130	1290.6054	1298.6626
1319.3133	1332.9772	1361.1839
1368.7554	1374.2653	1403.8779
1452.4921	1494.0312	1497.3015
1508.8776	1515.5679	1542.7531
1571.5010	1591.9652	1616.5945
1651.2290	1670.6837	1677.7059
1690.4843	1692.7774	1759.3552
3179.9336	3196.6035	3201.7225
3204.3259	3213.0937	3217.2504
3221.9688	3224.8203	3228.4858
3228.7238	3232.6038	3237.1462

hou-TS1'

Zero-point correction= 0.288944

Thermal correction to Energy= 0.313115

Thermal correction to Enthalpy= 0.314059

Thermal correction to Gibbs Free Energy= 0.233575

Sum of electronic and zero-point Energies= -2791.385445

Sum of electronic and thermal Energies= -2791.361274

Sum of electronic and thermal Enthalpies= -2791.360330

Sum of electronic and thermal Free Energies= -2791.440813

Cartesian coordinates

C	3.183225	1.983573	0.099891
C	1.810958	2.023316	0.312417
C	1.140549	1.034703	1.042601
C	1.924858	0.002213	1.578087
C	3.294110	-0.077556	1.368385
C	3.905943	0.922228	0.625758
H	3.669517	2.757676	-0.481361
H	3.864513	-0.904465	1.773771
Cl	1.144366	-1.224451	2.532801
Cl	0.887037	3.325148	-0.370885
Cl	5.623200	0.828072	0.327831
O	-0.188127	1.115251	1.232366
H	-0.594117	0.257752	0.953221
C	-4.582771	-0.705526	0.437393
C	-4.604333	0.359838	-0.489466
C	-5.761982	1.098147	-0.721693
C	-6.917400	0.770341	-0.017451
C	-6.909724	-0.284510	0.905142
C	-5.756889	-1.021979	1.136990
C	-2.456698	-0.846922	-0.211550
H	-5.764026	1.915273	-1.436903
H	-7.828289	1.335633	-0.186066
H	-7.818713	-0.528462	1.446626
H	-5.742818	-1.841319	1.849001
N	-3.379612	-1.358215	0.575953
S	-3.021244	0.531544	-1.215051
C	-1.112136	-1.295450	-0.270556
H	-0.878119	-2.136130	0.369174
C	-0.174333	-0.792871	-1.202819
O	-0.399313	0.175136	-1.963348
C	1.207005	-1.410982	-1.243041
C	2.217189	-0.691932	-1.888532
C	1.526642	-2.639866	-0.656595
C	3.520909	-1.174606	-1.931013
H	1.951532	0.257626	-2.341925
C	2.832256	-3.122411	-0.691244
H	0.755757	-3.230983	-0.173587
C	3.835288	-2.388786	-1.323118

H	4.297921	-0.597414	-2.424206
H	3.065314	-4.076311	-0.227647
H	4.853990	-2.764026	-1.346320

Vibrational frequencies

24.5509	26.7159	38.5632
48.6123	56.6660	72.1251
85.4489	93.8371	111.7812
130.2926	158.8076	172.1603
182.7335	189.9276	199.4822
199.8230	217.6912	224.0256
236.1748	237.0348	298.0439
322.2771	339.4191	372.3492
384.9236	388.3578	404.3702
428.7609	435.6245	440.3857
449.3899	479.2710	513.1262
517.9318	545.2966	556.3216
571.7094	578.4614	597.7899
627.8555	641.4663	644.7538
668.8199	707.4634	712.4198
714.9077	720.8132	729.2826
748.8721	748.9703	771.0468
779.5967	815.6369	819.2249
864.2665	875.2975	875.8950
883.0137	885.0013	886.7758
916.2295	952.9659	957.6994
998.9452	1005.7275	1017.1467
1030.4043	1054.0645	1066.2705
1088.3447	1102.1270	1110.5856
1122.4307	1147.2992	1169.4380
1173.4041	1174.3580	1195.7481
1215.8831	1240.0857	1262.6765
1280.8829	1288.0914	1321.7963
1327.4863	1336.7178	1361.2450
1363.1581	1380.9725	1452.9671
1473.2051	1490.2721	1496.8779
1505.4852	1532.8556	1541.0551
1555.1805	1644.7718	1648.5921
1651.8602	1675.9761	1684.2591
1689.8512	1693.9313	3193.8980
3194.0610	3200.8900	3203.9097
3209.6100	3214.2146	3221.2873
3222.4657	3225.4937	3239.4194
3248.0829	3259.9533	3347.4665

pre-TS1''

Zero-point correction= 0.489570

Thermal correction to Energy= 0.517159

Thermal correction to Enthalpy= 0.518103

Thermal correction to Gibbs Free Energy= 0.429282

Sum of electronic and zero-point Energies= -1476.482594

Sum of electronic and thermal Energies= -1476.455005

Sum of electronic and thermal Enthalpies= -1476.454061

Sum of electronic and thermal Free Energies= -1476.542883

Cartesian coordinates

N	-1.079957	2.362598	0.439550
C	-2.509754	2.336079	0.803519
H	-2.777921	3.257590	1.354099
C	-2.785784	1.137784	1.714173
H	-3.815754	1.172585	2.080685
H	-2.661743	0.213798	1.139997
H	-2.122336	1.098796	2.581000
C	-3.424934	2.228827	-0.414515
H	-4.450732	2.056945	-0.077564
H	-3.425311	3.127299	-1.035402
H	-3.128338	1.374330	-1.033167
C	-0.749391	3.227642	-0.709665
H	-1.363891	2.871558	-1.542729
C	-1.064169	4.714232	-0.494510
H	-0.437976	5.146164	0.292858
H	-0.872512	5.276120	-1.413397
H	-2.110829	4.871082	-0.216860
C	0.704959	3.034468	-1.136648
H	0.933137	1.978093	-1.307592
H	0.889567	3.582746	-2.065161
H	1.405711	3.418105	-0.387862
C	-0.228954	2.619354	1.616748
H	0.354455	3.536257	1.475179
H	-0.860024	2.813064	2.492188
C	0.718619	1.462289	1.909431
H	0.161887	0.527429	2.040121
H	1.417655	1.321161	1.078403
H	1.300013	1.648157	2.817938
C	3.472124	-0.428390	-0.848470
C	3.674531	-1.201249	0.308127
C	4.957535	-1.434232	0.809236
C	6.032769	-0.875272	0.134288
C	5.839642	-0.099470	-1.021181
C	4.567905	0.128599	-1.519446

C	1.353729	-0.907715	-0.420127
H	5.109364	-2.032391	1.701499
H	7.038560	-1.039301	0.506691
H	6.699698	0.326218	-1.527267
H	4.400927	0.723915	-2.410973
N	2.146730	-0.288061	-1.232180
S	2.138189	-1.754232	0.915299
C	-0.130534	-0.841651	-0.630213
H	-0.309162	-0.963349	-1.700805
C	-0.979157	-1.789413	0.184252
O	-0.553190	-2.286407	1.212209
C	-2.385893	-2.045975	-0.254482
C	-3.179911	-2.865337	0.556356
C	-2.935801	-1.477017	-1.407928
C	-4.502545	-3.115922	0.216832
H	-2.739489	-3.292085	1.450995
C	-4.264138	-1.723480	-1.742920
H	-2.341767	-0.835502	-2.050091
C	-5.046462	-2.543510	-0.933374
H	-5.113095	-3.753189	0.847737
H	-4.685922	-1.277143	-2.637086
H	-6.081206	-2.737055	-1.197370
H	-0.472186	0.181963	-0.367022

Vibrational frequencies

16.0019	18.8416	28.0864
33.2170	39.5960	57.8661
64.3032	71.2891	82.7815
96.4611	104.2146	125.7624
146.6260	151.8752	167.4375
180.4752	187.8435	198.6287
208.0562	228.9738	243.0029
247.5798	271.9558	289.6008
315.1476	320.1985	326.7103
335.6414	368.0045	394.2829
401.9569	409.8709	415.6072
428.6028	439.8148	454.1099
466.4315	485.8970	515.8029
516.3987	518.7417	540.9365
582.7540	583.3384	622.1681
626.0375	661.4514	674.4506
707.5984	713.8726	727.7509
743.2986	748.5960	779.4498
780.2957	788.4999	850.6744
869.5150	881.1209	883.6106

898.6691	904.9881	926.6966
938.7195	939.6127	959.9318
970.4245	972.5814	976.6163
981.1962	1011.4489	1013.0983
1016.4344	1025.4466	1038.1451
1041.0119	1051.7279	1069.7474
1083.9660	1096.0883	1112.4161
1124.2702	1139.7022	1140.9228
1151.1454	1163.8727	1182.2172
1185.0501	1187.9872	1204.5822
1206.1612	1218.7114	1245.5669
1247.1455	1254.2065	1263.3781
1280.5082	1316.1065	1345.0218
1345.6705	1363.5464	1367.2036
1367.7216	1368.3800	1376.7631
1390.8053	1406.9857	1407.1775
1411.9872	1419.2391	1425.1642
1428.8790	1434.3420	1442.8528
1484.0879	1488.1830	1490.0780
1492.2334	1494.0420	1498.3426
1501.9209	1503.2022	1508.0592
1512.0407	1514.1775	1518.7619
1526.9965	1540.0110	1551.3161
1618.5304	1649.4437	1674.1808
1691.3928	1693.0332	1817.3566
2932.9163	2964.7099	3053.0981
3060.4101	3063.1897	3067.5491
3069.3825	3073.4848	3099.9183
3102.1545	3136.5288	3139.4677
3140.9965	3142.6657	3143.7662
3144.1750	3145.5922	3149.8586
3156.1184	3164.8236	3166.5915
3205.6494	3211.7709	3214.4209
3221.4532	3226.6895	3229.4488
3230.9026	3242.6214	3247.4892

TS1''

Zero-point correction= 0.487396

Thermal correction to Energy= 0.513575

Thermal correction to Enthalpy= 0.514519

Thermal correction to Gibbs Free Energy= 0.430718

Sum of electronic and zero-point Energies= -1476.463005

Sum of electronic and thermal Energies= -1476.436826

Sum of electronic and thermal Enthalpies= -1476.435882

Sum of electronic and thermal Free Energies= -1476.519683

Cartesian coordinates

C	-3.370122	-0.346058	-0.850333
C	-3.600047	-1.146499	0.284753
C	-4.894036	-1.442824	0.714010
C	-5.961387	-0.926158	-0.009126
C	-5.743255	-0.126269	-1.141350
C	-4.457364	0.167860	-1.567986
C	-1.247738	-0.726472	-0.315247
H	-5.063520	-2.060731	1.589852
H	-6.976214	-1.144452	0.306799
H	-6.593779	0.266448	-1.689176
H	-4.273768	0.783852	-2.442303
N	-2.037706	-0.130109	-1.160687
S	-2.072035	-1.631581	0.973083
C	0.208524	-0.637304	-0.416062
H	0.555598	0.636787	0.046670
C	1.042701	-1.523846	0.383867
O	0.678109	-1.999636	1.462634
C	2.458044	-1.755913	-0.069994
C	3.456992	-1.825565	0.905951
C	2.799461	-1.918414	-1.414876
C	4.785092	-2.011983	0.539573
H	3.173295	-1.721284	1.948883
C	4.126081	-2.133148	-1.779972
H	2.028189	-1.894799	-2.179259
C	5.120949	-2.166544	-0.805520
H	5.558505	-2.045667	1.300301
H	4.382303	-2.271966	-2.825256
H	6.156369	-2.321478	-1.091817
H	0.507714	-0.530331	-1.457806
N	0.973479	1.882719	0.445303
C	2.460529	1.858034	0.180667
H	2.802631	1.054766	0.842701
C	2.889074	1.454177	-1.234492
H	3.843756	0.924971	-1.158923
H	2.182182	0.781957	-1.719748
H	3.042048	2.323636	-1.877810
C	3.161306	3.154824	0.584284
H	2.937258	3.456336	1.610169
H	4.241813	3.009620	0.503446
H	2.890469	3.973465	-0.088816
C	0.200629	2.951988	-0.277159
H	0.691907	3.909076	-0.053579

C	0.163917	2.731122	-1.789536
H	1.130425	2.841199	-2.274535
H	-0.253583	1.744324	-2.015434
H	-0.504920	3.477570	-2.225357
C	-1.248161	3.041867	0.207902
H	-1.341614	3.274396	1.269218
H	-1.736367	3.847525	-0.345505
H	-1.783987	2.112619	-0.010875
C	0.774485	1.979587	1.927596
H	1.721617	1.722754	2.406745
H	0.570601	3.023747	2.188612
C	-0.296787	1.050292	2.484480
H	-0.006689	0.003580	2.364251
H	-0.407687	1.249927	3.554067
H	-1.270595	1.189749	2.013201

Vibrational frequencies

-1239.2393	11.8881	28.3127
32.5220	49.4196	55.3988
77.7306	80.3689	93.4525
121.8724	127.1762	140.8929
146.6673	158.4369	191.9115
208.7191	211.5651	229.2834
232.2703	245.2326	262.5644
286.6106	291.8061	299.0812
309.1323	319.2718	331.5781
353.7855	370.7006	384.8431
398.3008	402.2571	417.6366
425.3474	444.4879	451.8517
475.0721	485.8846	499.6233
514.8525	540.9500	553.6773
567.8444	595.6053	624.8579
640.8043	656.2146	672.1263
700.3743	711.7641	721.3011
734.5148	744.9874	774.8632
793.5699	808.3478	817.9516
867.0031	872.6094	877.6058
877.7184	897.7476	909.2073
940.4357	945.4911	951.9299
960.8265	962.2425	964.2599
974.0134	980.7373	993.6917
1001.2457	1001.7992	1017.1156
1024.9508	1053.7454	1065.3577
1080.9099	1095.8450	1096.7883
1109.7936	1121.9390	1136.8237

1146.7465	1150.7324	1174.8012
1177.9462	1179.0584	1191.0987
1199.4663	1213.4335	1215.2822
1230.4551	1236.8844	1251.5797
1282.1541	1318.5324	1335.0747
1336.2507	1355.4282	1360.1551
1363.7253	1364.6317	1381.3665
1406.1046	1407.6900	1415.9171
1423.7930	1430.3827	1440.2669
1443.8828	1461.4403	1482.0267
1492.3955	1495.5201	1497.1222
1498.7704	1502.7008	1504.3952
1511.1640	1512.0071	1513.6241
1518.9063	1524.5921	1537.6168
1541.0655	1545.1774	1554.7739
1559.1537	1598.6645	1648.6150
1671.2942	1689.3896	1695.4880
1743.1443	3059.9428	3073.2574
3079.1952	3079.8374	3084.2191
3086.8270	3088.3430	3094.2080
3138.8129	3147.9024	3151.9822
3155.5297	3161.5954	3163.2292
3164.6151	3166.7956	3176.2993
3195.5465	3197.0471	3199.0137
3201.2663	3204.3055	3208.8650
3210.8600	3217.6400	3219.7193
3222.4920	3225.0798	3226.6170

hou-TS1''

Zero-point correction= 0.492366

Thermal correction to Energy= 0.519336

Thermal correction to Enthalpy= 0.520280

Thermal correction to Gibbs Free Energy= 0.435105

Sum of electronic and zero-point Energies= -1476.479513

Sum of electronic and thermal Energies= -1476.452543

Sum of electronic and thermal Enthalpies= -1476.451599

Sum of electronic and thermal Free Energies= -1476.536775

Cartesian coordinates

C	2.820964	-0.848100	-0.958512
C	2.911937	-1.798135	0.081586
C	4.143583	-2.206642	0.586020
C	5.302255	-1.663124	0.038121
C	5.225373	-0.721180	-0.996690
C	3.997832	-0.310589	-1.499568

C	0.631910	-1.127311	-0.619972
H	4.200746	-2.931397	1.392297
H	6.270768	-1.972683	0.416616
H	6.139420	-0.307795	-1.411586
H	3.928328	0.418678	-2.301050
N	1.544162	-0.488534	-1.330546
S	1.303160	-2.240551	0.613135
C	-0.760501	-0.939388	-0.770753
H	-1.064631	-0.356935	-1.631898
C	-1.711384	-1.522127	0.094283
O	-1.413603	-2.207736	1.098066
C	-3.172715	-1.236940	-0.158514
C	-4.048993	-1.327884	0.927431
C	-3.685474	-0.893167	-1.413845
C	-5.404620	-1.057780	0.771253
H	-3.637972	-1.616709	1.889786
C	-5.044087	-0.631853	-1.574135
H	-3.028470	-0.853172	-2.277468
C	-5.905753	-0.707409	-0.481552
H	-6.072697	-1.123024	1.624528
H	-5.431626	-0.375816	-2.555325
H	-6.963919	-0.501079	-0.608072
N	0.130006	2.013139	0.439368
C	-0.606666	2.848807	-0.598901
H	-0.494624	3.883689	-0.262808
C	-2.088107	2.483856	-0.616585
H	-2.577256	3.090812	-1.381082
H	-2.235467	1.430331	-0.870645
H	-2.588274	2.687451	0.331910
C	0.029172	2.656767	-1.972503
H	-0.641445	3.069073	-2.728369
H	0.987985	3.170865	-2.063074
H	0.190834	1.594583	-2.184747
C	1.642733	2.221303	0.417884
H	1.938554	1.893156	-0.579781
C	2.001298	3.682382	0.640333
H	1.593875	4.057143	1.584692
H	3.089487	3.757397	0.698932
H	1.667705	4.332198	-0.171230
C	2.321085	1.304537	1.431118
H	1.846593	0.319649	1.473797
H	3.356339	1.153494	1.114731
H	2.335584	1.735005	2.435554
C	-0.463628	2.167437	1.823698

H	0.358665	2.311667	2.521839
H	-1.056473	3.083425	1.826318
C	-1.282045	0.949252	2.219515
H	-2.149632	0.811820	1.569404
H	-0.685439	0.031758	2.177082
H	-1.637766	1.081013	3.243605
H	-0.025106	1.027609	0.151331

Vibrational frequencies

23.2138	28.3478	31.6530
40.9535	65.3230	70.7644
76.1455	93.7893	100.4268
116.2868	127.3480	155.7239
159.0359	160.3639	171.8513
207.1868	211.6805	221.5952
228.9191	232.7502	246.6243
250.6160	265.6278	280.5997
295.9686	316.4768	342.3960
344.2955	361.8344	390.2953
401.8155	413.0755	419.5870
432.4316	441.6323	448.0162
471.2478	488.2841	492.3411
512.1923	549.2281	565.5505
586.7127	628.8139	635.8977
646.1713	669.9566	709.4146
712.6516	717.3905	727.6781
744.3172	750.5300	777.9700
783.9514	793.2749	818.8369
863.0738	875.0866	878.7564
880.8190	905.1679	918.0205
945.4556	953.2479	958.5315
959.3891	960.0624	962.8517
974.1477	984.2677	1003.1038
1004.0418	1017.6159	1024.9579
1055.4826	1055.9056	1069.1074
1087.5407	1090.8289	1105.8424
1115.9726	1129.5341	1146.3861
1151.1797	1162.6817	1176.0722
1177.6066	1188.3238	1202.2157
1202.2888	1213.5600	1219.3640
1244.9521	1262.8170	1285.7125
1318.3882	1323.1461	1339.4240
1343.8732	1353.8775	1362.4010
1363.1537	1376.1751	1385.7252
1397.5808	1422.3810	1428.2961

1432.7158	1438.4379	1441.5244
1450.3204	1461.3074	1475.1641
1481.0387	1487.5898	1491.1597
1494.7724	1495.7076	1497.4836
1500.3848	1501.6802	1507.3336
1509.4972	1513.6577	1518.6979
1527.7859	1540.0329	1543.1367
1557.1530	1646.4774	1652.3727
1681.8371	1689.1949	1696.0516
3069.4742	3076.5411	3078.7521
3082.9903	3084.5753	3121.5121
3137.8414	3148.5120	3157.1712
3158.0859	3160.5012	3163.7171
3167.6542	3170.4757	3171.2991
3172.6254	3174.3169	3176.8508
3197.3734	3198.1115	3203.6537
3206.3519	3208.6074	3216.2937
3218.2430	3221.2462	3226.5341
3229.8915	3248.3040	3260.3715

***Re*-M1**

Zero-point correction= 0.481681

Thermal correction to Energy= 0.518237

Thermal correction to Enthalpy= 0.519181

Thermal correction to Gibbs Free Energy= 0.410369

Sum of electronic and zero-point Energies= -3456.576306

Sum of electronic and thermal Energies= -3456.539750

Sum of electronic and thermal Enthalpies= -3456.538806

Sum of electronic and thermal Free Energies= -3456.647618

Cartesian coordinates

C	-5.148982	-3.389985	0.592049
C	-5.052071	-4.033586	-0.648385
C	-3.944476	-3.847856	-1.464300
C	-2.937487	-2.998307	-1.012456
C	-3.045142	-2.350324	0.215518
C	-4.148931	-2.540510	1.045182
H	-6.019927	-3.558844	1.215247
H	-5.850937	-4.689463	-0.975261
H	-3.861483	-4.347425	-2.422966
H	-4.226564	-2.055860	2.011081
C	-0.995696	-1.575942	-0.483519
C	0.468218	-0.094710	0.841527
C	-0.854149	0.409011	1.450341
C	-1.794564	-0.755141	1.704127

H	-2.789994	-0.392594	1.968071
S	-1.434311	-2.599629	-1.819755
N	-1.929478	-1.542265	0.472577
N	0.171946	-0.908870	-0.369556
C	-0.664943	1.294962	2.705187
C	-0.507009	0.526262	4.024655
C	-1.840565	2.268021	2.841104
H	0.244204	1.887736	2.530204
H	0.266031	-0.243478	3.995306
H	-0.249267	1.230813	4.819960
H	-1.452959	0.052964	4.311537
H	-1.967093	2.874330	1.941839
H	-2.776615	1.728634	3.025566
H	-1.679228	2.938348	3.689786
H	-1.310169	1.037666	0.672491
H	0.987743	0.790289	0.470270
C	1.375058	-0.852397	1.786052
C	2.420570	-0.167253	2.410584
C	1.166859	-2.201413	2.079540
C	3.221312	-0.812357	3.347672
H	2.599880	0.877522	2.163979
C	1.969067	-2.847203	3.016582
H	0.382940	-2.760537	1.573066
C	2.991204	-2.151394	3.658251
H	4.028152	-0.271941	3.831284
H	1.797537	-3.894605	3.241230
H	3.615793	-2.655194	4.388346
C	2.547384	-0.620629	-1.054691
H	2.713179	0.182677	-0.352623
C	3.563024	-1.206455	-1.676892
H	3.421395	-1.999062	-2.404162
C	4.975927	-0.799210	-1.412957
F	5.699188	-1.837366	-0.962791
F	5.574190	-0.364624	-2.531605
F	5.067307	0.176957	-0.500350
O	0.912813	-1.744787	-2.353373
C	1.171836	-1.093266	-1.365958
H	-1.436929	-1.419122	2.498393
O	1.018941	1.371560	-1.901263
C	0.132125	2.152914	-1.456429
C	0.382421	3.171762	-0.474293
C	-1.252871	2.100936	-1.830766
C	-0.567348	4.052627	0.012050
C	-2.230576	2.963070	-1.362771

C	-1.877428	3.947960	-0.446522
H	-0.295000	4.803910	0.745838
H	-3.254577	2.867094	-1.706624
Cl	-1.707258	0.836154	-2.951563
Cl	-3.098888	5.046353	0.164379
Cl	2.024310	3.275242	0.134830

Vibrational frequencies

13.7524	22.2914	26.0474
31.4119	37.5011	38.8447
44.3023	54.9628	64.9514
67.2472	71.8458	81.3557
84.5107	97.8311	110.6027
122.1098	127.0080	134.6147
151.1445	164.5071	174.0822
178.0728	186.7647	195.9117
205.0733	209.5212	225.8975
228.3988	241.0043	246.5584
261.1736	264.8817	274.4175
296.9505	299.2274	312.3748
318.8281	336.0574	344.9014
376.7515	378.7173	391.2116
393.3675	408.6437	420.4301
430.6872	434.6691	439.4995
443.0318	470.0922	489.6922
494.2569	516.5410	520.7524
545.4629	548.2039	560.4455
562.7474	581.1874	611.3124
612.2818	625.4077	627.4644
640.7943	658.7946	670.1428
709.8920	718.2851	726.4904
733.5809	734.6667	750.0741
762.3688	764.8839	775.8625
792.9330	799.3860	825.8962
865.5119	872.3137	884.1259
886.5027	886.8864	887.0768
890.3683	894.3900	920.3296
935.0917	945.9324	964.6865
970.2876	978.7802	991.8040
1001.9132	1010.3404	1012.5893
1019.0108	1024.1666	1036.1378
1042.1824	1060.4942	1068.0314
1070.6970	1090.7158	1092.6440
1113.0449	1126.5209	1144.3412
1155.3168	1158.9399	1176.0609

1179.7203	1185.6258	1190.9148
1191.5034	1203.7426	1212.1050
1213.5320	1237.6811	1243.5881
1263.1319	1270.8710	1277.9785
1291.5190	1307.3805	1315.5480
1324.8784	1330.0212	1348.9279
1359.5791	1362.7170	1364.5634
1372.7613	1379.9158	1384.0650
1386.6730	1405.3125	1407.0676
1413.3801	1431.9993	1437.5387
1452.7982	1461.3086	1485.3122
1493.5370	1504.5953	1508.3063
1512.8134	1515.0631	1522.1694
1528.3169	1554.1864	1585.2393
1590.9610	1603.2347	1659.7372
1677.4914	1679.9376	1688.8378
1700.5282	1793.6229	1840.4579
3057.4722	3061.2737	3066.4454
3070.4422	3102.0680	3133.0449
3136.9204	3164.7265	3166.5636
3171.6770	3173.2529	3193.7576
3198.2283	3213.1728	3219.2439
3220.2893	3228.4239	3230.1332
3230.7752	3239.5426	3241.0600
3246.0456	3247.2135	3298.0610

M1-OAR

Zero-point correction= 0.416658

Thermal correction to Energy= 0.442585

Thermal correction to Enthalpy= 0.443529

Thermal correction to Gibbs Free Energy= 0.359547

Sum of electronic and zero-point Energies= -1771.035698

Sum of electronic and thermal Energies= -1771.009771

Sum of electronic and thermal Enthalpies= -1771.008827

Sum of electronic and thermal Free Energies= -1771.092810

Cartesian coordinates

C	-5.837317	-0.662048	0.331909
C	-5.776092	-2.040700	0.578313
C	-4.566743	-2.719954	0.548994
C	-3.417314	-1.985300	0.264592
C	-3.484667	-0.617927	0.010442
C	-4.695817	0.072201	0.044694
H	-6.794615	-0.154908	0.369154
H	-6.686707	-2.585405	0.799582

H	-4.514809	-3.785036	0.743053
H	-4.749720	1.139686	-0.132568
C	-1.224252	-0.966370	-0.185537
C	0.431142	0.824594	-0.607740
C	-0.727322	1.480191	-1.379366
C	-2.020111	1.334291	-0.596961
H	-2.873550	1.643445	-1.203420
S	-1.771168	-2.574509	0.165303
N	-2.217685	-0.081079	-0.258375
N	0.078135	-0.600379	-0.335633
C	-0.441190	2.947336	-1.784967
C	-0.872937	3.990321	-0.747005
C	-1.106413	3.248822	-3.130797
H	0.644115	3.032630	-1.923628
H	-0.477408	3.793034	0.252629
H	-0.516407	4.975087	-1.058848
H	-1.965131	4.049141	-0.682164
H	-0.734653	2.586182	-3.916756
H	-2.193525	3.127206	-3.067040
H	-0.907406	4.280770	-3.430538
H	-0.836792	0.893798	-2.300851
H	1.276129	0.792360	-1.300388
C	0.843077	1.544101	0.658641
C	1.910896	2.443757	0.603556
C	0.153289	1.370293	1.860760
C	2.262288	3.187570	1.726208
H	2.467741	2.566682	-0.322530
C	0.505685	2.115574	2.983144
H	-0.656203	0.647680	1.936887
C	1.554372	3.029887	2.915182
H	3.091516	3.884607	1.672047
H	-0.036387	1.976503	3.912302
H	1.827348	3.608403	3.791113
C	2.494943	-1.112091	-0.185307
H	2.733809	-0.080527	0.041664
C	3.455321	-2.005481	-0.398161
H	3.240532	-3.048391	-0.611148
C	4.904536	-1.626207	-0.352461
F	5.549982	-2.346730	0.571995
F	5.493770	-1.864456	-1.530663
F	5.081097	-0.332660	-0.060990
O	0.785529	-2.752698	-0.113174
C	1.085386	-1.582340	-0.208952
H	-2.014775	1.912484	0.331878

Vibrational frequencies

22.0135	28.8385	36.7441
43.7646	61.4978	62.1024
78.7375	85.1018	95.5454
115.7904	123.6911	129.4569
157.5260	177.2986	181.1586
219.1464	221.5224	236.1446
244.5676	253.6967	275.9622
291.0313	306.9613	310.9744
316.5193	335.3131	378.8816
389.0809	406.5054	418.2629
432.1921	434.8688	443.2477
465.4941	489.1633	514.2300
522.3315	543.6566	547.6574
560.0109	578.2426	609.1709
624.0933	627.5620	641.3260
658.0857	672.9078	715.3459
727.7845	729.6817	735.5168
740.4531	765.6694	775.2540
791.7783	825.4675	864.0812
874.0154	878.5444	882.7538
919.5649	925.4696	938.1290
948.1712	964.7518	974.5870
980.5366	1006.0579	1007.5310
1011.4007	1019.3012	1028.8366
1029.2841	1040.1112	1042.8289
1062.5307	1067.5456	1070.3034
1090.7563	1111.0100	1128.2174
1153.6948	1158.8489	1176.9429
1185.9987	1187.2263	1192.5814
1205.5844	1209.4873	1215.8764
1238.6916	1255.8464	1258.8396
1272.7881	1291.6099	1309.4131
1320.6705	1328.9490	1332.2302
1343.9711	1351.4285	1359.1227
1364.5802	1367.3111	1379.6658
1381.7432	1396.1585	1409.2937
1419.0361	1428.2714	1438.0564
1443.5445	1488.8035	1495.9987
1506.1329	1509.6271	1515.5419
1518.8899	1521.0510	1526.7022
1553.5402	1604.7602	1679.4411
1681.9467	1690.6019	1696.0049
1785.6806	1829.5056	3063.7751

3069.0303	3074.3595	3078.2665
3110.2261	3129.1550	3141.6726
3146.5422	3158.2738	3164.1434
3175.8322	3192.9742	3198.1488
3221.2824	3225.4237	3225.7047
3232.1616	3241.2928	3245.9580
3249.5988	3250.8858	3274.0244

***Si*-M1**

Zero-point correction= 0.481701

Thermal correction to Energy= 0.518069

Thermal correction to Enthalpy= 0.519013

Thermal correction to Gibbs Free Energy= 0.411965

Sum of electronic and zero-point Energies= -3456.573613

Sum of electronic and thermal Energies= -3456.537245

Sum of electronic and thermal Enthalpies= -3456.536301

Sum of electronic and thermal Free Energies= -3456.643349

Cartesian coordinates

C	5.890973	1.283232	-0.464673
C	5.753016	1.564312	-1.829766
C	4.660196	1.098382	-2.549129
C	3.709061	0.339233	-1.872130
C	3.855750	0.058052	-0.515408
C	4.945038	0.527277	0.214796
H	6.748507	1.666738	0.076592
H	6.507188	2.158608	-2.333065
H	4.545446	1.321053	-3.603881
H	5.045308	0.327940	1.275373
C	1.842625	-0.960546	-0.938203
C	0.485946	-2.131523	0.760983
C	1.859727	-2.468354	1.370495
C	2.752433	-1.236833	1.338163
H	3.777735	-1.499109	1.609899
S	2.238851	-0.360079	-2.515907
N	2.789632	-0.709473	-0.030231
N	0.709205	-1.619739	-0.621655
C	1.769393	-3.099047	2.781950
C	1.765457	-2.086601	3.934268
C	2.913144	-4.098494	2.976772
H	0.826386	-3.659652	2.819279
H	0.998788	-1.315856	3.824618
H	1.582042	-2.612575	4.874758
H	2.740278	-1.594489	4.025406
H	2.879291	-4.895585	2.229104

H	3.886334	-3.600692	2.900076
H	2.854448	-4.556148	3.967710
H	2.309003	-3.212477	0.699861
H	-0.044664	-3.080458	0.634902
C	-0.358327	-1.208525	1.612743
C	-1.353621	-1.761167	2.423785
C	-0.137655	0.167605	1.637979
C	-2.105610	-0.947119	3.265676
H	-1.547021	-2.831061	2.390517
C	-0.898968	0.983963	2.470696
H	0.591234	0.613460	0.966854
C	-1.878041	0.427603	3.290215
H	-2.877369	-1.384494	3.890341
H	-0.740288	2.058577	2.453348
H	-2.475412	1.065804	3.932997
C	-1.660620	-2.057718	-1.150451
H	-1.935250	-1.826728	-0.129098
C	-2.551723	-2.526377	-2.014944
H	-2.307170	-2.732164	-3.052186
C	-3.973467	-2.753675	-1.612929
F	-4.798809	-1.941227	-2.288821
F	-4.355422	-4.012664	-1.877031
F	-4.178004	-2.536458	-0.307199
O	0.009823	-1.673449	-2.792214
C	-0.286797	-1.764666	-1.623788
H	2.399472	-0.448253	2.009251
O	-0.615699	0.741202	-1.270477
C	-1.022737	1.800006	-0.719833
C	-0.164882	2.885653	-0.333014
C	-2.387610	2.048681	-0.344549
C	-0.580885	4.047299	0.295733
C	-2.839482	3.193598	0.285617
C	-1.928852	4.197873	0.600283
H	0.136661	4.820087	0.549734
H	-3.888758	3.299462	0.538174
Cl	-3.531521	0.762874	-0.667714
Cl	-2.485963	5.661041	1.394734
Cl	1.551048	2.677387	-0.651837

Vibrational frequencies

18.5144	25.4730	32.7485
37.8690	42.5721	47.3454
53.7104	56.9176	67.0993
70.9449	80.8185	86.6750
98.5164	100.0412	111.2769

122.4245 127.1209 135.9568
148.4103 155.6941 171.4279
183.4704 187.5034 193.6704
203.7090 223.0172 227.6741
230.0092 232.3348 247.7719
261.6993 271.8035 276.8025
304.0935 307.4647 308.0585
322.7615 327.2414 346.6010
368.7066 378.8303 389.8733
396.7875 410.9355 431.0421
432.0255 434.0908 436.7038
446.2885 468.9447 492.3935
495.7481 512.2816 522.4655
544.6163 549.1983 558.2505
559.0330 575.5018 610.7088
613.5566 620.1028 625.2271
639.3870 656.6589 671.8778
714.8875 718.8726 728.2968
734.2593 735.5953 752.2021
757.9356 765.4717 768.8296
793.1809 794.5869 826.8088
865.9595 875.2482 876.4508
880.9620 883.8464 886.2101
888.6719 914.3846 917.7971
930.2903 944.4598 961.6246
972.6689 974.7214 1005.5035
1007.8754 1012.7225 1017.6367
1019.5855 1022.3233 1034.0564
1045.6207 1060.5283 1065.1681
1070.4346 1087.0091 1088.2831
1113.2805 1127.0698 1151.0218
1156.5365 1159.2227 1171.3541
1182.2808 1183.2235 1187.3064
1189.4723 1198.9208 1210.4098
1213.9269 1236.3879 1243.3451
1246.6932 1267.2299 1279.4211
1291.5838 1307.8442 1312.5126
1322.0621 1327.0272 1347.8559
1355.4179 1362.4922 1364.3794
1367.9115 1380.6989 1381.7238
1387.8758 1398.0536 1407.7634
1419.5250 1431.2865 1438.3452
1443.1123 1469.0336 1493.9780
1499.6571 1506.0300 1512.1092

1514.2627	1517.8187	1519.1420
1528.3951	1550.1632	1586.6107
1600.0402	1611.3469	1665.3495
1680.4376	1682.0211	1690.8425
1696.0420	1798.2652	1847.8478
3060.2972	3063.3209	3069.0714
3073.2659	3106.0500	3110.6995
3137.8679	3141.4175	3154.1865
3165.2414	3166.5107	3186.3104
3205.3540	3216.3642	3219.2852
3219.6474	3221.2575	3223.9386
3228.3152	3236.8962	3240.1686
3241.6632	3252.6368	3279.2605

TS2*SS*

Zero-point correction= 0.628904

Thermal correction to Energy= 0.669066

Thermal correction to Enthalpy= 0.670011

Thermal correction to Gibbs Free Energy= 0.555378

Sum of electronic and zero-point Energies= -2876.466535

Sum of electronic and thermal Energies= -2876.426372

Sum of electronic and thermal Enthalpies= -2876.425428

Sum of electronic and thermal Free Energies= -2876.540061

Cartesian coordinates

C	6.816518	-1.863603	-0.331986
C	6.359070	-2.894573	-1.161049
C	5.036581	-2.934317	-1.584196
C	4.181074	-1.922603	-1.155742
C	4.638029	-0.907761	-0.318935
H	7.045574	-3.670030	-1.481794
H	4.677972	-3.727188	-2.231416
C	2.429147	-0.296443	-0.557091
C	1.381393	1.644488	0.539059
C	2.506391	1.466081	1.573218
C	3.817953	1.148877	0.877238
H	4.580075	0.876109	1.610077
S	2.483356	-1.727451	-1.544643
N	3.614154	-0.006349	0.000531
N	1.339961	0.468443	-0.365764
C	2.624810	2.638927	2.575172
C	3.568760	3.762101	2.130529
C	3.061021	2.105753	3.942909
H	1.619792	3.063903	2.689905
H	3.334205	4.146765	1.135097

H	3.500512	4.593406	2.837056
H	4.610148	3.421181	2.132678
H	2.348548	1.372486	4.330959
H	4.044360	1.625870	3.881083
H	3.138645	2.922601	4.665172
H	2.233764	0.572690	2.143982
H	0.444366	1.606227	1.100994
C	1.461379	2.932888	-0.253040
C	0.735110	4.047857	0.171501
C	2.295089	3.044929	-1.367782
C	0.866714	5.266657	-0.487666
H	0.063376	3.962521	1.022301
C	2.427678	4.264302	-2.026932
H	2.836703	2.176623	-1.736091
C	1.720343	5.378928	-1.582858
H	0.297583	6.126351	-0.149889
H	3.079711	4.339990	-2.890740
H	1.822781	6.328614	-2.097225
C	-1.029761	0.962217	-0.838058
H	-0.954318	1.914356	-0.333763
C	-2.251521	0.510947	-1.251446
C	-3.352252	1.517895	-1.384948
F	-4.540190	0.965125	-1.653545
F	-3.488565	2.271177	-0.277548
F	-3.095205	2.373239	-2.393903
O	0.122868	-0.900791	-1.724337
C	0.107480	0.105852	-1.025108
H	4.187319	1.987504	0.277956
C	0.089621	-2.131249	1.236438
C	-0.186948	-3.246207	0.418450
C	0.747657	-4.265270	0.240941
C	1.975413	-4.165626	0.887505
C	2.254248	-3.076515	1.725547
C	1.317876	-2.067770	1.911184
C	-1.972289	-1.555968	0.630225
H	0.522450	-5.118745	-0.390830
H	2.719680	-4.943486	0.750111
H	3.207447	-3.027489	2.243535
H	1.499978	-1.250280	2.601548
N	-0.911802	-1.183266	1.317050
S	-1.803064	-3.113377	-0.224496
C	-4.365685	-1.320188	0.011681
O	-4.372313	-2.322259	-0.717752
C	-5.685600	-0.718200	0.420263

C	-6.841922	-1.449319	0.133125
C	-5.806938	0.509963	1.078236
C	-8.094329	-0.972907	0.504921
H	-6.732861	-2.396869	-0.383116
C	-7.060215	0.991602	1.443446
H	-4.929569	1.111983	1.284787
C	-8.206438	0.250058	1.163687
H	-8.983285	-1.553996	0.280400
H	-7.142812	1.949743	1.946753
H	-9.182222	0.625708	1.455321
C	5.966108	-0.853762	0.100606
H	6.332952	-0.053727	0.732522
H	7.854977	-1.847361	-0.020720
C	-3.137540	-0.748149	0.506181
H	-3.174696	0.070483	1.214454
H	-2.336965	-0.365289	-1.887274

Vibrational frequencies

-187.0339	14.4161	21.0237
27.5752	32.5295	37.7688
50.3177	55.2777	59.6016
65.3696	67.8370	78.8502
80.5313	83.1534	92.8033
101.8147	106.5527	109.7632
118.3345	134.7602	135.5125
157.5593	163.5357	167.5455
184.0490	189.0437	195.0022
224.0483	226.1383	229.0747
239.9222	247.2183	248.2065
256.8656	273.5749	276.5021
289.7532	311.4535	312.7963
320.4338	331.0499	337.3403
347.2730	388.5317	391.4909
408.3726	416.8838	421.2488
426.3769	433.5286	438.8406
445.5167	451.1287	460.2419
472.6221	479.5597	490.4339
512.3433	515.2601	522.7946
545.8015	547.8538	551.3996
564.5099	576.0855	587.4693
612.6028	620.2956	627.8952
628.6289	639.8356	641.7048
655.7989	662.2649	670.2454
681.7664	695.3323	707.1740
711.0265	721.5216	723.9447

725.7590	730.3091	732.4329
733.7601	750.3231	764.4056
771.7560	776.5253	780.9634
791.1338	818.0906	824.0258
849.4821	864.9277	874.3430
877.0713	877.6091	879.2912
881.0297	882.1047	916.4819
919.6183	937.1225	945.4650
958.4986	961.3150	966.0667
971.7211	975.9471	986.6335
998.5661	1005.5058	1006.0913
1008.7857	1014.2327	1018.1643
1019.4412	1023.7760	1030.1845
1030.5883	1050.6092	1057.7779
1062.3690	1068.5854	1071.3847
1072.6705	1084.0010	1092.9538
1099.7536	1121.3148	1126.2102
1130.0682	1152.5964	1153.7099
1163.8130	1176.7342	1179.9258
1183.3608	1185.8115	1185.9812
1191.9891	1194.0481	1203.2915
1212.6084	1212.8219	1221.3171
1227.6224	1246.5346	1255.6750
1266.3435	1269.7577	1287.9677
1294.6632	1295.5735	1305.7569
1318.1113	1319.6754	1331.8096
1334.2702	1342.9264	1349.4899
1362.7858	1363.7115	1367.2001
1370.4630	1375.0655	1382.8673
1387.5656	1398.7749	1408.8992
1418.5110	1433.2580	1437.3000
1437.8091	1445.8257	1493.8739
1497.0279	1497.6337	1499.6784
1507.8344	1508.8407	1511.7663
1517.2958	1517.9151	1520.2728
1531.6352	1533.5443	1552.2262
1554.3247	1588.9673	1620.2627
1646.6498	1668.6205	1680.1441
1680.8021	1682.0118	1689.2651
1695.7503	1699.6259	1718.5097
1766.8495	3063.4733	3065.9351
3080.0548	3104.5351	3120.8641
3127.1588	3139.2536	3142.5992
3157.7451	3161.7381	3167.9978

3191.4014	3194.4266	3199.6424
3202.5658	3215.3508	3215.4384
3215.5924	3217.8607	3218.9995
3223.6713	3224.8683	3226.3145
3229.5029	3234.4335	3234.6660
3235.2744	3235.6420	3236.9013
3247.9399	3250.1916	3271.4647

TS2*SS*'

Zero-point correction= 0.628431

Thermal correction to Energy= 0.668856

Thermal correction to Enthalpy= 0.669800

Thermal correction to Gibbs Free Energy= 0.553712

Sum of electronic and zero-point Energies= -2876.461377

Sum of electronic and thermal Energies= -2876.420953

Sum of electronic and thermal Enthalpies= -2876.420009

Sum of electronic and thermal Free Energies= -2876.536097

Cartesian coordinates

C	6.212267	3.846026	-0.408317
C	5.480954	5.018265	-0.181400
C	4.110127	4.972440	0.038202
C	3.487825	3.727248	0.022681
C	4.218382	2.566139	-0.213160
H	5.990707	5.975048	-0.173217
H	3.540170	5.877007	0.219208
C	2.112218	1.677155	0.079130
C	1.582411	-0.727092	-0.004358
C	2.779646	-0.786542	-0.971696
C	3.912637	0.082348	-0.454062
H	4.700097	0.174130	-1.205326
S	1.785099	3.380094	0.267882
N	3.400076	1.428968	-0.190915
N	1.202175	0.695816	0.215190
C	3.250753	-2.227357	-1.289828
C	4.316831	-2.779393	-0.334974
C	3.766652	-2.299670	-2.729803
H	2.368089	-2.873708	-1.219304
H	4.027576	-2.707277	0.716374
H	4.489975	-3.834453	-0.562740
H	5.272668	-2.260191	-0.467971
H	3.006852	-1.978117	-3.448181
H	4.646503	-1.660129	-2.865073
H	4.061424	-3.322971	-2.978261
H	2.422610	-0.335552	-1.907549

H	0.735717	-1.174466	-0.530906
C	1.797701	-1.474818	1.292463
C	1.336230	-2.791922	1.382806
C	2.487409	-0.911094	2.366515
C	1.597162	-3.547395	2.521646
H	0.770160	-3.224860	0.557050
C	2.746326	-1.668830	3.506276
H	2.816108	0.125146	2.325893
C	2.310260	-2.989635	3.581400
H	1.236272	-4.568737	2.583340
H	3.283884	-1.224104	4.337181
H	2.513499	-3.577796	4.470117
C	-1.012504	-0.007955	1.027431
H	-0.646732	-1.016810	1.155910
C	-2.316304	0.283191	1.308953
C	-3.045084	-0.611040	2.270314
F	-4.384649	-0.561428	2.171878
F	-2.680325	-1.890860	2.167321
F	-2.756939	-0.219462	3.529487
O	-0.443700	2.240888	0.555901
C	-0.153015	1.053302	0.579360
H	4.347681	-0.314260	0.468696
C	-1.868938	-3.380073	-1.089816
C	-0.950567	-2.739725	-1.950730
C	0.140395	-3.422476	-2.488671
C	0.328341	-4.756018	-2.142500
C	-0.571553	-5.400334	-1.278393
C	-1.668255	-4.729737	-0.758119
C	-2.788616	-1.358341	-1.053323
H	0.829938	-2.922614	-3.163391
H	1.176341	-5.300346	-2.546129
H	-0.408071	-6.441621	-1.019317
H	-2.370354	-5.221395	-0.092654
N	-2.893863	-2.591850	-0.622843
S	-1.396566	-1.064749	-2.136383
C	-3.481467	1.025849	-1.182875
O	-2.533703	1.339154	-1.923859
C	-4.495277	2.083762	-0.834247
C	-4.541166	3.223540	-1.643148
C	-5.371716	1.984693	0.251074
C	-5.458070	4.236418	-1.388764
H	-3.844503	3.291503	-2.471774
C	-6.283662	3.004611	0.512540
H	-5.332273	1.123578	0.909859

C	-6.334071	4.128218	-0.309423
H	-5.490325	5.112037	-2.029512
H	-6.954751	2.921990	1.361598
H	-7.050104	4.918600	-0.107202
C	5.595028	2.602060	-0.426552
H	6.169447	1.697959	-0.590260
H	7.282619	3.905710	-0.569909
C	-3.621833	-0.284561	-0.625955
H	-4.536951	-0.575667	-0.129077
H	-2.657813	1.314167	1.299948

Vibrational frequencies

-187.0166	14.0982	15.8502
26.8385	38.9702	39.3933
42.8778	47.0674	50.9216
61.4999	62.9238	67.5429
73.2765	85.5310	91.6236
94.4748	98.7612	109.4256
113.5698	126.0399	134.3114
135.8042	154.5632	170.3761
180.0334	184.2639	196.0267
222.8881	224.5739	231.8284
237.6541	240.6152	245.1233
255.0049	274.6455	282.3056
291.7177	304.6924	307.3846
318.7242	325.4917	333.4321
345.3960	377.4700	391.7885
401.8917	416.7215	423.7881
425.8141	431.6053	438.4629
442.2338	449.0822	456.8453
476.1422	487.8568	491.9107
510.6837	514.0610	522.3093
547.9461	549.3474	551.3716
564.6049	574.8244	587.3189
615.1933	625.0182	628.4765
631.1992	640.6109	642.5900
648.0706	664.3883	668.7260
672.9298	708.1270	714.9292
716.0585	719.0554	721.0212
727.3657	729.1034	734.4503
735.2358	747.8151	764.3803
768.6388	776.7578	791.4970
802.1464	813.7455	827.0569
836.5930	864.9077	874.6629
876.8618	879.6038	882.4345

882.7517	885.6835	914.0301
919.7979	930.8440	945.6856
963.5853	965.0661	966.4042
970.7865	974.6764	996.6190
1002.3390	1006.3253	1010.4693
1010.6746	1013.0227	1018.2691
1018.5733	1021.7115	1027.9829
1031.8667	1050.1068	1050.7746
1057.1609	1070.2381	1070.5646
1072.3882	1087.7775	1089.7358
1101.7265	1121.1863	1128.3571
1129.8683	1148.0004	1152.5824
1160.9482	1171.5827	1177.3314
1180.7381	1182.7069	1186.6132
1187.2330	1190.0995	1205.6060
1210.5361	1213.0806	1214.5554
1219.7735	1246.7835	1252.8741
1257.5494	1266.6133	1276.9551
1295.0471	1300.1292	1309.8849
1317.8883	1326.1126	1333.6528
1339.9624	1347.4649	1350.3235
1360.6604	1364.5504	1365.9617
1368.3871	1372.4549	1383.3631
1389.0828	1392.7688	1410.8193
1418.8557	1432.9459	1436.4061
1444.6716	1457.1656	1483.8881
1493.7721	1498.6714	1504.2131
1505.0026	1506.4029	1510.5118
1515.7684	1518.4193	1519.4730
1534.1934	1551.1787	1553.3399
1560.1685	1591.5633	1617.7893
1639.5335	1669.1112	1678.0041
1683.9115	1684.4537	1692.7511
1697.8876	1698.5743	1705.8684
1776.8205	3056.6648	3062.5439
3069.9442	3097.7254	3111.0745
3132.3405	3139.7469	3152.3058
3152.7008	3162.3679	3170.0910
3175.0870	3193.8618	3193.9667
3203.4906	3205.2587	3213.2522
3214.6203	3215.4118	3217.5704
3222.9465	3223.3166	3225.0318
3226.8006	3229.6764	3232.1446
3233.7260	3234.6265	3238.2010

3239.9966 3267.8907 3274.8256

TS2*SS*''

Zero-point correction= 0.628434

Thermal correction to Energy= 0.668900

Thermal correction to Enthalpy= 0.669845

Thermal correction to Gibbs Free Energy= 0.553841

Sum of electronic and zero-point Energies= -2876.460168

Sum of electronic and thermal Energies= -2876.419702

Sum of electronic and thermal Enthalpies= -2876.418757

Sum of electronic and thermal Free Energies= -2876.534761

Cartesian coordinates

C	6.517117	4.027474	-0.366575
C	5.685654	5.140879	-0.193057
C	4.315951	4.989807	-0.021200
C	3.796435	3.697770	-0.030517
C	4.626557	2.595544	-0.214805
H	6.115963	6.135891	-0.188475
H	3.668246	5.848072	0.117521
C	2.591777	1.544963	0.014118
C	2.269931	-0.900048	-0.014199
C	3.492889	-0.878963	-0.947673
C	4.535767	0.091727	-0.421796
H	5.329700	0.236631	-1.157354
S	2.119920	3.214725	0.157629
N	3.902942	1.395629	-0.201353
N	1.759971	0.490733	0.138505
C	4.086151	-2.278892	-1.233261
C	5.142052	-2.747951	-0.224346
C	4.683661	-2.307202	-2.643270
H	3.247567	-2.986638	-1.206675
H	6.062086	-2.160530	-0.319350
H	4.802145	-2.691086	0.812229
H	5.402819	-3.788273	-0.435388
H	3.948256	-2.020984	-3.401009
H	5.531507	-1.617612	-2.723834
H	5.051481	-3.308489	-2.882815
H	3.121385	-0.476114	-1.899173
H	1.484856	-1.440615	-0.551561
C	2.508962	-1.564939	1.323284
C	2.152501	-2.907656	1.471368
C	3.118893	-0.894731	2.385142
C	2.436726	-3.584035	2.653472
H	1.645704	-3.420066	0.655294

C	3.402377	-1.572227	3.568656
H	3.366104	0.161428	2.302704
C	3.070363	-2.918448	3.701124
H	2.156500	-4.626675	2.759108
H	3.878604	-1.045661	4.388903
H	3.291132	-3.443655	4.624259
C	-0.410423	-0.416672	0.861107
H	0.006146	-1.411846	0.906744
C	-1.718837	-0.223735	1.140180
C	-2.483709	-1.358275	1.757124
F	-3.801980	-1.255794	1.601025
F	-2.096021	-2.545707	1.266423
F	-2.251135	-1.394000	3.085642
O	-0.043820	1.868298	0.377518
C	0.378901	0.725200	0.451373
H	4.980742	-0.245645	0.519845
C	-5.737969	2.025608	-0.095865
C	-6.620900	0.936924	-0.263211
C	-7.988164	1.067338	-0.027025
C	-8.478393	2.304555	0.377367
C	-7.612098	3.394173	0.546201
C	-6.250467	3.265150	0.313664
C	-4.230535	0.514168	-0.720778
H	-8.657314	0.222291	-0.156097
H	-9.540451	2.425496	0.564340
H	-8.012961	4.351425	0.864785
H	-5.571258	4.101931	0.441655
N	-4.410237	1.763888	-0.356507
S	-5.717098	-0.474893	-0.755811
C	-2.771842	-1.387322	-1.417057
O	-3.650531	-2.268949	-1.327872
C	-1.399083	-1.804235	-1.885924
C	-0.553254	-0.962012	-2.615028
C	-0.990180	-3.116832	-1.627004
C	0.655375	-1.441848	-3.123677
H	-0.863581	0.054280	-2.838375
C	0.228339	-3.588440	-2.104944
H	-1.659103	-3.756419	-1.061001
C	1.044308	-2.757135	-2.875883
H	1.279261	-0.794624	-3.734119
H	0.532549	-4.611245	-1.902644
H	1.971653	-3.141489	-3.289861
C	6.003003	2.737826	-0.379100
H	6.654797	1.880628	-0.500644

H	7.584476	4.170981	-0.490803
C	-2.962606	-0.028763	-1.067002
H	-2.172629	0.699088	-1.203885
H	-2.164621	0.762720	1.211195

Vibrational frequencies

-101.0629	14.6392	17.6212
25.1086	33.6534	40.8111
45.8682	49.5211	59.3200
66.1122	67.5744	71.2906
73.3869	81.2776	85.7380
96.0615	100.5060	121.3499
121.9672	124.5101	131.2794
137.6487	157.0331	164.4978
166.7689	186.5149	211.2929
215.4473	222.9317	225.2815
233.3925	239.4962	242.6458
253.2517	270.2060	270.4383
283.2580	303.8764	307.3247
308.4429	319.1171	335.3474
342.6571	378.8712	394.1617
399.2457	416.7574	422.0188
424.2999	426.7978	431.4534
437.1899	445.5694	448.1281
471.4875	491.7198	498.2476
514.0917	515.0408	521.8787
546.7661	551.1774	552.8455
566.5688	572.8136	585.5683
613.4405	624.2553	627.1855
627.8578	641.5739	644.4718
649.5517	661.4612	668.6793
673.8021	704.3902	715.5731
716.9972	720.9569	724.3237
726.7522	732.7941	733.1945
739.1818	747.4515	764.5216
764.9995	775.2419	790.2739
798.2410	820.4482	826.1416
855.0781	866.4949	870.5176
875.2928	876.8199	878.6494
885.8837	886.9887	915.3119
921.9365	938.0647	950.3918
955.8923	964.0107	967.3992
967.6783	968.4845	976.2713
998.0984	1007.1590	1009.8291
1012.5159	1013.5282	1016.5070

1018.8129	1021.3849	1031.2911
1035.0502	1049.0607	1056.5234
1060.5351	1064.6092	1065.6478
1068.8906	1089.3776	1091.1722
1104.8161	1116.3181	1124.4499
1130.1738	1151.6697	1152.3661
1163.0727	1176.4220	1178.2527
1179.8072	1182.9799	1183.8460
1190.1726	1195.5740	1198.2539
1205.5633	1211.5369	1222.9360
1232.8257	1246.5730	1258.2628
1263.8994	1270.0460	1284.8121
1290.9358	1308.2836	1312.1377
1323.7415	1327.2949	1330.3872
1337.0738	1346.6264	1350.2842
1358.0503	1359.1097	1363.4130
1364.9105	1372.8951	1382.9080
1390.0270	1398.4517	1411.9285
1420.4189	1431.9388	1437.8498
1447.4930	1467.2055	1489.3444
1493.4721	1496.2882	1499.2394
1506.9111	1509.5108	1511.7841
1515.3698	1517.4414	1518.1898
1529.8789	1540.1470	1552.3597
1557.5196	1600.1057	1632.4065
1646.9971	1664.7581	1679.0669
1682.8702	1685.1155	1685.7037
1688.4037	1699.0330	1701.4866
1782.4125	3058.5646	3065.2053
3073.7370	3078.1101	3111.6006
3132.2910	3134.1652	3144.3107
3149.9543	3168.1129	3173.7001
3190.5319	3198.6769	3199.1626
3204.1078	3204.7300	3210.0055
3214.4474	3214.8602	3217.9898
3221.0926	3225.6615	3226.1214
3228.2014	3231.7557	3232.7566
3240.0198	3240.7709	3242.5253
3244.0216	3248.0633	3279.6269

TS2*RS*

Zero-point correction= 0.628657

Thermal correction to Energy= 0.668897

Thermal correction to Enthalpy= 0.669841

Thermal correction to Gibbs Free Energy= 0.554461

Sum of electronic and zero-point Energies= -2876.468000

Sum of electronic and thermal Energies= -2876.427761

Sum of electronic and thermal Enthalpies= -2876.426817

Sum of electronic and thermal Free Energies= -2876.542196

Cartesian coordinates

C	-7.011154	-0.522772	0.122212
C	-7.117909	0.592547	-0.716599
C	-5.985885	1.181772	-1.266465
C	-4.745253	0.630376	-0.958999
C	-4.645038	-0.472535	-0.114303
H	-8.095967	1.002008	-0.943049
H	-6.062424	2.044214	-1.919382
C	-2.420668	-0.124920	-0.609764
C	-0.566630	-1.486263	0.252330
C	-1.501095	-1.677007	1.458511
C	-2.919390	-1.940534	0.983546
H	-3.616802	-1.927934	1.824218
S	-3.166782	1.178524	-1.498116
N	-3.312134	-0.860747	0.072806
N	-1.112175	-0.409123	-0.613414
C	-0.994828	-2.728908	2.472075
C	-1.466327	-4.160354	2.189014
C	-1.400400	-2.319537	3.890647
H	0.101495	-2.711062	2.421879
H	-2.543952	-4.258126	2.363828
H	-1.252449	-4.486902	1.168133
H	-0.965466	-4.849612	2.874004
H	-0.986984	-1.341965	4.154069
H	-2.491027	-2.267421	3.988340
H	-1.038884	-3.050906	4.618328
H	-1.511171	-0.703952	1.969284
H	0.374418	-1.087910	0.645609
C	-0.282149	-2.747345	-0.531822
C	0.891141	-3.453195	-0.253143
C	-1.174225	-3.248773	-1.482104
C	1.147742	-4.667542	-0.882876
H	1.604217	-3.038264	0.456350
C	-0.915809	-4.462276	-2.114613
H	-2.069933	-2.689342	-1.742966
C	0.239527	-5.178237	-1.808205
H	2.059770	-5.210167	-0.657336
H	-1.615364	-4.846189	-2.849741
H	0.438507	-6.124137	-2.300972

C	1.165260	0.050972	-1.396963
H	1.446526	-0.971255	-1.189970
C	2.133092	1.000055	-1.631526
C	3.447051	0.545122	-2.192761
F	3.353046	0.412177	-3.530857
F	4.455921	1.400607	-1.971805
F	3.817349	-0.651055	-1.710266
O	-0.665751	1.520743	-1.754503
C	-0.194993	0.482751	-1.301455
H	-3.012381	-2.898853	0.462677
C	-0.255488	3.751305	0.461609
C	-0.840792	2.771397	1.290904
C	-2.176891	2.849064	1.687135
C	-2.935483	3.921522	1.237241
C	-2.365411	4.903638	0.410485
C	-1.036773	4.830056	0.023115
C	1.506233	2.413176	0.626206
H	-2.614890	2.084987	2.323304
H	-3.978939	3.998795	1.525162
H	-2.976993	5.733109	0.070048
H	-0.591007	5.582463	-0.619041
N	1.061917	3.532232	0.120633
S	0.331202	1.532432	1.633690
C	3.236066	0.628230	0.921606
O	2.429485	-0.214444	1.360463
C	4.703957	0.307266	0.950766
C	5.696235	1.287413	0.866938
C	5.081186	-1.030531	1.100909
C	7.041823	0.933358	0.922020
H	5.424443	2.334068	0.777238
C	6.423129	-1.386495	1.148655
H	4.299408	-1.779428	1.173510
C	7.408365	-0.403118	1.058416
H	7.804272	1.703351	0.860431
H	6.704580	-2.429397	1.255973
H	8.457769	-0.678056	1.097509
C	-5.774999	-1.073616	0.436136
H	-5.701135	-1.945103	1.076221
H	-7.908376	-0.970299	0.534751
C	2.794568	1.853502	0.320391
H	3.514899	2.568209	-0.056443
H	1.836443	1.999890	-1.938268

Vibrational frequencies

-255.1829	9.1185	19.5298

29.9567	37.5880	38.8365
43.2376	45.1730	58.7372
63.7996	67.8574	70.8474
83.4988	86.5882	90.8015
93.9101	100.0892	108.8350
124.8494	132.6227	136.4344
140.1751	159.7586	170.4256
184.0244	191.2371	209.6053
214.8450	224.7229	231.4718
237.6505	239.4093	253.1711
258.0129	272.7212	278.9545
295.6675	306.2552	313.5576
322.2914	329.4273	335.9096
343.0134	378.7603	396.7259
402.4281	414.5004	425.4668
431.3297	433.4953	434.2393
439.3985	443.7214	465.7145
481.4946	490.6063	491.0604
512.9771	517.1534	521.8402
546.4943	549.2162	551.8998
561.7695	581.5014	591.9068
613.7891	621.0632	626.7334
629.3766	639.3977	641.3390
653.0366	665.1833	671.7423
675.2582	696.1437	709.8489
716.7347	720.1036	723.8147
727.7551	729.9377	734.0218
735.2969	744.4259	765.2263
770.6126	773.1825	781.4417
794.6123	821.5803	829.6405
851.0704	865.8020	871.6687
872.3115	875.1383	880.4768
882.5892	889.1401	915.5836
921.4222	934.6503	948.7942
953.9780	957.2268	967.8224
971.9685	978.9025	999.4380
1000.9417	1006.7814	1013.5571
1014.6463	1016.8511	1019.2739
1022.9873	1025.0462	1032.5898
1033.4591	1051.2050	1054.5886
1058.3642	1066.6148	1068.3922
1074.4279	1089.1177	1094.6255
1101.7406	1120.6920	1123.0495
1130.5920	1152.4421	1157.4085

1161.1490	1173.9482	1174.8571
1175.5175	1177.9483	1188.1024
1188.6456	1191.3938	1195.8741
1207.5213	1215.3129	1218.3155
1227.4683	1242.5567	1250.8144
1259.9837	1266.6469	1282.8016
1293.3013	1294.5920	1315.0880
1323.0393	1326.5198	1330.5285
1337.3335	1343.3840	1352.9027
1359.9597	1361.0997	1364.8570
1368.8768	1369.5763	1381.3553
1392.6902	1396.6542	1416.8664
1421.6390	1434.9001	1437.8888
1451.9680	1454.5861	1488.9287
1495.0353	1498.9538	1500.5577
1509.0541	1511.9955	1514.9726
1518.0738	1519.1125	1519.9650
1532.7430	1547.6630	1559.0942
1560.2635	1581.4287	1611.3511
1643.3164	1662.8644	1680.7867
1682.8270	1687.9301	1689.9731
1691.4955	1698.0820	1702.7328
1759.5325	3059.5441	3060.5055
3062.8992	3071.9490	3099.7133
3121.4507	3135.7262	3138.7211
3155.8711	3157.9392	3163.1590
3193.9510	3200.9615	3202.5008
3206.8240	3207.6597	3208.0516
3214.8387	3217.3681	3218.7190
3219.3913	3220.2771	3228.4169
3228.9008	3229.6712	3230.0456
3232.8944	3237.4226	3241.6654
3243.9001	3264.1734	3279.3448

TS2*RS*'

Zero-point correction= 0.628924

Thermal correction to Energy= 0.669220

Thermal correction to Enthalpy= 0.670165

Thermal correction to Gibbs Free Energy= 0.554338

Sum of electronic and zero-point Energies= -2876.463070

Sum of electronic and thermal Energies= -2876.422773

Sum of electronic and thermal Enthalpies= -2876.421829

Sum of electronic and thermal Free Energies= -2876.537655

Cartesian coordinates

C	5.723003	4.515413	-0.352951
C	4.933052	5.496646	0.256180
C	3.646914	5.205476	0.695467
C	3.169921	3.911007	0.511615
C	3.957075	2.941875	-0.105151
H	5.329444	6.496682	0.390770
H	3.031851	5.961728	1.170520
C	2.062722	1.707864	0.345648
C	1.806499	-0.678781	-0.142906
C	2.746202	-0.372232	-1.321930
C	3.869125	0.547901	-0.871532
H	4.434463	0.914934	-1.731655
S	1.589915	3.276209	0.949339
N	3.288167	1.714315	-0.200299
N	1.323238	0.598106	0.437412
C	3.268040	-1.645186	-2.033177
C	4.588630	-2.191939	-1.478426
C	3.403612	-1.385758	-3.535796
H	2.501108	-2.417107	-1.897264
H	5.422089	-1.519749	-1.711785
H	4.564060	-2.350195	-0.397116
H	4.807028	-3.152659	-1.952274
H	3.779899	-2.276830	-4.046194
H	2.442215	-1.115713	-3.982927
H	4.108538	-0.569744	-3.732257
H	2.131644	0.186884	-2.040407
H	0.916502	-1.141565	-0.574519
C	2.396588	-1.601207	0.899458
C	2.110665	-2.967437	0.818606
C	3.254494	-1.138268	1.898714
C	2.708341	-3.862990	1.700377
H	1.413199	-3.327158	0.062491
C	3.850962	-2.035345	2.781740
H	3.454274	-0.073888	2.001583
C	3.586421	-3.399072	2.677953
H	2.481126	-4.921613	1.628553
H	4.518666	-1.667105	3.553609
H	4.050522	-4.096560	3.367369
C	-0.626231	-0.562353	1.351874
H	-0.059043	-1.483264	1.357071
C	-1.999798	-0.604690	1.502472
C	-2.596289	-1.709850	2.321386
F	-2.092066	-2.914300	1.993587
F	-2.324378	-1.527255	3.627316

F	-3.928692	-1.790067	2.217962
O	-0.472425	1.800928	1.191037
C	-0.014464	0.675446	1.014437
H	4.559180	0.052366	-0.180976
C	-5.589777	1.391311	-0.322107
C	-4.727697	2.327083	-0.927905
C	-5.148299	3.625573	-1.212474
C	-6.449813	3.984275	-0.882609
C	-7.317841	3.060897	-0.280637
C	-6.899649	1.769296	0.001760
C	-3.811908	0.077918	-0.516418
H	-4.475769	4.339382	-1.677038
H	-6.797003	4.990419	-1.093683
H	-8.330384	3.362616	-0.032602
H	-7.562633	1.045846	0.464905
N	-5.045035	0.140187	-0.099244
S	-3.174980	1.585123	-1.217012
C	-1.799318	-1.268294	-1.157602
O	-1.127804	-0.291505	-1.526428
C	-1.236290	-2.639838	-1.410782
C	-1.645965	-3.789359	-0.727345
C	-0.224483	-2.748773	-2.373786
C	-1.039272	-5.015779	-0.989716
H	-2.416272	-3.730570	0.031137
C	0.366598	-3.976542	-2.650570
H	0.083008	-1.849072	-2.899443
C	-0.035200	-5.114266	-1.950659
H	-1.353555	-5.897802	-0.441184
H	1.141470	-4.046817	-3.408667
H	0.428877	-6.073653	-2.156125
C	5.249057	3.223017	-0.542858
H	5.869984	2.464794	-1.005495
H	6.726123	4.763073	-0.681416
C	-2.997360	-1.111525	-0.384718
H	-3.586969	-1.992211	-0.157364
H	-2.538720	0.335125	1.589590

Vibrational frequencies

-309.3708	14.7714	20.4308
25.3675	30.1208	35.2864
41.7155	47.9093	50.5596
59.2273	65.6870	68.0820
71.8730	81.3273	87.3549
97.8581	111.1742	117.8397
126.3155	133.0712	135.0465

147.4745 164.3076 177.6881
181.0927 190.8923 203.0338
208.9108 218.4635 222.6974
230.1557 237.2717 243.8333
253.4027 272.4997 281.2105
298.3615 300.2565 305.3728
321.7309 325.6332 338.4364
341.2477 373.0901 393.4808
406.2903 420.6169 427.4767
429.0671 433.3814 438.0483
444.0278 447.2524 466.4764
477.7534 486.6891 492.8624
512.4426 516.3706 519.5397
548.8210 550.4361 551.7301
561.9560 578.9202 590.5733
613.7473 621.8055 627.0172
627.6880 638.8356 643.8196
655.4555 664.1622 671.3150
677.1692 706.2794 716.7867
717.6958 723.6340 724.7989
727.1124 733.5482 734.3358
744.4413 747.7605 765.7493
773.5574 779.9455 791.5889
802.0352 823.7503 831.3809
863.6969 867.1298 876.6441
880.8704 881.6215 884.0311
894.2641 899.2707 920.6622
925.0484 936.8772 946.3292
963.5638 966.5835 971.5697
977.5329 979.3690 1005.7518
1006.5022 1008.6191 1014.1490
1018.7733 1020.5177 1022.5205
1025.0264 1031.0943 1036.7210
1048.8860 1053.9100 1058.2308
1062.5683 1064.6607 1069.0935
1069.9569 1088.0721 1091.1545
1100.7742 1117.9962 1123.6090
1126.6513 1154.6113 1157.4664
1159.9772 1171.1812 1176.2826
1176.7798 1177.7347 1181.5075
1186.6669 1190.0764 1203.6906
1206.0053 1208.8580 1219.3363
1231.2728 1243.2923 1252.6603
1255.7154 1266.1029 1286.1632

1287.5704	1293.9764	1310.8460
1316.9379	1324.1256	1327.3596
1335.9290	1344.4273	1348.0755
1362.1842	1362.3534	1362.8863
1363.8243	1372.3407	1382.6390
1388.4395	1394.5348	1406.3480
1418.6025	1429.9566	1436.5637
1448.7784	1449.9730	1492.9188
1495.9363	1498.6750	1499.1268
1505.0847	1509.7327	1510.8249
1515.2637	1517.9862	1518.8174
1530.3316	1548.0552	1552.4200
1566.7081	1584.7433	1614.2957
1647.3627	1663.4300	1678.7811
1681.3587	1689.4798	1689.7922
1690.4691	1697.9933	1705.5541
1756.8571	3054.7470	3060.3841
3069.1875	3096.7026	3106.4961
3132.2189	3138.7336	3145.1709
3156.7524	3162.9049	3163.3123
3181.2045	3188.9027	3203.8069
3205.7232	3211.7301	3213.6172
3215.4332	3216.2085	3220.4911
3220.6539	3221.9772	3224.0351
3226.1575	3231.2208	3231.5765
3234.9346	3236.0951	3241.5350
3246.0687	3265.0779	3268.5353

TS2*RS*''

Zero-point correction= 0.628055

Thermal correction to Energy= 0.668551

Thermal correction to Enthalpy= 0.669495

Thermal correction to Gibbs Free Energy= 0.553209

Sum of electronic and zero-point Energies= -2876.458531

Sum of electronic and thermal Energies= -2876.418035

Sum of electronic and thermal Enthalpies= -2876.417091

Sum of electronic and thermal Free Energies= -2876.533377

Cartesian coordinates

C	6.935958	-2.788573	-1.131375
C	6.233153	-3.841555	-1.730063
C	4.849868	-3.800676	-1.846218
C	4.184549	-2.685920	-1.342266
C	4.887889	-1.646606	-0.739261
H	6.775120	-4.698974	-2.112883

H	4.302066	-4.609558	-2.316481
C	2.734674	-0.844922	-0.569014
C	2.111688	1.297877	0.475470
C	3.404394	1.089031	1.284286
C	4.509868	0.575848	0.379859
H	5.384031	0.292895	0.969334
S	2.459437	-2.364391	-1.375943
N	4.029191	-0.628401	-0.303742
N	1.775475	0.045821	-0.251728
C	3.831115	2.325520	2.109837
C	4.757131	3.297001	1.367695
C	4.496677	1.869642	3.411806
H	2.913248	2.863900	2.378636
H	5.743920	2.847816	1.207947
H	4.360992	3.612604	0.399155
H	4.906344	4.192152	1.977063
H	3.818238	1.260672	4.016358
H	5.394797	1.275428	3.207854
H	4.801917	2.733153	4.008511
H	3.175901	0.281205	1.987838
H	1.310401	1.428935	1.209588
C	2.150175	2.488657	-0.458202
C	1.646697	3.714458	-0.015541
C	2.732592	2.406608	-1.724574
C	1.758902	4.850674	-0.810440
H	1.166327	3.780599	0.957911
C	2.844569	3.543902	-2.520501
H	3.093127	1.453042	-2.103604
C	2.366404	4.768943	-2.061645
H	1.366154	5.797333	-0.454839
H	3.300229	3.469061	-3.502218
H	2.451977	5.653777	-2.683418
C	-0.561257	0.821513	-0.464666
H	-0.300683	1.797166	-0.080317
C	-1.858208	0.518992	-0.761884
C	-2.834950	1.654469	-0.901677
F	-3.024989	2.326498	0.241813
F	-2.371607	2.557441	-1.792590
F	-4.024126	1.250332	-1.357583
O	0.203993	-1.267565	-1.252239
C	0.425615	-0.202881	-0.692328
H	4.813851	1.310896	-0.372238
C	-6.490730	0.061805	0.433252
C	-6.527520	-1.095131	-0.374876

C	-7.691465	-1.486403	-1.034383
C	-8.830211	-0.702192	-0.892335
C	-8.806566	0.452530	-0.095624
C	-7.651347	0.838083	0.567717
C	-4.380474	-0.565493	0.718949
H	-7.707112	-2.380829	-1.649225
H	-9.744214	-0.985953	-1.403756
H	-9.706376	1.052031	0.001573
H	-7.624660	1.729052	1.186703
N	-5.281324	0.332165	1.034023
S	-4.964104	-1.870685	-0.350666
C	-2.144048	-1.621393	1.052255
O	-2.410949	-2.640684	0.391202
C	-0.812796	-1.553185	1.760331
C	-0.425989	-0.495540	2.590301
C	0.088254	-2.603337	1.547275
C	0.825339	-0.498447	3.206523
H	-1.098360	0.333353	2.781530
C	1.339050	-2.605394	2.151724
H	-0.219291	-3.405082	0.884706
C	1.708673	-1.554025	2.992639
H	1.105064	0.324496	3.858722
H	2.025691	-3.428285	1.976345
H	2.677697	-1.563091	3.484427
C	6.276963	-1.674415	-0.628965
H	6.829437	-0.857848	-0.179643
H	8.016555	-2.838761	-1.059940
C	-3.012913	-0.490118	1.122613
H	-2.803123	0.331454	1.793527
H	-2.106172	-0.397025	-1.289925

Vibrational frequencies

-186.1851	13.0476	18.5113
22.5105	32.2931	38.0236
43.3629	53.7804	57.2980
60.3752	64.0187	67.7564
79.2944	82.4706	87.1139
98.2258	101.2091	107.5233
126.1823	128.9572	133.3855
138.3466	156.8600	171.3211
178.6003	182.7976	206.1631
215.4794	220.6942	223.7986
228.3600	239.8394	247.6280
252.2941	261.4776	270.8156
280.8217	301.3159	304.0809

314.4421	332.0540	334.0852
343.1608	386.6845	390.6795
403.1600	417.8649	420.6884
425.0078	431.2603	440.7470
444.0428	448.6485	462.5514
467.7727	478.5915	489.8331
513.0828	513.7627	522.0468
545.5754	547.3866	551.9378
563.8000	575.2533	585.1868
611.8323	623.5646	626.6791
627.9072	639.6315	642.0134
645.3880	661.3333	668.7838
672.7262	695.0798	705.3610
715.7654	719.3066	721.8858
726.1112	729.0308	731.9362
734.2160	749.6657	762.4990
770.7233	775.7508	778.1610
792.0350	814.8160	824.0021
828.5189	864.6245	874.4600
876.6864	882.2604	884.7782
886.6990	887.0671	912.7144
919.1076	934.9092	946.0546
962.0381	962.8403	966.9009
974.6584	975.5694	981.8390
1000.1426	1003.1299	1011.0185
1012.4098	1013.4925	1017.2464
1020.4057	1020.9056	1034.4149
1035.5876	1049.3280	1059.0190
1060.3843	1067.3356	1069.0914
1072.1927	1083.6866	1090.4005
1096.0004	1117.7667	1124.9476
1127.5013	1151.0701	1153.1889
1164.5036	1174.8753	1177.4537
1179.1695	1179.8981	1181.8843
1188.8272	1196.5289	1203.4239
1210.9209	1212.3280	1213.0044
1222.4998	1240.8368	1249.2094
1263.1059	1268.1801	1289.6476
1292.8221	1299.8582	1305.1681
1319.7655	1324.2501	1328.2878
1331.3846	1342.7301	1347.7957
1356.9505	1363.2451	1364.1583
1364.8245	1369.1748	1380.7058
1382.3515	1393.6276	1408.6677

1418.7363	1430.1522	1437.4820
1443.8515	1452.4379	1490.3639
1492.2175	1495.9736	1497.3083
1504.4712	1508.0701	1510.1057
1515.5161	1516.7842	1519.6508
1529.6486	1542.8895	1555.0561
1561.7538	1588.1437	1613.1734
1646.1183	1661.4712	1676.4709
1681.1142	1687.6500	1689.8057
1689.8528	1700.2875	1704.2181
1769.8530	3062.6323	3066.9626
3071.9039	3102.4669	3111.6531
3112.9591	3137.7698	3141.9358
3159.0304	3165.2568	3174.0454
3185.5959	3196.2685	3199.4505
3200.4610	3207.7857	3209.0575
3213.8215	3218.3262	3220.3705
3222.2180	3223.3320	3230.2910
3233.3234	3234.2175	3234.6391
3236.5251	3243.0244	3243.8063
3249.4016	3261.9048	3267.1216

TS2*RS*'''

Zero-point correction= 0.628598

Thermal correction to Energy= 0.668998

Thermal correction to Enthalpy= 0.669942

Thermal correction to Gibbs Free Energy= 0.553750

Sum of electronic and zero-point Energies= -2876.463253

Sum of electronic and thermal Energies= -2876.422853

Sum of electronic and thermal Enthalpies= -2876.421909

Sum of electronic and thermal Free Energies= -2876.538101

Cartesian coordinates

C	6.428598	3.505009	-1.187079
C	5.695371	4.694632	-1.274470
C	4.321505	4.702991	-1.069516
C	3.698161	3.492860	-0.777251
C	4.431067	2.311315	-0.701583
H	6.206085	5.623594	-1.501149
H	3.749752	5.622236	-1.131196
C	2.322213	1.520915	-0.220381
C	1.791204	-0.825077	0.307074
C	2.994526	-1.123319	-0.607111
C	4.127229	-0.155793	-0.308663
H	4.922290	-0.256174	-1.050484

S	1.991853	3.212681	-0.474460
N	3.612615	1.214038	-0.401077
N	1.412687	0.603801	0.155270
C	3.453229	-2.602309	-0.570090
C	4.499123	-2.918779	0.506950
C	3.995421	-3.016850	-1.941611
H	2.559421	-3.207520	-0.370086
H	5.462996	-2.457986	0.262984
H	4.202948	-2.589925	1.505842
H	4.660105	-3.999229	0.544371
H	3.248143	-2.891405	-2.730924
H	4.874246	-2.422074	-2.214793
H	4.301005	-4.066578	-1.927114
H	2.652181	-0.901114	-1.626998
H	0.942113	-1.385034	-0.096412
C	2.005709	-1.199595	1.756888
C	1.561273	-2.447515	2.201283
C	2.688328	-0.360726	2.639604
C	1.832100	-2.868224	3.499532
H	1.002250	-3.090526	1.524389
C	2.958222	-0.781623	3.939337
H	3.005467	0.630506	2.323265
C	2.539434	-2.039070	4.367830
H	1.484544	-3.839570	3.834867
H	3.491658	-0.124239	4.617857
H	2.750433	-2.365555	5.380681
C	-0.817942	0.098273	1.079576
H	-0.523104	-0.910028	1.327490
C	-2.100918	0.510735	1.257585
C	-3.029649	-0.335898	2.070945
F	-2.886346	-1.641892	1.804743
F	-2.774172	-0.180592	3.387088
F	-4.314798	-0.014197	1.893568
O	-0.259644	2.151612	0.065155
C	0.061649	1.020445	0.412468
H	4.551341	-0.305480	0.688957
C	-0.948401	-2.478577	-1.803361
C	-2.059517	-3.340659	-1.693292
C	-1.931374	-4.715409	-1.882032
C	-0.676221	-5.235883	-2.182257
C	0.432879	-4.389357	-2.312512
C	0.301388	-3.019013	-2.134352
C	-2.477639	-0.935021	-1.323212
H	-2.793597	-5.369121	-1.795654

H	-0.559312	-6.304916	-2.325857
H	1.403303	-4.807340	-2.565482
H	1.144199	-2.348601	-2.270997
N	-1.199677	-1.138783	-1.582336
S	-3.488578	-2.404890	-1.327904
C	-4.396796	0.579570	-0.819098
O	-5.250225	-0.321447	-0.863842
C	-4.848542	1.991946	-0.535393
C	-3.975041	3.078991	-0.407418
C	-6.221121	2.208814	-0.379834
C	-4.469578	4.352081	-0.133331
H	-2.901617	2.948540	-0.513853
C	-6.715319	3.479253	-0.108527
H	-6.884367	1.356069	-0.476229
C	-5.839171	4.556567	0.015559
H	-3.780925	5.185353	-0.035682
H	-7.783839	3.631842	0.008141
H	-6.221847	5.549893	0.228391
C	5.810435	2.295396	-0.898435
H	6.386482	1.380839	-0.820885
H	7.501105	3.524561	-1.343693
C	-2.998126	0.336627	-0.984130
H	-2.315914	1.157435	-1.167272
H	-2.374791	1.555993	1.175093

Vibrational frequencies

-172.5106	15.1856	17.0662
25.8121	31.9909	37.4700
41.6958	45.8517	54.8412
56.9599	62.2196	68.7072
72.7990	81.9952	88.4857
96.7739	104.9060	115.9108
119.3916	122.3956	134.4461
139.7258	157.4386	172.6403
183.0820	185.4529	190.9654
220.2393	222.7992	227.6974
230.0239	244.2496	245.3542
257.0682	272.9759	278.0289
293.5848	304.0849	311.3464
321.2047	327.7830	337.1167
342.2371	379.9678	397.0766
406.1822	417.4358	421.5977
429.9744	435.6677	441.0474
449.3310	450.0346	459.5979
468.5230	474.1101	490.5205

516.9068	517.0860	522.3196
547.2611	549.0227	551.9026
564.9370	575.9705	587.1592
615.3174	624.5834	627.2653
627.7061	641.9391	646.8346
655.2150	659.8702	671.2968
679.0560	698.0373	714.1723
718.8252	720.8893	723.8210
725.2412	727.8485	732.6469
734.9643	750.0296	764.0279
773.1801	773.9279	784.7435
793.1580	813.8510	826.9011
839.5032	865.2455	876.0951
877.7053	879.6308	881.4088
882.7517	887.5907	915.4930
925.4287	937.6040	948.8831
954.6643	959.2463	966.2230
974.3269	975.4061	980.5612
995.9063	1006.2870	1010.7760
1013.7549	1015.2419	1016.4414
1022.8656	1023.1005	1030.5795
1032.7856	1050.6978	1060.9341
1064.7726	1067.4863	1067.9044
1072.1772	1089.7663	1090.5964
1102.3459	1119.3009	1123.1312
1125.8852	1150.3221	1155.7878
1165.3921	1176.5018	1177.7755
1177.8939	1178.4898	1181.1971
1189.7877	1193.5600	1204.2990
1211.3803	1212.6296	1222.5568
1228.7430	1249.0932	1262.3635
1266.3866	1279.7627	1289.5963
1297.0889	1305.9687	1309.0596
1317.9620	1323.3538	1332.7575
1340.6191	1344.4749	1350.4265
1357.5751	1363.3356	1363.6715
1365.0704	1369.1864	1382.0216
1386.6195	1398.6050	1408.4234
1421.0183	1433.8831	1441.9630
1447.8032	1452.9569	1492.5418
1495.1632	1498.1482	1499.6430
1505.7560	1506.2135	1512.3806
1517.6698	1518.1881	1520.4936
1531.1722	1539.4014	1555.0465

1556.5443	1598.3275	1626.4791
1646.4821	1666.4634	1679.8567
1682.7061	1683.0989	1690.3169
1693.8014	1699.7606	1712.3980
1758.0122	3061.9326	3066.2048
3070.1061	3079.2721	3111.9158
3137.2482	3141.0463	3145.4834
3158.6322	3162.3875	3171.4615
3188.4951	3190.0442	3192.8733
3197.7915	3205.1526	3208.2727
3212.1840	3212.6513	3218.6875
3221.7803	3221.8157	3223.7127
3226.1438	3230.7145	3231.1168
3235.7990	3236.8716	3238.7061
3244.1650	3246.6920	3290.4202

TS2*RR*

Zero-point correction= 0.628869

Thermal correction to Energy= 0.669003

Thermal correction to Enthalpy= 0.669948

Thermal correction to Gibbs Free Energy= 0.555918

Sum of electronic and zero-point Energies= -2876.462743

Sum of electronic and thermal Energies= -2876.422609

Sum of electronic and thermal Enthalpies= -2876.421665

Sum of electronic and thermal Free Energies= -2876.535694

Cartesian coordinates

C	-0.994409	0.882679	1.210603
H	-0.944264	1.876863	0.788915
C	-2.197104	0.344668	1.530495
C	-3.375408	1.262035	1.677856
F	-4.495697	0.606961	1.998917
F	-3.614932	1.986195	0.573550
F	-3.156055	2.151083	2.669689
O	0.202147	-1.077438	1.791138
C	0.185275	0.059296	1.344989
C	0.237098	-2.061723	-1.299172
C	-0.050043	-3.247530	-0.587687
C	0.870655	-4.290281	-0.508288
C	2.094104	-4.154263	-1.158185
C	2.379088	-3.000272	-1.901651
C	1.462139	-1.960543	-1.980734
C	-1.829905	-1.540380	-0.662391
H	0.635409	-5.195021	0.043771
H	2.824647	-4.955322	-1.103387

H	3.328054	-2.920213	-2.423946
H	1.660432	-1.091556	-2.599455
N	-0.758675	-1.107435	-1.297468
S	-1.671076	-3.168511	0.053232
C	-4.233957	-1.361960	-0.051602
O	-4.262811	-2.427310	0.591455
C	-5.540668	-0.661941	-0.331515
C	-6.667021	-1.086355	0.379999
C	-5.680565	0.364771	-1.269202
C	-7.905526	-0.492055	0.169786
H	-6.541925	-1.887512	1.100500
C	-6.921657	0.959545	-1.484088
H	-4.826808	0.695854	-1.850412
C	-8.035918	0.535467	-0.764249
H	-8.771054	-0.826468	0.733530
H	-7.019236	1.751835	-2.219601
H	-9.002370	1.000776	-0.931591
C	-3.016026	-0.776680	-0.517322
H	-3.025308	0.147505	-1.079467
H	-2.278965	-0.626630	2.008728
C	6.758639	-1.702340	-0.314699
C	6.308618	-2.935319	0.175600
C	5.032196	-3.068803	0.706323
C	4.218022	-1.939368	0.743679
C	4.671506	-0.716815	0.255852
H	6.962524	-3.799117	0.135521
H	4.672191	-4.022435	1.076853
C	2.521465	-0.161878	0.856035
C	1.551361	2.101215	0.678002
C	3.011895	2.538712	0.897091
C	3.935808	1.683580	0.044400
H	4.981418	1.893569	0.280341
S	2.568549	-1.835363	1.320630
N	3.689715	0.275544	0.366897
N	1.441839	0.640991	0.948356
C	3.247677	4.055029	0.691962
C	3.627349	4.450543	-0.740624
C	4.324591	4.545481	1.664172
H	2.310411	4.564137	0.949027
H	2.925825	4.075103	-1.489430
H	3.651612	5.540460	-0.819851
H	4.629665	4.086407	-0.992499
H	4.031832	4.375426	2.703716
H	5.274908	4.028312	1.489492

H	4.502225	5.615532	1.528956
H	3.236603	2.305443	1.946202
H	0.960970	2.588023	1.459784
C	0.993999	2.476501	-0.677316
C	0.285548	3.671555	-0.824046
C	1.224526	1.675723	-1.793652
C	-0.152429	4.076233	-2.081388
H	0.072970	4.286383	0.047383
C	0.786125	2.078126	-3.052063
H	1.727986	0.721588	-1.671861
C	0.104794	3.283987	-3.198693
H	-0.700643	5.006506	-2.186769
H	0.967921	1.444429	-3.914131
H	-0.239905	3.598359	-4.178121
H	3.775116	1.841170	-1.026435
C	5.948529	-0.574806	-0.284293
H	6.295792	0.371486	-0.682487
H	7.755495	-1.623769	-0.733634

Vibrational frequencies

-141.7050	18.8015	20.9389
32.2083	34.1655	42.7642
44.3671	50.8335	65.6317
68.4080	70.6507	77.3293
82.3252	88.7129	91.0271
93.3428	105.8569	111.6357
129.7919	131.6823	145.5414
153.7130	166.0116	170.8268
176.3755	187.3002	204.3343
222.3713	229.8890	233.0182
236.8055	242.6459	247.4865
257.2712	269.7941	275.6567
293.4255	304.1238	311.1802
317.5557	326.0902	336.2133
345.7222	377.0124	393.9266
404.4650	414.5973	422.3869
424.6767	435.7053	442.6358
443.7263	444.9146	458.4564
475.7047	482.5296	491.0470
511.8980	514.7030	523.7032
545.5117	546.2711	551.5764
569.1908	573.5748	582.6964
615.4222	619.2191	627.3303
628.6015	639.5023	646.0589
652.2163	661.2606	669.9870

678.2612	696.2760	712.3507
716.5576	720.1355	720.9375
726.2647	727.4518	733.0504
733.1519	754.9952	764.1120
778.5660	782.3682	791.3105
796.6325	820.3212	825.8594
851.1203	866.2886	873.1982
874.2377	877.5034	878.8374
884.3140	889.0408	916.5491
918.4172	930.7479	944.6480
959.0084	959.4854	964.6088
973.4366	977.1071	979.6918
998.2613	1002.4368	1005.6878
1008.2169	1014.6111	1017.5162
1023.5446	1026.8171	1029.8874
1030.6547	1049.3858	1057.9514
1059.3497	1067.6993	1068.6690
1072.4550	1086.4678	1090.8349
1098.5533	1119.0747	1124.2226
1126.4540	1149.9430	1153.2204
1162.5640	1177.5298	1178.5273
1179.0359	1179.3289	1182.3761
1189.0442	1198.4191	1202.4856
1211.4686	1212.4906	1216.8701
1226.4158	1244.0805	1248.6367
1260.8943	1265.2064	1282.3317
1292.6871	1305.1169	1305.5767
1315.7782	1318.5795	1329.1033
1340.4926	1341.2008	1343.9355
1359.7835	1360.1905	1365.7420
1368.3354	1373.0067	1380.9012
1386.2951	1399.0103	1410.1330
1419.0158	1431.3993	1436.0372
1442.6518	1447.3745	1489.9033
1494.7269	1497.9196	1499.0641
1505.3833	1505.6665	1510.3452
1514.5363	1516.8837	1522.2233
1531.9430	1536.9037	1552.4551
1554.3619	1592.9213	1631.4686
1643.0750	1670.4782	1678.8193
1679.0312	1681.0528	1688.4406
1692.8601	1701.6768	1708.3667
1776.8913	3060.6911	3064.1825
3072.8541	3077.3832	3104.9162

3122.4755	3136.7334	3141.6037
3156.1445	3168.7021	3175.8150
3195.9156	3197.6260	3207.7662
3208.0010	3209.7742	3215.3188
3216.8988	3220.7366	3223.7885
3228.4129	3229.8959	3229.9110
3232.6395	3234.7723	3238.0799
3240.5295	3243.7697	3251.2613
3255.0401	3259.8228	3269.7566

TS2*RR*'

Zero-point correction= 0.627997

Thermal correction to Energy= 0.668143

Thermal correction to Enthalpy= 0.669087

Thermal correction to Gibbs Free Energy= 0.553900

Sum of electronic and zero-point Energies= -2876.438335

Sum of electronic and thermal Energies= -2876.398189

Sum of electronic and thermal Enthalpies= -2876.397245

Sum of electronic and thermal Free Energies= -2876.512432

Cartesian coordinates

C	-6.313270	3.587082	0.129791
C	-5.508054	4.568089	-0.463059
C	-4.129867	4.414616	-0.526724
C	-3.576092	3.250799	0.002674
C	-4.380178	2.278990	0.587357
H	-5.965272	5.461092	-0.873978
H	-3.499401	5.173758	-0.976330
C	-2.298771	1.312053	0.870791
C	-1.965485	-0.911256	1.840977
C	-3.391139	-1.190627	1.301077
C	-4.247718	0.011114	1.640943
H	-5.245831	-0.081012	1.215864
S	-1.878902	2.829648	0.112251
N	-3.621380	1.196814	1.053624
N	-1.413998	0.342025	1.214494
C	-3.415071	-1.607930	-0.202141
C	-3.537646	-3.131281	-0.335485
C	-4.525819	-0.964528	-1.040605
H	-2.465191	-1.296418	-0.654890
H	-4.552865	-3.444858	-0.065409
H	-2.835178	-3.665510	0.307100
H	-3.349107	-3.432975	-1.370420
H	-5.520067	-1.250567	-0.679798
H	-4.437854	-1.326765	-2.069127

H	-4.468651	0.127462	-1.076429
H	-3.767406	-2.022748	1.906132
H	-2.052128	-0.694792	2.912076
C	-1.144276	-2.177449	1.700365
C	-1.161970	-3.056192	2.783869
C	-0.473168	-2.544506	0.534324
C	-0.518436	-4.289148	2.705536
H	-1.680482	-2.774476	3.697003
C	0.193918	-3.761990	0.464819
H	-0.425832	-1.852747	-0.299674
C	0.165027	-4.641837	1.545532
H	-0.539548	-4.962349	3.556077
H	0.747030	-4.009622	-0.434422
H	0.684651	-5.592620	1.486795
C	1.033870	-0.171216	1.558650
H	0.847067	-1.178264	1.878294
C	2.331927	0.237350	1.354278
C	3.399744	-0.622298	1.962937
F	3.244914	-1.915707	1.635628
F	3.356526	-0.558501	3.309356
F	4.639317	-0.259263	1.608324
O	0.214036	1.916581	0.909456
C	-0.004197	0.750811	1.222375
H	-4.338555	0.156175	2.721061
C	0.628382	-2.140650	-2.511555
C	-0.218359	-1.022076	-2.664814
C	-1.472578	-1.130164	-3.269198
C	-1.876070	-2.375796	-3.733510
C	-1.034420	-3.493554	-3.607240
C	0.209637	-3.386676	-3.005863
C	1.932995	-0.640113	-1.515723
H	-2.118221	-0.262322	-3.369206
H	-2.848246	-2.484419	-4.204208
H	-1.365568	-4.455012	-3.986341
H	0.865901	-4.246056	-2.908020
N	1.811270	-1.903966	-1.843955
S	0.545623	0.379311	-1.971549
C	3.422917	1.290733	-1.000284
O	2.604473	2.162292	-1.322052
C	4.833359	1.719503	-0.691826
C	5.034912	3.050650	-0.315343
C	5.936198	0.867338	-0.797757
C	6.312136	3.519518	-0.028230
H	4.170107	3.703390	-0.255007

C	7.216669	1.338635	-0.523992
H	5.800821	-0.162766	-1.111208
C	7.406705	2.662932	-0.133263
H	6.456376	4.551932	0.274567
H	8.068019	0.671911	-0.617227
H	8.405853	3.026875	0.085195
C	-5.764817	2.429951	0.666180
H	-6.396934	1.686505	1.136702
H	-7.386626	3.732104	0.177030
C	3.064283	-0.094749	-0.823987
H	3.848272	-0.822455	-0.652814
H	2.559535	1.293567	1.259972

Vibrational frequencies

-244.8460	11.1160	16.1117
26.0190	37.2276	40.3557
43.5175	50.5240	54.9427
61.5193	69.0513	72.8768
79.1408	83.4404	89.1588
101.9030	110.9734	115.9059
125.7711	130.3885	144.8587
147.6423	158.2535	164.5025
168.8133	192.5055	205.2616
209.5909	218.9272	228.7766
234.4888	243.5383	253.0625
262.5562	278.6406	300.7815
307.5171	314.6635	320.5782
322.8607	342.0216	353.8958
356.2511	379.4432	395.1831
400.3289	416.7747	423.4172
428.5745	431.3047	438.0418
441.6166	451.0785	456.2384
472.7514	492.6683	494.2126
517.8127	522.8552	530.9015
546.1789	550.1555	553.2672
563.1224	573.8943	593.3148
614.7579	624.3750	626.9824
629.5603	634.0758	638.3464
653.8050	666.5808	672.0434
699.4073	707.2635	715.8581
716.6166	722.1640	725.3115
727.8080	729.1193	731.8478
735.2646	747.0772	757.8738
772.3159	782.7421	787.8147
789.4129	816.9931	828.9161

839.4411 852.4779 868.2552
871.6323 875.1782 878.4442
879.3031 883.7881 911.2312
922.8745 928.3614 937.9460
944.1498 956.3537 960.7953
968.0388 973.5425 973.9741
993.8962 998.1601 1005.7829
1008.5937 1009.5145 1018.1580
1020.9503 1021.7521 1024.1581
1024.9741 1032.1088 1051.4198
1063.6884 1065.6366 1068.9753
1079.1017 1083.7845 1092.7565
1098.3538 1116.2472 1121.1028
1127.7376 1130.9067 1150.4962
1152.8816 1166.0895 1175.1799
1176.6081 1181.6359 1181.7573
1185.7118 1188.2091 1196.6911
1202.7623 1208.8392 1220.5905
1225.2718 1240.5509 1241.8766
1253.8738 1261.9621 1276.3874
1279.1397 1289.9010 1299.2757
1317.9340 1318.8722 1328.8513
1337.2045 1339.3349 1344.6570
1355.7185 1360.2083 1362.0468
1364.3280 1372.6903 1378.1279
1383.7998 1385.2563 1401.4932
1408.4733 1409.5924 1428.4358
1431.5451 1434.3828 1483.6871
1489.8821 1497.6512 1500.4558
1501.4190 1507.9302 1511.2221
1514.4502 1518.3380 1521.6863
1527.9499 1541.7717 1551.1528
1554.2108 1571.9055 1595.2530
1640.5405 1668.1338 1680.6478
1681.7568 1682.4047 1687.1094
1694.6767 1701.5135 1706.6676
1749.1847 3058.5159 3060.1619
3087.5727 3089.0482 3101.8964
3119.4033 3134.5207 3140.0646
3148.7793 3167.1842 3192.2064
3197.2016 3197.3266 3199.2333
3204.6879 3206.7201 3212.0285
3213.0634 3220.1267 3220.2392
3222.3817 3228.1668 3228.3370

3228.9576	3232.5241	3233.3568
3235.8796	3243.4628	3243.8051
3244.3534	3249.9017	3336.7010

TS2*RR*''

Zero-point correction= 0.628113

Thermal correction to Energy= 0.668144

Thermal correction to Enthalpy= 0.669088

Thermal correction to Gibbs Free Energy= 0.554862

Sum of electronic and zero-point Energies= -2876.449264

Sum of electronic and thermal Energies= -2876.409233

Sum of electronic and thermal Enthalpies= -2876.408289

Sum of electronic and thermal Free Energies= -2876.522515

Cartesian coordinates

C	7.630591	0.465945	1.036535
C	7.658057	-0.820328	0.482790
C	6.483582	-1.465936	0.121725
C	5.281207	-0.788684	0.311447
C	5.258404	0.491457	0.864762
H	8.608798	-1.320135	0.336304
H	6.497917	-2.464154	-0.301304
C	3.009532	0.131697	0.541249
C	1.277009	1.890720	0.688306
C	2.481031	2.871187	0.655002
C	3.573273	2.275085	1.535172
H	4.460080	2.906976	1.540088
S	3.662060	-1.376094	-0.022060
N	3.948429	0.969652	0.982246
N	1.702594	0.470033	0.532795
C	3.060244	3.374539	-0.698689
C	3.485484	2.297009	-1.706030
C	2.186162	4.428789	-1.393045
H	3.974160	3.904748	-0.396218
H	2.668267	1.607490	-1.933953
H	4.351126	1.717379	-1.374738
H	3.769274	2.779824	-2.645309
H	1.347968	3.986636	-1.935719
H	2.800876	4.973648	-2.115645
H	1.785064	5.153673	-0.678193
H	2.116987	3.763134	1.177408
H	0.850060	1.972080	1.694850
C	0.216739	2.286831	-0.320933
C	-0.586201	3.383609	-0.000649
C	0.085161	1.677621	-1.567031

C	-1.459538	3.914789	-0.944524
H	-0.508300	3.840318	0.983651
C	-0.782569	2.215654	-2.513943
H	0.632353	0.770384	-1.799631
C	-1.540133	3.345177	-2.214305
H	-2.068788	4.776405	-0.690614
H	-0.881820	1.733275	-3.480734
H	-2.215692	3.760691	-2.955340
C	-0.553386	-0.330605	1.184047
H	-0.914126	0.680731	1.308300
C	-1.302702	-1.398340	1.565697
C	-2.435274	-1.207139	2.526793
F	-3.080210	-0.046027	2.347329
F	-1.952172	-1.182894	3.790426
F	-3.332640	-2.195950	2.491001
O	1.156353	-1.737602	0.353819
C	0.749579	-0.620765	0.626011
H	3.236805	2.127665	2.565770
C	-5.475672	0.156091	0.155480
C	-4.712683	1.216332	-0.380839
C	-5.222847	2.511576	-0.463866
C	-6.510823	2.749909	0.001082
C	-7.279358	1.705238	0.537605
C	-6.775336	0.415833	0.616979
C	-3.642042	-0.996579	-0.317390
H	-4.622410	3.315365	-0.880157
H	-6.924898	3.751653	-0.052243
H	-8.283591	1.910679	0.895365
H	-7.363444	-0.397425	1.030455
N	-4.856441	-1.072511	0.176625
S	-3.153830	0.617094	-0.883250
C	-1.548730	-2.090281	-1.130227
O	-1.080454	-1.048471	-1.634745
C	-0.798085	-3.384886	-1.318454
C	0.184937	-3.427632	-2.311152
C	-1.030194	-4.530299	-0.551082
C	0.911055	-4.589599	-2.543762
H	0.365896	-2.525652	-2.886331
C	-0.297782	-5.693574	-0.776387
H	-1.772486	-4.518960	0.241348
C	0.671064	-5.729122	-1.776001
H	1.665974	-4.610508	-3.324246
H	-0.485854	-6.573359	-0.168769
H	1.236729	-6.638150	-1.955345

C	6.434504	1.140278	1.239649
H	6.426489	2.129028	1.682397
H	8.560211	0.947387	1.318193
C	-2.732711	-2.096053	-0.347163
H	-3.158093	-3.029872	-0.002391
H	-0.880570	-2.398023	1.545509

Vibrational frequencies

-153.0839	9.4096	24.0394
30.8647	34.9553	45.2515
48.6789	53.1360	55.4448
60.1264	62.6279	68.9399
86.9469	89.3460	99.2794
106.7432	116.0743	120.0887
136.4623	142.2380	146.5565
151.2944	167.7681	180.7635
183.6631	185.3900	198.7417
211.0648	214.8717	223.7773
241.0835	245.3746	253.9391
265.8135	277.5345	294.0671
302.5110	322.1390	328.0754
329.2342	330.1516	344.1009
347.6022	363.4164	395.9072
404.0036	416.1115	420.1536
424.5946	430.6936	439.3651
442.3847	444.4787	451.6126
473.0477	486.2452	506.6829
517.3440	522.3776	533.9206
545.9205	547.1045	551.4802
565.0679	571.7291	578.7085
610.1669	617.4364	624.9988
631.0623	642.6111	643.8075
649.6510	660.6297	672.3160
688.5055	706.9280	712.6144
714.5762	721.3690	722.0154
724.7802	727.9230	730.0957
731.3232	746.7608	763.3591
772.8891	774.3918	781.7166
791.6062	806.4441	816.4266
822.7696	850.4997	866.1210
874.1289	876.0012	877.3690
877.6971	882.7658	911.7650
920.4809	932.8965	935.6156
953.0879	955.0464	956.7449
961.6808	966.8900	973.4890

985.2699	995.7484	1004.7888
1006.9332	1016.7777	1017.1617
1023.5530	1024.1179	1024.3107
1028.2311	1029.5072	1053.8181
1060.4714	1065.2026	1068.3641
1073.3380	1087.6836	1095.1226
1099.5164	1108.8013	1123.9428
1127.3266	1141.0460	1148.1887
1148.8495	1165.8158	1174.5201
1175.2136	1177.4508	1183.7130
1185.0469	1192.7175	1193.2273
1202.6898	1216.2931	1218.8849
1228.1365	1241.4575	1244.2530
1264.3733	1273.8224	1282.1660
1293.9218	1301.4168	1307.3910
1309.8912	1323.4453	1334.1203
1336.1215	1341.0502	1351.5618
1354.9325	1362.4069	1364.7145
1368.4066	1372.5904	1376.7536
1380.7510	1392.4252	1399.2619
1414.5532	1418.7265	1435.7755
1436.6144	1463.9583	1487.6941
1492.9291	1495.6143	1498.7287
1503.0715	1508.8382	1509.7933
1516.8283	1518.7712	1519.8341
1527.2734	1542.8288	1554.2464
1558.6219	1595.9899	1614.0922
1643.4133	1662.9754	1678.8386
1679.3687	1686.0102	1689.4470
1691.6967	1696.2023	1696.5772
1782.1210	3043.9829	3071.0327
3076.5805	3084.2836	3098.6628
3113.7301	3144.8295	3146.6248
3165.8018	3173.1275	3192.9139
3194.2708	3194.7853	3198.2902
3198.6106	3200.8289	3208.2942
3211.9301	3217.9478	3219.7051
3220.5077	3221.1515	3224.4781
3226.0238	3228.0971	3229.0973
3233.9204	3236.1201	3242.6316
3244.7749	3254.4915	3271.8471

TS2*RR*'''

Zero-point correction= 0.627864

Thermal correction to Energy= 0.668278
Thermal correction to Enthalpy= 0.669222
Thermal correction to Gibbs Free Energy= 0.553098
Sum of electronic and zero-point Energies= -2876.440856
Sum of electronic and thermal Energies= -2876.400443
Sum of electronic and thermal Enthalpies= -2876.399499
Sum of electronic and thermal Free Energies= -2876.515623
Cartesian coordinates

C	6.395796	-4.330505	-0.006952
C	5.650053	-5.014432	-0.975512
C	4.417325	-4.534832	-1.397117
C	3.952323	-3.347331	-0.835904
C	4.698982	-2.669911	0.125662
H	6.037690	-5.933537	-1.399839
H	3.833547	-5.063559	-2.142164
C	2.853963	-1.300007	-0.010142
C	2.652923	0.895711	1.116056
C	4.199737	0.812643	1.186825
C	4.541438	-0.610774	1.604440
H	5.615098	-0.758405	1.693569
S	2.428570	-2.538114	-1.153401
N	4.041405	-1.513012	0.561621
N	2.092914	-0.231171	0.312135
C	4.942018	1.279447	-0.101697
C	5.240472	2.784597	-0.056556
C	6.270448	0.551465	-0.342212
H	4.292473	1.076248	-0.963997
H	5.949016	2.992127	0.753615
H	4.353966	3.398812	0.102131
H	5.706605	3.098637	-0.994500
H	6.955654	0.693464	0.501305
H	6.752893	0.973021	-1.227400
H	6.155693	-0.520849	-0.519418
H	4.490343	1.468338	2.015705
H	2.268660	0.774451	2.135431
C	2.197047	2.234439	0.576792
C	2.096086	3.294820	1.478194
C	1.970520	2.456191	-0.781232
C	1.804131	4.577086	1.022964
H	2.257743	3.117500	2.538718
C	1.685014	3.740529	-1.234726
H	2.024653	1.632575	-1.488151
C	1.606158	4.802580	-0.337027
H	1.728156	5.396202	1.730259

H	1.516512	3.911288	-2.292156
H	1.372991	5.799785	-0.695883
C	-0.219195	0.452414	0.902968
H	0.103382	1.374030	1.365455
C	-1.485853	-0.011272	1.085049
C	-2.302178	0.642627	2.163115
F	-2.301115	1.979916	2.052201
F	-1.775065	0.362743	3.376079
F	-3.566825	0.226380	2.194787
O	0.287498	-1.188965	-0.712835
C	0.664613	-0.346901	0.086483
H	4.070698	-0.880628	2.554229
C	-4.475675	-2.951804	-0.472644
C	-5.715323	-2.397847	-0.089191
C	-6.816013	-3.205686	0.191254
C	-6.674077	-4.584761	0.080949
C	-5.448058	-5.147215	-0.301773
C	-4.350896	-4.344179	-0.578657
C	-3.880457	-0.807566	-0.548769
H	-7.764009	-2.768471	0.489160
H	-7.520687	-5.229247	0.294278
H	-5.356926	-6.225928	-0.383043
H	-3.398144	-4.769386	-0.877767
N	-3.467129	-2.043185	-0.717505
S	-5.580968	-0.658121	-0.020623
C	-3.522405	1.660348	-0.567735
O	-4.587493	1.939297	0.012617
C	-2.682642	2.797323	-1.086335
C	-2.746756	4.024035	-0.418870
C	-1.936768	2.700078	-2.263870
C	-2.074922	5.134574	-0.915830
H	-3.340815	4.083345	0.487403
C	-1.288953	3.820317	-2.779592
H	-1.902125	1.759226	-2.804723
C	-1.354165	5.037346	-2.106068
H	-2.122201	6.080828	-0.385351
H	-0.737691	3.744069	-3.712277
H	-0.845082	5.908908	-2.507598
C	5.933197	-3.151411	0.560542
H	6.511767	-2.638752	1.319934
H	7.351742	-4.728979	0.313327
C	-3.046419	0.330690	-0.753513
H	-2.147579	0.144450	-1.327625
H	-1.767918	-1.019211	0.795937

Vibrational frequencies

-161.6364	13.8619	20.9830
29.4426	33.1423	37.7268
40.1783	47.1962	52.0010
59.4334	61.5630	70.3630
74.0992	78.8358	88.0230
98.7940	102.5414	111.1954
118.9932	128.1880	138.3365
148.6878	154.8578	163.0797
166.7263	188.9037	203.6947
207.9825	211.0163	225.8448
229.8725	234.0340	250.5412
259.2482	268.8685	290.7927
293.3193	300.4084	314.7980
320.7423	337.3402	339.0333
366.5533	387.3325	398.6284
401.9223	415.9477	420.3276
422.0204	429.5967	436.4250
441.2176	444.2475	449.3406
475.4234	490.1117	501.9007
513.0583	521.8285	529.7096
547.5637	551.8665	557.6708
565.6520	571.6563	586.9364
613.6428	616.1607	627.0484
627.6454	635.1679	639.7472
654.1872	657.6800	670.3314
692.9801	707.3445	709.6105
716.1286	719.7978	721.6182
727.9644	730.2385	732.2219
741.9594	747.1517	766.5840
774.3055	777.3468	788.3987
796.6059	817.6174	828.3488
838.7692	859.3831	872.0025
876.8396	877.0892	877.8549
879.3034	880.7343	916.5196
923.2224	930.7633	937.1928
947.8553	953.7020	958.0791
961.4797	975.2854	977.3392
994.2925	1000.0400	1002.4870
1006.8088	1012.0687	1018.6767
1020.8794	1023.2578	1025.0464
1027.9528	1029.9791	1056.2989
1062.0544	1067.3489	1071.3475
1071.7912	1089.3666	1099.3744

1103.6175	1118.2312	1122.8797
1123.5580	1137.0669	1151.3181
1153.6591	1170.7880	1175.5404
1176.2081	1181.2972	1183.8400
1189.2802	1195.2775	1198.9016
1203.4679	1206.8854	1210.4916
1237.2571	1244.8602	1246.7827
1254.0177	1260.8795	1284.3722
1287.5500	1303.8396	1309.2041
1313.8339	1323.1966	1332.9048
1337.1456	1338.9174	1342.2670
1355.8692	1361.2310	1363.4840
1364.0258	1365.9143	1373.3551
1379.6468	1390.1444	1399.2952
1405.5843	1415.4796	1434.3061
1437.6225	1457.2581	1491.8431
1493.0735	1497.1974	1502.5144
1504.0003	1507.1323	1513.0454
1516.1379	1519.9123	1530.6945
1532.8173	1540.9414	1553.2840
1553.9474	1592.0020	1619.2375
1645.3459	1666.7529	1679.6134
1682.2960	1682.5015	1689.0955
1695.6603	1699.4082	1700.4984
1778.6056	3060.5087	3062.7910
3070.3657	3087.1958	3095.8130
3117.9026	3137.7661	3143.0006
3161.1203	3180.8560	3189.2478
3197.0952	3200.6114	3200.8301
3201.5786	3208.0562	3208.3374
3208.3730	3211.7059	3216.2051
3217.4571	3226.0238	3226.5947
3227.7612	3228.6875	3228.9976
3233.8387	3235.0826	3238.4358
3245.1258	3251.4708	3269.7398

TS2*SR*

Zero-point correction= 0.627851

Thermal correction to Energy= 0.668497

Thermal correction to Enthalpy= 0.669441

Thermal correction to Gibbs Free Energy= 0.552984

Sum of electronic and zero-point Energies= -2876.460548

Sum of electronic and thermal Energies= -2876.419902

Sum of electronic and thermal Enthalpies= -2876.418958

Sum of electronic and thermal Free Energies= -2876.535415

Cartesian coordinates

C	-5.757886	-3.602581	0.089965
C	-4.859527	-4.675871	0.099209
C	-3.519464	-4.489664	-0.217579
C	-3.098539	-3.203553	-0.544649
C	-3.999563	-2.140045	-0.558699
H	-5.211148	-5.667156	0.361680
H	-2.819915	-5.317840	-0.206510
C	-2.053255	-1.045313	-1.110558
C	-1.868722	1.380015	-1.487719
C	-3.299717	1.215966	-2.035983
C	-4.104312	0.320033	-1.104863
H	-5.069599	0.068918	-1.551419
S	-1.483323	-2.686108	-0.997165
N	-3.373351	-0.937258	-0.911758
N	-1.274717	0.023070	-1.324394
C	-4.007637	2.560620	-2.330530
C	-4.802033	3.135562	-1.152018
C	-4.924780	2.408141	-3.547186
H	-3.223351	3.281780	-2.594196
H	-5.681250	2.518924	-0.934146
H	-4.208763	3.224784	-0.238797
H	-5.165373	4.132470	-1.414527
H	-4.363541	2.102690	-4.434327
H	-5.702509	1.658617	-3.361978
H	-5.425429	3.354309	-3.768580
H	-3.193641	0.679594	-2.988015
H	-1.273206	1.859495	-2.270889
C	-1.781787	2.217516	-0.230637
C	-1.453614	3.571505	-0.336398
C	-2.047882	1.673616	1.024275
C	-1.419524	4.374778	0.799639
H	-1.214864	3.995646	-1.308643
C	-1.997302	2.471672	2.164327
H	-2.265448	0.615764	1.130262
C	-1.692756	3.826034	2.051424
H	-1.164244	5.425317	0.708512
H	-2.180541	2.021795	3.135240
H	-1.652162	4.449984	2.938073
C	0.979333	0.951119	-1.141186
H	0.566896	1.767709	-0.562670
C	2.315486	0.830956	-1.317701
C	3.199391	1.974243	-0.914226

F	2.987826	3.042435	-1.711688
F	2.956790	2.377143	0.338442
F	4.499594	1.678050	-1.012230
O	0.542268	-1.242796	-1.926911
C	0.148247	-0.168404	-1.508547
H	-4.275364	0.785019	-0.129333
C	-0.071264	-0.766535	2.345828
C	0.606193	-0.046525	3.353720
C	-0.024492	0.303168	4.546265
C	-1.345726	-0.086838	4.742668
C	-2.023653	-0.824216	3.760981
C	-1.395897	-1.170743	2.572089
C	1.920098	-0.662329	1.352263
H	0.507636	0.857452	5.313075
H	-1.850509	0.171339	5.667940
H	-3.047844	-1.137794	3.937915
H	-1.911918	-1.760478	1.817837
N	0.666819	-1.056565	1.218840
S	2.260424	0.226986	2.862768
C	4.291999	-0.618820	0.597715
O	4.703095	0.026305	1.578826
C	5.299987	-1.100393	-0.420133
C	6.648222	-0.833837	-0.164211
C	4.959204	-1.771169	-1.599918
C	7.636127	-1.231981	-1.057209
H	6.894777	-0.304868	0.749790
C	5.947040	-2.166759	-2.498523
H	3.922354	-1.994698	-1.832153
C	7.287726	-1.900568	-2.229939
H	8.678873	-1.019577	-0.841945
H	5.667871	-2.686394	-3.409748
H	8.055948	-2.212455	-2.930643
C	-5.343120	-2.317909	-0.237668
H	-6.038718	-1.486835	-0.228923
H	-6.797153	-3.772132	0.347863
C	2.915094	-0.909835	0.379819
H	2.601086	-1.598456	-0.392991
H	2.745196	0.095243	-1.986910

Vibrational frequencies

-115.2862	18.8937	23.0822
27.4104	31.4194	33.7206
35.3161	44.2889	53.4607
60.1492	61.2882	64.4245
73.1760	77.2543	90.0743

94.6349	104.7910	113.4220
117.9003	123.7350	131.8705
137.2858	153.6505	165.5849
177.4684	182.8916	194.3799
210.7990	215.8967	220.2339
228.4956	243.9743	247.9193
258.2130	270.9705	275.0035
282.4104	293.6020	307.9104
315.0694	322.6947	328.3833
339.0886	358.9684	396.8920
404.1383	415.5001	426.4859
427.2060	432.5941	435.4140
445.8483	446.7707	456.3089
469.4799	476.1768	495.0142
510.6034	513.0071	520.2774
545.3258	546.4160	547.8547
566.7963	573.9816	581.3165
613.7135	614.9302	628.3059
628.8492	635.1062	638.8669
650.2582	658.0325	671.5986
674.7137	700.0373	711.7120
715.3764	719.1429	720.9157
725.0352	727.1770	728.6396
734.9386	745.6002	763.6999
767.5032	774.5923	795.4714
797.4374	813.4298	828.5498
849.2166	866.0692	873.7743
875.2326	877.1572	877.8987
884.2663	885.1239	916.0086
920.2629	931.1121	946.1165
953.9551	956.3000	962.3547
967.1590	969.6250	976.0838
993.2600	1006.7746	1009.9514
1010.8676	1014.7910	1018.0021
1018.9837	1023.7879	1032.3490
1038.6019	1048.5642	1055.0385
1055.8138	1067.1167	1068.4779
1070.1030	1084.8104	1086.9600
1098.5143	1117.6186	1122.4482
1127.7023	1145.4414	1152.5015
1155.7460	1175.0177	1175.4791
1176.0709	1176.5198	1182.6688
1187.6964	1195.4771	1204.2152
1204.9722	1212.2946	1220.6846

1223.0241	1238.7208	1244.2522
1259.2600	1274.5487	1287.3277
1291.7521	1305.4446	1310.0424
1313.1111	1320.5774	1325.0858
1341.3441	1344.5469	1345.4532
1359.4377	1361.7664	1364.2191
1365.3076	1368.8607	1378.5711
1379.7814	1395.4516	1409.1356
1418.2715	1427.4274	1437.0136
1444.4745	1454.3308	1491.3500
1496.6588	1498.2042	1499.1486
1505.1044	1506.8668	1511.9783
1516.7576	1518.5261	1521.1318
1532.0249	1539.9593	1550.6632
1557.0944	1605.7917	1641.6433
1643.8459	1671.6797	1679.9114
1680.6259	1681.4834	1690.9990
1696.5243	1696.6966	1712.7197
1793.7368	3065.1721	3067.1029
3070.6458	3073.6253	3106.8721
3118.1315	3139.7876	3143.2557
3157.3380	3163.4332	3173.2295
3193.6892	3193.7854	3200.2651
3204.5177	3212.4490	3214.1302
3216.5208	3221.2694	3222.3547
3222.9125	3224.9397	3227.0952
3229.1496	3231.4530	3234.9771
3237.8914	3241.6454	3242.6891
3249.1871	3254.3907	3259.9138

TS2*SR*'

Zero-point correction= 0.628962

Thermal correction to Energy= 0.669125

Thermal correction to Enthalpy= 0.670069

Thermal correction to Gibbs Free Energy= 0.555577

Sum of electronic and zero-point Energies= -2876.456317

Sum of electronic and thermal Energies= -2876.416154

Sum of electronic and thermal Enthalpies= -2876.415210

Sum of electronic and thermal Free Energies= -2876.529703

Cartesian coordinates

C	-6.502968	3.070592	-1.761599
C	-5.699396	4.043430	-2.369571
C	-4.321379	4.041838	-2.197701
C	-3.765616	3.041881	-1.403872

C	-4.570341	2.083937	-0.793158
H	-6.157999	4.807639	-2.986738
H	-3.694458	4.790037	-2.669420
C	-2.495384	1.398448	-0.076578
C	-2.097775	-0.645380	1.221301
C	-3.466901	-0.323513	1.852637
C	-4.440409	0.128614	0.778101
H	-5.338134	0.558645	1.228627
S	-2.073592	2.806969	-1.007109
N	-3.814469	1.183052	-0.030375
N	-1.610283	0.567837	0.514775
C	-4.032444	-1.472136	2.723788
C	-4.901512	-2.484679	1.967614
C	-4.823187	-0.890219	3.899214
H	-3.168633	-2.008817	3.136864
H	-5.855195	-2.035538	1.668523
H	-4.415383	-2.889225	1.076095
H	-5.135495	-3.321838	2.630228
H	-4.198461	-0.243660	4.521182
H	-5.676438	-0.301503	3.544290
H	-5.216350	-1.692743	4.528688
H	-3.285839	0.535515	2.511720
H	-1.405523	-0.798295	2.051255
C	-2.105527	-1.875851	0.340128
C	-1.700152	-3.094589	0.888990
C	-2.637534	-1.854493	-0.952685
C	-1.886161	-4.282443	0.186206
H	-1.255156	-3.117172	1.880880
C	-2.833813	-3.043219	-1.650916
H	-2.907655	-0.913689	-1.425423
C	-2.477695	-4.261127	-1.073935
H	-1.569499	-5.222684	0.625094
H	-3.261312	-3.015407	-2.647661
H	-2.637451	-5.187217	-1.616487
C	0.704940	-0.019930	1.127724
H	0.481232	-1.078332	1.154764
C	1.927674	0.447784	1.472033
C	2.872637	-0.466954	2.188091
F	2.598600	-0.474052	3.511021
F	2.754426	-1.734692	1.766774
F	4.149570	-0.102749	2.065946
O	0.097007	2.020100	0.104556
C	-0.224175	0.927078	0.548775
H	-4.735630	-0.687392	0.111637

C	1.871300	-2.575311	-1.574712
C	3.169303	-3.118416	-1.457730
C	3.400911	-4.481784	-1.628783
C	2.319790	-5.313022	-1.908370
C	1.025687	-4.784887	-2.016409
C	0.795609	-3.425876	-1.856490
C	2.936683	-0.684575	-1.096686
H	4.403039	-4.889728	-1.538980
H	2.482589	-6.377995	-2.039538
H	0.190092	-5.446793	-2.226123
H	-0.201300	-3.004565	-1.933112
N	1.767681	-1.213754	-1.388492
S	4.303230	-1.841745	-1.084962
C	4.372641	1.256314	-0.469858
O	5.437717	0.612010	-0.468726
C	4.427895	2.730381	-0.139903
C	5.691389	3.313384	0.000265
C	3.292117	3.529470	0.040508
C	5.823818	4.663421	0.304146
H	6.560466	2.678715	-0.136344
C	3.424790	4.881482	0.349905
H	2.295894	3.106954	-0.055586
C	4.688382	5.452988	0.480265
H	6.811685	5.102296	0.405760
H	2.536287	5.489732	0.489661
H	4.787924	6.507364	0.718908
C	-5.953393	2.075715	-0.964139
H	-6.578831	1.318902	-0.505299
H	-7.575647	3.089504	-1.916792
C	3.101615	0.675183	-0.741462
H	2.237541	1.300812	-0.924099
H	2.139237	1.508273	1.548098

Vibrational frequencies

-142.7982	15.8834	28.1328
29.1984	34.7175	40.3509
45.1140	49.9117	57.9840
62.2993	70.7413	73.2586
80.3818	91.0016	91.8268
102.0014	105.9542	113.0947
122.4750	130.0127	136.6864
139.8115	163.5017	172.5673
180.6553	185.7739	192.0039
220.1865	220.8422	226.5051
234.2525	242.8336	244.4083

258.6637	278.3286	283.9183
299.3647	314.3361	315.8798
325.1371	329.8839	338.8380
344.9998	383.5226	397.1070
406.5472	417.8984	424.8688
425.4516	432.3188	439.9109
444.8308	447.1652	453.8282
475.2929	478.9174	489.5050
515.4384	515.5318	523.0671
547.2801	548.6751	556.0284
565.6156	579.2927	584.0002
613.2327	623.6376	628.0435
628.9333	641.5321	644.2587
650.3108	662.3000	673.9421
675.9727	703.0527	714.4607
717.3177	721.6381	724.0988
726.3924	728.2491	733.2037
734.2616	750.4916	763.4615
771.6702	777.8950	792.2159
795.8613	815.0791	828.9719
850.0701	866.0867	875.4871
876.7640	881.3140	884.3232
885.8958	887.2099	917.2439
922.8802	932.2138	942.7253
949.7048	961.3971	966.3327
973.3720	973.6445	977.2576
998.4311	1006.9315	1007.4909
1014.3936	1016.4057	1019.7304
1021.4599	1023.2251	1030.9627
1031.9729	1047.2027	1061.6500
1063.3064	1064.6800	1067.5522
1070.7500	1088.3278	1090.3882
1106.0668	1116.2814	1122.1762
1126.3784	1151.1118	1155.7460
1162.9850	1174.6727	1174.8778
1176.8941	1179.7269	1181.5027
1188.8272	1192.6271	1203.4073
1208.8586	1212.2492	1222.6670
1234.7576	1248.0364	1255.8652
1266.1920	1279.5932	1290.7467
1291.0284	1311.4259	1312.0639
1324.8338	1327.3596	1330.5549
1341.9819	1346.0607	1346.6515
1360.9963	1363.6296	1364.8571

1365.9433	1370.4143	1381.8954
1383.6845	1395.6506	1411.4803
1418.0162	1431.6627	1436.2136
1450.2587	1460.7511	1494.5655
1495.5134	1499.5716	1500.7077
1505.4451	1508.3051	1511.5668
1517.1248	1519.4692	1521.3010
1529.0894	1544.3740	1552.0490
1559.8748	1600.8470	1636.4125
1645.8706	1669.0734	1677.5800
1682.7789	1686.9545	1690.4191
1694.3016	1697.5209	1709.6940
1769.4702	3063.1439	3065.8672
3073.2357	3075.7820	3103.9370
3138.2008	3141.7436	3142.1187
3159.8647	3161.1180	3168.3211
3188.4497	3193.5621	3196.1142
3198.0542	3208.5531	3209.3839
3210.2221	3216.5787	3220.6606
3221.9658	3223.0605	3225.3268
3228.1915	3230.2654	3231.4235
3234.6145	3239.6105	3241.7773
3246.2885	3249.7573	3260.7951

TS2*SR*''

Zero-point correction= 0.627845

Thermal correction to Energy= 0.668206

Thermal correction to Enthalpy= 0.669151

Thermal correction to Gibbs Free Energy= 0.553928

Sum of electronic and zero-point Energies= -2876.455096

Sum of electronic and thermal Energies= -2876.414734

Sum of electronic and thermal Enthalpies= -2876.413790

Sum of electronic and thermal Free Energies= -2876.529012

Cartesian coordinates

C	6.661773	2.899778	-0.065275
C	5.874506	4.046424	-0.227015
C	4.520694	3.947559	-0.522553
C	3.972459	2.674165	-0.651255
C	4.761455	1.537272	-0.491772
H	6.325860	5.025972	-0.117206
H	3.905716	4.832140	-0.647241
C	2.711199	0.577111	-0.884573
C	2.262775	-1.832698	-0.733701
C	3.693581	-1.965398	-1.291581

C	4.613421	-0.973497	-0.596101
H	5.577960	-0.919848	-1.107526
S	2.313227	2.260074	-1.037620
N	4.013243	0.364002	-0.656236
N	1.817713	-0.428074	-0.917076
C	4.236907	-3.414881	-1.248324
C	4.983357	-3.779670	0.040774
C	5.140580	-3.666520	-2.458482
H	3.368924	-4.080826	-1.336710
H	5.936521	-3.243302	0.105295
H	4.406456	-3.568838	0.945017
H	5.215188	-4.847728	0.032377
H	4.601100	-3.518186	-3.397716
H	6.003238	-2.990769	-2.451655
H	5.523967	-4.690019	-2.442498
H	3.626475	-1.664278	-2.344929
H	1.614526	-2.430713	-1.380093
C	2.108491	-2.304115	0.696147
C	1.634755	-3.595402	0.938625
C	2.483201	-1.499588	1.774057
C	1.566295	-4.087655	2.238941
H	1.317339	-4.218424	0.105838
C	2.412531	-1.990974	3.075119
H	2.818440	-0.479164	1.605376
C	1.961525	-3.288093	3.308856
H	1.196618	-5.092129	2.415299
H	2.708141	-1.359542	3.907032
H	1.906039	-3.669702	4.322719
C	-0.539969	-1.098206	-0.736446
H	-0.245997	-1.991353	-0.200382
C	-1.852748	-0.817041	-0.950084
C	-2.844380	-1.924958	-0.707117
F	-2.450247	-3.048231	-1.346447
F	-2.948507	-2.252514	0.586270
F	-4.061104	-1.632504	-1.172654
O	0.161303	0.978945	-1.613016
C	0.430710	-0.111322	-1.137748
H	4.784647	-1.231954	0.453552
C	-6.312364	-0.104107	0.534044
C	-6.458463	0.763917	-0.569341
C	-7.682583	0.918279	-1.217796
C	-8.772861	0.185637	-0.762012
C	-8.640867	-0.683309	0.331151
C	-7.425165	-0.831801	0.982153

C	-4.216682	0.629097	0.459225
H	-7.782273	1.594245	-2.061431
H	-9.733285	0.288277	-1.256607
H	-9.503861	-1.246982	0.671944
H	-7.314979	-1.500787	1.829611
N	-5.053988	-0.159070	1.089107
S	-4.934633	1.551737	-0.894519
C	-2.053412	1.842522	0.314125
O	-2.415289	2.592639	-0.610978
C	-0.765774	2.157400	1.034185
C	-0.307899	3.478651	0.976085
C	-0.033603	1.220340	1.772034
C	0.838137	3.868659	1.659356
H	-0.880037	4.188138	0.387600
C	1.122070	1.611309	2.450130
H	-0.359078	0.183949	1.825681
C	1.558760	2.933430	2.401701
H	1.170486	4.901714	1.616513
H	1.667086	0.883055	3.042528
H	2.451310	3.234488	2.941688
C	6.119298	1.627528	-0.193702
H	6.730064	0.742948	-0.055404
H	7.715234	3.002682	0.169169
C	-2.827391	0.730726	0.767293
H	-2.521670	0.178179	1.647192
H	-2.161728	0.004909	-1.588658

Vibrational frequencies

-184.3509	13.9545	24.5292
26.8159	30.7238	37.6455
47.7936	52.9066	58.6425
63.9141	71.3204	75.4716
82.4362	85.1416	91.2500
97.5461	107.7468	112.7051
125.4600	131.5986	137.1703
140.1674	150.7942	162.4084
170.5116	189.2303	207.9708
216.2830	221.3744	224.7179
233.2707	237.1075	244.8580
257.9645	269.3141	277.3312
285.9476	301.2781	310.1106
314.4101	325.6731	332.3694
345.5330	370.9134	396.2802
402.6088	419.8904	425.5024
428.6050	431.4715	435.8914

439.1727	447.0569	453.4297
476.9226	489.7514	491.9751
512.1909	515.0360	524.4631
547.6484	550.7684	553.0938
565.4830	580.4688	582.2474
613.2753	618.9165	626.3549
627.0120	637.1547	640.0213
646.5833	661.2627	670.7804
672.5022	703.7467	712.4409
717.2760	720.4293	722.7593
728.2785	732.4854	734.5387
737.7741	748.9341	760.9821
764.1271	771.3378	776.6548
794.1727	816.3842	824.3638
836.6567	866.1025	872.4094
875.3741	875.8300	877.1809
879.4092	886.5882	913.9347
918.5163	929.7512	945.5033
952.7977	956.7961	963.0469
968.6068	976.5323	976.9508
998.7264	1005.9457	1007.6303
1010.7129	1013.9691	1016.2564
1023.7226	1024.0980	1026.1575
1036.3549	1048.5755	1056.8106
1060.1678	1063.8316	1065.6461
1072.5931	1086.4933	1089.6976
1096.6039	1114.9067	1119.3630
1128.0050	1152.5748	1152.6223
1163.3696	1172.7488	1174.0332
1180.0856	1181.1973	1182.5791
1189.9857	1190.9147	1201.1298
1211.3909	1215.0088	1217.1692
1227.0136	1239.2369	1250.1330
1255.8615	1261.9700	1285.0237
1292.6316	1304.5994	1308.0679
1318.5825	1321.6772	1328.4791
1333.3867	1336.3573	1343.6077
1358.0391	1359.5763	1364.6685
1365.1368	1369.0939	1379.8012
1382.6295	1395.1471	1408.6588
1416.3882	1431.6108	1435.3123
1445.6464	1448.2750	1489.9434
1493.4858	1493.8225	1500.1205
1505.1052	1510.2141	1510.8648

1516.1694	1518.6722	1519.6873
1529.8529	1538.9660	1553.2273
1554.2995	1596.9510	1622.0770
1646.7821	1662.0850	1679.7189
1680.1402	1685.1482	1687.4922
1690.7078	1698.1016	1699.3906
1783.6157	3059.0089	3064.3147
3073.4078	3080.3288	3107.7083
3128.9574	3135.9741	3142.3203
3152.0384	3162.1866	3162.8312
3195.2694	3199.0992	3200.4291
3201.1001	3203.4113	3205.5156
3211.4933	3215.5455	3216.2784
3219.9167	3222.6342	3223.2569
3225.2309	3227.8134	3229.8906
3230.7084	3232.8687	3234.4402
3247.4686	3251.9923	3257.4373

TS2*SR*'''

Zero-point correction= 0.627752

Thermal correction to Energy= 0.668022

Thermal correction to Enthalpy= 0.668966

Thermal correction to Gibbs Free Energy= 0.554672

Sum of electronic and zero-point Energies= -2876.460981

Sum of electronic and thermal Energies= -2876.420710

Sum of electronic and thermal Enthalpies= -2876.419766

Sum of electronic and thermal Free Energies= -2876.534060

Cartesian coordinates

C	6.736431	0.097315	-0.908458
C	6.686440	-1.259090	-0.561411
C	5.561719	-1.799543	0.048041
C	4.488262	-0.949722	0.305100
C	4.544043	0.398223	-0.041877
H	7.536028	-1.897567	-0.775732
H	5.513859	-2.849593	0.315120
C	2.416904	0.272219	0.820374
C	0.814669	2.142833	0.846605
C	2.084419	2.997583	1.020281
C	3.172382	2.503967	0.081806
H	4.124956	2.990200	0.304911
S	2.959169	-1.361003	1.052367
N	3.357198	1.063978	0.289177
N	1.171447	0.718082	1.086527
C	1.828766	4.518534	0.888814

C	1.939583	5.065291	-0.540029
C	2.782436	5.287663	1.807792
H	0.805936	4.699151	1.243589
H	2.977019	5.032614	-0.891245
H	1.314545	4.525454	-1.255248
H	1.631402	6.114078	-0.548715
H	2.686570	4.963216	2.847484
H	3.824386	5.143403	1.500354
H	2.571917	6.359405	1.763832
H	2.428915	2.805999	2.044946
H	0.145112	2.418653	1.665575
C	0.098815	2.339628	-0.470938
C	-0.981908	3.221081	-0.526073
C	0.533413	1.715117	-1.639936
C	-1.598402	3.503431	-1.741066
H	-1.340605	3.693431	0.385921
C	-0.087733	1.990660	-2.853546
H	1.343876	0.990758	-1.607833
C	-1.147359	2.892148	-2.908065
H	-2.435771	4.193113	-1.773627
H	0.251804	1.493299	-3.756160
H	-1.630774	3.105026	-3.855916
C	-1.194789	0.209121	1.584714
H	-1.505985	1.164583	1.187870
C	-2.107139	-0.703207	1.984826
C	-3.496789	-0.271390	2.341103
F	-3.574100	0.031623	3.654187
F	-3.873743	0.823127	1.669338
F	-4.406026	-1.228959	2.124594
O	0.587904	-1.309786	1.940257
C	0.197893	-0.219027	1.560979
H	2.921728	2.677595	-0.969250
C	0.202184	-3.957239	-0.261823
C	0.849746	-2.992873	-1.064166
C	2.158315	-3.172726	-1.508889
C	2.841977	-4.322134	-1.128345
C	2.216771	-5.281183	-0.315505
C	0.908663	-5.112325	0.113307
C	-1.474037	-2.500163	-0.377693
H	2.642235	-2.421491	-2.127870
H	3.860666	-4.480795	-1.468332
H	2.763687	-6.173306	-0.026105
H	0.418169	-5.855614	0.733641
N	-1.094164	-3.667800	0.093778

S	-0.211169	-1.631086	-1.313242
C	-3.111739	-0.699081	-0.806441
O	-2.245671	0.093854	-1.237084
C	-4.559963	-0.284827	-0.910696
C	-4.826336	1.011191	-1.363614
C	-5.633929	-1.123947	-0.601087
C	-6.134248	1.461408	-1.502780
H	-3.978749	1.647704	-1.599309
C	-6.944928	-0.675058	-0.739424
H	-5.457291	-2.134626	-0.249519
C	-7.199917	0.617935	-1.190667
H	-6.326166	2.470538	-1.855412
H	-7.769501	-1.337995	-0.496083
H	-8.222521	0.965829	-1.299805
C	5.667442	0.947250	-0.657249
H	5.705148	1.991714	-0.944181
H	7.623637	0.493866	-1.389060
C	-2.761406	-1.927281	-0.192500
H	-3.516094	-2.606914	0.191820
H	-1.794471	-1.663483	2.384713

Vibrational frequencies

-117.0127	14.4167	24.2975
32.6575	39.3857	41.4433
44.2620	50.4382	58.7379
62.5240	73.0816	77.9119
84.6082	89.8994	91.4168
102.1539	108.7461	118.0267
124.5868	134.5435	136.5891
141.9579	160.9304	175.0746
180.8300	190.2118	203.8186
210.4637	224.4962	226.6586
230.6116	238.3561	243.2297
254.0776	270.6256	273.4866
286.3446	304.8989	309.2022
318.6679	334.7193	336.0114
341.7555	378.2724	394.6855
408.2392	415.5808	419.6242
420.2534	432.6240	439.4227
443.3567	448.6315	460.4261
473.9373	480.5692	487.6351
510.0497	514.4312	522.0430
543.7259	545.7928	548.3347
564.1041	570.3249	579.6368
612.8240	621.4492	625.1721

627.2072 639.3874 640.0497
644.1060 663.3748 670.4802
671.2565 700.5418 709.6977
714.1012 716.7892 719.2290
721.1164 726.2164 730.6690
732.9343 748.3159 762.6615
774.6924 776.4203 788.0819
792.2279 816.0652 822.3132
838.8834 859.8226 866.4933
875.1568 876.6825 877.8871
881.9857 884.5254 915.5934
919.1150 930.8207 936.3596
953.0023 955.4021 960.1320
966.4764 975.5341 976.4923
990.5980 997.3748 1005.8940
1006.6085 1013.5500 1018.3263
1020.9282 1023.3761 1023.5113
1024.6747 1047.1038 1055.8778
1061.2015 1067.5790 1067.9688
1070.8150 1088.9637 1089.8732
1100.4647 1115.1906 1123.0695
1125.6654 1151.6820 1153.6349
1162.8511 1171.6290 1172.6093
1175.7689 1178.1038 1179.0600
1187.3188 1189.0819 1198.9721
1205.9607 1211.2401 1222.0311
1228.8353 1241.6786 1251.7518
1255.8748 1263.9797 1284.5107
1291.6422 1308.4215 1309.3219
1317.4381 1327.1941 1327.8506
1340.1951 1342.7195 1346.4493
1354.5260 1360.7339 1363.1518
1366.4018 1367.1160 1380.8794
1383.3495 1393.7392 1408.0917
1416.5998 1431.4498 1434.8708
1443.8028 1467.0928 1487.6832
1492.0895 1497.8499 1498.3864
1505.7543 1506.5872 1510.1818
1514.1393 1515.1313 1518.7390
1529.2904 1540.8522 1554.3722
1555.7157 1597.7091 1627.9613
1641.8495 1671.7200 1678.5540
1683.2463 1684.9015 1690.6833
1694.3830 1699.7099 1701.5482

1791.9825	3058.2661	3065.8246
3072.0328	3073.9797	3102.3428
3123.3763	3135.1917	3144.2387
3151.5878	3161.5365	3170.4265
3186.1236	3186.8144	3188.2698
3194.5173	3203.0978	3203.6597
3208.6858	3209.7333	3213.9888
3216.4852	3219.8505	3222.4525
3225.3701	3227.1005	3228.7185
3232.2930	3232.5511	3234.3197
3243.1842	3251.4218	3278.767

M2*SS*

Zero-point correction= 0.630916

Thermal correction to Energy= 0.671445

Thermal correction to Enthalpy= 0.672390

Thermal correction to Gibbs Free Energy= 0.555753

Sum of electronic and zero-point Energies= -2876.492107

Sum of electronic and thermal Energies= -2876.451577

Sum of electronic and thermal Enthalpies= -2876.450633

Sum of electronic and thermal Free Energies= -2876.567269

Cartesian coordinates

C	-7.415384	-1.897922	-0.782820
C	-7.065627	-3.152418	-1.289871
C	-5.729776	-3.510648	-1.445714
C	-4.753879	-2.590956	-1.079047
C	-5.110472	-1.337785	-0.584025
H	-7.842586	-3.857650	-1.563151
H	-5.454259	-4.483698	-1.837894
C	-2.807527	-1.182075	-0.480428
C	-1.591668	0.694828	0.460555
C	-2.761454	1.529236	-0.097155
C	-4.079417	0.824762	0.187990
H	-4.896971	1.303091	-0.358021
S	-3.002607	-2.769765	-1.198526
N	-3.986827	-0.559694	-0.279867
N	-1.647891	-0.660629	-0.123649
C	-2.753029	3.003876	0.367229
C	-3.503034	3.268142	1.678558
C	-3.317629	3.902293	-0.736413
H	-1.699838	3.281201	0.509730
H	-3.191638	2.607482	2.491356
H	-3.323685	4.299024	1.996229
H	-4.584590	3.157744	1.539213

H	-2.750390	3.794350	-1.664828
H	-4.366581	3.658865	-0.942608
H	-3.275392	4.952823	-0.433667
H	-2.619963	1.526052	-1.186394
H	-0.665883	1.133680	0.075985
C	-1.517859	0.665151	1.972602
C	-0.660028	1.555087	2.623245
C	-2.322355	-0.187151	2.731945
C	-0.639051	1.624608	4.013306
H	-0.001768	2.187953	2.031063
C	-2.300634	-0.118686	4.122667
H	-2.962392	-0.917481	2.242347
C	-1.467709	0.794203	4.765442
H	0.029571	2.321437	4.508237
H	-2.931288	-0.782824	4.704570
H	-1.452234	0.846731	5.849059
C	0.704283	-1.031655	0.293986
H	0.640744	-0.338866	1.120635
C	2.056085	-1.475519	-0.157015
C	2.611582	-2.595719	0.696291
F	3.826681	-3.004620	0.263922
F	2.780112	-2.211241	1.978730
F	1.818326	-3.669933	0.704120
O	-0.500207	-2.235316	-1.368938
C	-0.383090	-1.396413	-0.446575
H	-4.323066	0.824650	1.255717
C	1.395134	2.901862	-0.581263
C	1.120845	2.590228	-1.927422
C	0.386007	3.459570	-2.736718
C	-0.072070	4.643502	-2.175291
C	0.199342	4.965829	-0.835017
C	0.932095	4.105175	-0.032953
C	2.415184	0.946547	-0.663335
H	0.179081	3.217717	-3.773532
H	-0.650969	5.330883	-2.783507
H	-0.170746	5.900063	-0.425710
H	1.158021	4.342757	1.001902
N	2.121669	1.940032	0.108081
S	1.856033	1.062604	-2.328081
C	4.322054	-0.627161	-0.981674
O	4.184198	-0.820348	-2.175191
C	5.669460	-0.657538	-0.343085
C	6.786443	-0.525221	-1.175135
C	5.846318	-0.836662	1.032497

C	8.066097	-0.549807	-0.635843
H	6.628734	-0.398062	-2.241095
C	7.129975	-0.877819	1.567365
H	4.993866	-0.985404	1.687147
C	8.238076	-0.726540	0.736974
H	8.929669	-0.435335	-1.282598
H	7.264842	-1.030230	2.632868
H	9.237723	-0.750722	1.158981
C	-6.442881	-0.970845	-0.421782
H	-6.717585	-0.002256	-0.019708
H	-8.461711	-1.639487	-0.663659
C	3.081616	-0.298419	-0.144774
H	3.340026	-0.063148	0.889519
H	1.983662	-1.874922	-1.176140

Vibrational frequencies

14.6928	17.1043	20.3012
34.6061	39.7757	41.7145
46.9827	53.2274	63.4021
65.6116	69.0945	71.0643
77.9569	79.3674	90.3734
105.6263	107.7889	119.1384
129.2396	134.6339	140.7008
149.7720	169.5448	174.9653
179.4907	198.3918	206.3474
214.0300	223.5852	233.9735
245.1721	257.9516	268.5293
274.8887	281.3942	284.5931
304.3192	308.7030	313.4833
320.5660	330.8138	343.1125
375.1342	388.7066	394.4261
414.1359	420.6586	425.0347
430.0130	437.2467	441.6879
443.7135	472.6143	485.0030
489.4515	489.9123	509.3722
515.1475	519.9610	540.6544
544.1226	550.5986	561.0417
583.6729	591.0482	613.8282
622.7030	624.9865	626.6989
626.9928	635.3768	656.2421
668.2477	675.0865	684.2508
696.4096	705.3693	714.0618
718.9354	722.0335	724.6523
729.3158	731.8929	732.9635
749.7065	755.4416	762.6200

765.0999 784.8389 793.2675
824.7696 832.3141 858.3709
866.1084 871.9959 875.5312
877.1516 879.5224 892.2673
894.7744 910.2902 926.6230
937.7261 953.9050 964.0835
964.2485 971.5830 979.7819
1004.2382 1006.2619 1008.5461
1010.2099 1011.2109 1015.6119
1017.2057 1026.7301 1029.7841
1031.2757 1033.1979 1046.2654
1055.4252 1056.7651 1058.3446
1067.4588 1069.7777 1071.2266
1088.8246 1092.1059 1119.2797
1126.4438 1127.6439 1143.4096
1148.0650 1155.8254 1157.1842
1169.6191 1172.6484 1177.0169
1181.5074 1183.6130 1184.4304
1190.6407 1198.3456 1206.0472
1209.2202 1209.4228 1217.4023
1217.9669 1250.6041 1256.6923
1266.7101 1275.2410 1283.3023
1291.4681 1308.4742 1310.1762
1318.2957 1320.6885 1328.8484
1330.3786 1343.0080 1347.4472
1361.9048 1363.4733 1365.5019
1366.7441 1373.1967 1383.9775
1384.4119 1392.6888 1408.6679
1413.1646 1417.6119 1427.3330
1436.1202 1445.6612 1487.0320
1493.3442 1494.7393 1501.9640
1502.5626 1505.5955 1510.5071
1512.0209 1516.7711 1518.7296
1522.1832 1538.2101 1549.7084
1551.0722 1617.8983 1644.3477
1646.4989 1674.4128 1678.9322
1684.4994 1688.3917 1692.0357
1694.6441 1697.5993 1759.9806
1818.9011 3059.4306 3060.3843
3063.7213 3074.4310 3098.3550
3102.8233 3123.3105 3135.4513
3139.7236 3151.0671 3154.2096
3162.1733 3162.7281 3193.2951
3200.7215 3203.9748 3211.3219

3211.5792	3214.3122	3216.5740
3218.2745	3219.3037	3222.5857
3226.5670	3230.0325	3230.6105
3233.3043	3233.8324	3234.1447
3239.4431	3244.4141	3265.8381

M2*RS*

Zero-point correction= 0.630651

Thermal correction to Energy= 0.671225

Thermal correction to Enthalpy= 0.672169

Thermal correction to Gibbs Free Energy= 0.555341

Sum of electronic and zero-point Energies= -2876.493171

Sum of electronic and thermal Energies= -2876.452598

Sum of electronic and thermal Enthalpies= -2876.451653

Sum of electronic and thermal Free Energies= -2876.568481

Cartesian coordinates

C	-7.174414	-2.957821	-0.410498
C	-6.571352	-4.217774	-0.358256
C	-5.188476	-4.341481	-0.266046
C	-4.423844	-3.180418	-0.226692
C	-5.031325	-1.928838	-0.290201
H	-7.186593	-5.110142	-0.385199
H	-4.716170	-5.316982	-0.220890
C	-2.812549	-1.302477	-0.109249
C	-2.027841	0.997057	0.041653
C	-3.263321	1.313912	-0.825129
C	-4.461279	0.518362	-0.332637
H	-5.289826	0.596744	-1.041291
S	-2.667112	-3.050279	-0.125266
N	-4.089493	-0.892890	-0.242352
N	-1.800734	-0.463665	0.053749
C	-3.569624	2.825196	-0.953467
C	-4.486975	3.391531	0.137991
C	-4.178216	3.119423	-2.327458
H	-2.605317	3.346974	-0.896559
H	-5.506551	3.005362	0.028917
H	-4.140420	3.167826	1.149608
H	-4.542767	4.478569	0.034415
H	-3.520350	2.790265	-3.136652
H	-5.140886	2.609830	-2.448099
H	-4.357097	4.191879	-2.446283
H	-3.013569	0.939663	-1.827325
H	-1.160239	1.421170	-0.474535
C	-2.097038	1.573266	1.440322

C	-1.489386	2.805423	1.692861
C	-2.801503	0.937024	2.464175
C	-1.617585	3.414108	2.937786
H	-0.911417	3.285343	0.905168
C	-2.929387	1.545168	3.710712
H	-3.244837	-0.042379	2.298546
C	-2.346588	2.788276	3.946922
H	-1.143686	4.372847	3.121256
H	-3.479685	1.043433	4.499847
H	-2.447831	3.259729	4.918857
C	0.515984	-0.166246	0.722204
H	0.291849	0.843213	1.035397
C	1.947161	-0.606577	0.736176
C	2.523187	-0.589796	2.137007
F	2.578017	0.661491	2.633104
F	1.784385	-1.318496	2.984314
F	3.774506	-1.085459	2.194986
O	-0.315382	-2.216708	-0.136726
C	-0.425300	-1.019567	0.219896
H	-4.806385	0.859888	0.648950
C	6.410041	0.066142	0.016762
C	6.387761	-1.184706	-0.628044
C	7.562253	-1.903475	-0.859928
C	8.759381	-1.353473	-0.425127
C	8.792388	-0.107741	0.223074
C	7.627899	0.608000	0.445722
C	4.234084	-0.064945	-0.326818
H	7.539173	-2.864458	-1.362290
H	9.684801	-1.895560	-0.589114
H	9.743428	0.296833	0.552898
H	7.636414	1.571736	0.943679
N	5.170806	0.669742	0.173891
S	4.747964	-1.581337	-1.063525
C	2.046159	0.230462	-1.549860
O	2.149319	-0.776882	-2.221800
C	1.144918	1.345844	-1.978151
C	1.212757	2.637097	-1.446407
C	0.182749	1.049020	-2.950618
C	0.325216	3.618808	-1.882415
H	1.957998	2.894520	-0.701729
C	-0.707501	2.026882	-3.377407
H	0.144855	0.041493	-3.351365
C	-0.637068	3.314892	-2.843702
H	0.389881	4.622056	-1.473805

H	-1.451413	1.789130	-4.131853
H	-1.329870	4.081116	-3.179331
C	-6.414043	-1.793231	-0.376345
H	-6.888164	-0.818981	-0.406163
H	-8.254117	-2.881297	-0.475628
C	2.784948	0.307416	-0.210582
H	2.769324	1.316457	0.204251
H	2.004480	-1.640288	0.377175

Vibrational frequencies

13.1621	18.7076	20.3070
33.1300	38.8887	45.6598
50.7897	51.5310	59.4829
64.0092	66.4199	69.6934
77.4035	83.6843	86.9497
95.2218	111.3204	119.2208
132.4262	133.0498	145.5452
154.7443	161.9162	173.9287
189.9497	202.1376	204.0480
222.2839	223.0097	233.1629
244.1410	254.2985	260.6952
273.7945	277.9109	288.5167
302.9645	306.3522	316.4030
320.9626	328.8810	336.2301
375.2511	389.3571	393.8249
411.7536	418.3356	430.4482
431.6973	435.5624	438.8131
442.6362	457.1651	478.6519
488.0655	498.4027	508.0923
515.8467	518.9617	543.0654
548.3056	550.5038	561.3513
573.1040	592.8120	616.7353
620.2124	625.5443	628.3605
633.6113	643.3632	652.7478
661.5431	668.7021	675.2396
687.2167	705.4009	713.0608
719.7825	722.4436	724.1310
728.3813	731.2964	732.2303
750.9993	751.1769	760.4521
773.4183	784.1411	793.1604
816.4916	825.2136	861.6147
867.0015	870.0428	876.4282
878.1553	880.9175	885.2027
895.3005	924.3892	931.0213
942.1376	957.5492	965.1345

966.0910	972.6746	974.1322
1002.3724	1007.2298	1010.1837
1013.4048	1014.7573	1015.3567
1019.3926	1025.2049	1028.0318
1033.4986	1037.8533	1047.7907
1053.8177	1056.6175	1058.8770
1062.8306	1068.4433	1072.3345
1089.7253	1092.9886	1115.5103
1117.4246	1126.1053	1140.4797
1152.3352	1152.3486	1156.7383
1172.5013	1175.2899	1176.4870
1180.7576	1184.2418	1187.8364
1190.3373	1193.6615	1199.9969
1210.1480	1214.0461	1216.3383
1222.0555	1255.6109	1258.4938
1260.5635	1262.0870	1281.1294
1292.5047	1295.7759	1309.4255
1316.3787	1317.9749	1322.0689
1331.5499	1335.7049	1349.1563
1361.0369	1362.0854	1364.4249
1366.8149	1372.1474	1379.5882
1386.1976	1392.9746	1406.4127
1408.3120	1415.6855	1426.9347
1434.5374	1443.9415	1484.8175
1490.1190	1493.6377	1495.8701
1500.2386	1505.6774	1509.3705
1514.6677	1515.1360	1519.1488
1520.5547	1536.4369	1541.4986
1555.5364	1622.6384	1639.1369
1650.4135	1668.3437	1678.5285
1681.2035	1687.0511	1689.7890
1691.8810	1698.3452	1752.4046
1822.6283	3058.7198	3064.0191
3067.4451	3076.6277	3095.0202
3116.9085	3134.0686	3134.7880
3140.9034	3149.9918	3150.8654
3151.7182	3163.3274	3188.6774
3202.5709	3204.7488	3207.4483
3212.3827	3214.8855	3219.0688
3219.1735	3221.7484	3222.2823
3224.4189	3229.2204	3231.7349
3233.0968	3233.9391	3236.3321
3242.8394	3249.6185	3267.5533

M2*RR*

Zero-point correction= 0.630873

Thermal correction to Energy= 0.671134

Thermal correction to Enthalpy= 0.672078

Thermal correction to Gibbs Free Energy= 0.557289

Sum of electronic and zero-point Energies= -2876.491703

Sum of electronic and thermal Energies= -2876.451443

Sum of electronic and thermal Enthalpies= -2876.450498

Sum of electronic and thermal Free Energies= -2876.565288

Cartesian coordinates

C	0.925874	1.023637	-1.123645
H	0.845378	1.909604	-0.511172
C	2.290944	0.484521	-1.393418
C	3.215122	1.622036	-1.767016
F	4.472287	1.213884	-2.032670
F	3.315729	2.522617	-0.764144
F	2.789716	2.285004	-2.848076
O	-0.161613	-0.909281	-1.957329
C	-0.140258	0.216145	-1.402883
C	0.150589	-2.228680	1.221946
C	0.438542	-3.304983	0.362031
C	-0.385363	-4.431981	0.314361
C	-1.506844	-4.459296	1.132308
C	-1.795613	-3.395091	2.003260
C	-0.969001	-2.284828	2.061854
C	1.936996	-1.379115	0.248681
H	-0.162059	-5.258601	-0.351888
H	-2.166381	-5.320861	1.103568
H	-2.676375	-3.446140	2.635220
H	-1.167087	-1.460066	2.738929
N	1.027401	-1.159267	1.138731
S	1.875676	-2.952393	-0.548932
C	4.272803	-0.886811	-0.472067
O	4.353757	-1.776872	-1.300341
C	5.486533	-0.408599	0.254641
C	6.624343	-1.222312	0.214737
C	5.529403	0.807501	0.943202
C	7.785356	-0.835267	0.870885
H	6.574854	-2.157550	-0.332895
C	6.698968	1.199955	1.587263
H	4.670177	1.469175	0.952447
C	7.822959	0.377602	1.558729
H	8.661584	-1.474578	0.847085
H	6.732400	2.149001	2.111737

H	8.730153	0.683012	2.070341
C	2.900392	-0.296031	-0.158337
H	2.935509	0.393444	0.687038
H	2.271105	-0.211737	-2.239267
C	-6.552817	-2.069191	0.380690
C	-5.964057	-3.283204	0.013753
C	-4.667729	-3.322213	-0.490635
C	-3.973192	-2.123850	-0.619373
C	-4.568292	-0.918650	-0.253573
H	-6.521418	-4.206633	0.125750
H	-4.202879	-4.261515	-0.771806
C	-2.470624	-0.178843	-0.877554
C	-1.689904	2.101294	-0.580612
C	-3.149910	2.489480	-0.890361
C	-4.095426	1.544350	-0.165117
H	-5.119720	1.674441	-0.525113
S	-2.332121	-1.891127	-1.214143
N	-3.700986	0.163872	-0.443537
N	-1.478665	0.695347	-0.971723
C	-3.474347	3.978948	-0.622584
C	-3.963144	4.283121	0.798995
C	-4.507194	4.476956	-1.638147
H	-2.546035	4.540497	-0.789963
H	-3.297791	3.891938	1.572664
H	-4.034726	5.365825	0.933146
H	-4.964918	3.870720	0.963833
H	-4.140453	4.374611	-2.663012
H	-5.442333	3.911536	-1.553681
H	-4.741709	5.530193	-1.461891
H	-3.273904	2.310406	-1.966247
H	-1.047427	2.683525	-1.247026
C	-1.275711	2.364198	0.853314
C	-0.624495	3.559192	1.167160
C	-1.579803	1.466735	1.878489
C	-0.313957	3.869983	2.488060
H	-0.358379	4.249851	0.370402
C	-1.269327	1.775943	3.200130
H	-2.045674	0.511299	1.648874
C	-0.643946	2.981682	3.509043
H	0.191107	4.802426	2.717847
H	-1.511473	1.071485	3.989712
H	-0.401983	3.220817	4.539342
H	-4.082157	1.702768	0.918390
C	-5.863597	-0.867243	0.253462

H	-6.318467	0.070685	0.551647
H	-7.562416	-2.059807	0.776228

Vibrational frequencies

18.1431	19.9309	25.1722
32.0599	39.7591	44.2606
52.7282	60.6401	64.3508
72.0064	73.9663	81.3302
85.1704	93.1457	96.3260
104.0761	114.2245	126.5947
136.6006	142.7028	143.2033
163.9764	167.8733	177.3603
185.7772	188.9079	215.6782
224.9713	227.9958	235.5502
245.7630	256.1680	263.2729
276.3919	286.0286	290.7617
305.6524	310.4057	318.7229
324.4762	333.8458	344.6686
381.1111	391.2989	398.0053
415.3536	422.0701	427.1564
429.4696	437.9585	441.4909
444.6666	466.3983	476.7721
488.9334	497.5397	510.7067
516.5992	519.5594	542.1937
546.7837	550.1973	559.8200
582.7238	583.7656	610.1164
616.1560	626.7559	627.1767
630.2200	637.1785	644.4594
655.4847	663.8399	667.6313
693.9191	706.9483	712.4872
718.2788	722.1583	726.8139
727.9590	730.8722	732.2783
750.9666	752.0984	763.5205
769.6658	780.7325	790.7576
823.3218	827.3377	862.4279
867.2384	872.1172	875.4415
879.0174	881.7396	883.0538
900.6488	919.2323	934.7052
939.6064	955.4957	965.1899
965.9243	969.8466	975.4331
994.3508	1001.2869	1005.2349
1006.6933	1011.6228	1012.4638
1013.4135	1016.8029	1028.5311
1030.3381	1034.2523	1035.8897
1050.5834	1057.2440	1060.9687

1068.3200	1069.1709	1073.5670
1087.0217	1096.1856	1117.4080
1125.5680	1129.2915	1141.7269
1152.9503	1154.6624	1157.6497
1162.1858	1171.1683	1181.4711
1184.8783	1184.9778	1187.7931
1190.4210	1193.2957	1204.6868
1211.6625	1214.8077	1217.4726
1225.1013	1248.7191	1253.7210
1259.8719	1272.0323	1285.6581
1290.6980	1292.5664	1307.9798
1308.7144	1317.7104	1321.2027
1328.8699	1343.0772	1345.8717
1361.9625	1365.2314	1366.9094
1371.8956	1374.3888	1377.1364
1381.6716	1391.7706	1392.7125
1409.0543	1418.8065	1428.3947
1438.2428	1445.6214	1483.4644
1495.6275	1496.3471	1501.6315
1505.5174	1506.4503	1510.8168
1515.0225	1516.9506	1519.3202
1520.3793	1537.5882	1548.9151
1554.6327	1611.7569	1634.5214
1648.1443	1676.1536	1682.3785
1683.4180	1690.5512	1691.5996
1694.7903	1697.0155	1747.4991
1811.1288	3058.6091	3064.6160
3070.1806	3072.3550	3092.6834
3110.7404	3126.7236	3135.6388
3143.5183	3147.1667	3147.9896
3154.3463	3164.8495	3186.3863
3194.3702	3207.5745	3209.0488
3210.3162	3211.6501	3215.1386
3216.5068	3219.5515	3220.5201
3223.9545	3225.8345	3227.1110
3233.9880	3234.4144	3239.7892
3240.7814	3242.8232	3269.4962

M2*SR*

Zero-point correction= 0.630998

Thermal correction to Energy= 0.671388

Thermal correction to Enthalpy= 0.672332

Thermal correction to Gibbs Free Energy= 0.556326

Sum of electronic and zero-point Energies= -2876.490377

Sum of electronic and thermal Energies= -2876.449987

Sum of electronic and thermal Enthalpies= -2876.449043

Sum of electronic and thermal Free Energies= -2876.565049

Cartesian coordinates

C	-6.828150	-0.673229	0.802781
C	-6.543055	-2.020910	0.563655
C	-5.308238	-2.406861	0.050739
C	-4.367147	-1.418411	-0.216061
C	-4.661247	-0.076748	0.018817
H	-7.290831	-2.775559	0.780782
H	-5.079780	-3.451325	-0.134499
C	-2.486823	0.097806	-0.743120
C	-1.198752	2.154977	-0.734765
C	-2.549457	2.837111	-1.026192
C	-3.637182	2.209386	-0.168076
H	-4.626015	2.539625	-0.497961
S	-2.745205	-1.630231	-0.872995
N	-3.583779	0.754046	-0.312966
N	-1.334709	0.707146	-0.977682
C	-2.508899	4.379505	-0.910809
C	-2.833946	4.924191	0.485079
C	-3.454103	5.004268	-1.941256
H	-1.487007	4.689024	-1.165901
H	-2.230990	4.464452	1.272089
H	-2.650396	6.001649	0.506292
H	-3.891701	4.771217	0.727209
H	-3.180568	4.716699	-2.960033
H	-4.488470	4.687811	-1.764825
H	-3.427161	6.095266	-1.874971
H	-2.777904	2.588288	-2.070702
H	-0.488107	2.504397	-1.488604
C	-0.634705	2.451745	0.641313
C	0.307403	3.473485	0.781965
C	-1.066186	1.764737	1.778397
C	0.791318	3.822061	2.039584
H	0.669475	3.994336	-0.101434
C	-0.582537	2.112632	3.037207
H	-1.767127	0.938210	1.687712
C	0.341413	3.146344	3.171485
H	1.524981	4.615901	2.134192
H	-0.922708	1.569236	3.912705
H	0.719316	3.414374	4.152562
C	1.062868	0.464517	-1.291989
H	1.232356	1.400923	-0.783018

C	2.231227	-0.395846	-1.626287
C	3.321753	0.400495	-2.304564
F	2.920456	0.881122	-3.489391
F	3.712995	1.457283	-1.564055
F	4.427455	-0.335470	-2.538294
O	-0.483005	-1.242659	-1.851240
C	-0.173912	-0.102457	-1.427668
H	-3.519493	2.459633	0.891640
C	0.531011	-3.992362	0.017249
C	-0.197062	-3.284724	0.990999
C	-1.350497	-3.822320	1.567663
C	-1.769119	-5.076075	1.146662
C	-1.048562	-5.790658	0.174089
C	0.099685	-5.261034	-0.390833
C	1.766028	-2.164477	0.064225
H	-1.910945	-3.268915	2.314431
H	-2.666164	-5.510979	1.575607
H	-1.398872	-6.768959	-0.137875
H	0.664057	-5.799107	-1.145082
N	1.645318	-3.332127	-0.474836
S	0.551696	-1.741818	1.270708
C	3.335967	-0.276505	0.677542
O	2.535759	0.252357	1.429289
C	4.796620	0.028671	0.803817
C	5.152353	1.086053	1.650654
C	5.799034	-0.690288	0.146097
C	6.485787	1.424011	1.832782
H	4.360936	1.631680	2.153396
C	7.136987	-0.354409	0.335951
H	5.555876	-1.515755	-0.512041
C	7.481871	0.701132	1.175110
H	6.752543	2.249118	2.484932
H	7.910361	-0.919599	-0.173214
H	8.525889	0.961215	1.318020
C	-5.891284	0.320231	0.535374
H	-6.112924	1.362752	0.733226
H	-7.794388	-0.392014	1.206806
C	2.830699	-1.213363	-0.407839
H	3.630190	-1.842054	-0.800823
H	1.916750	-1.162310	-2.342992

Vibrational frequencies

14.6426	16.4533	22.2295
27.7757	31.8371	40.1991
52.7226	57.8182	65.1801

71.2513	77.9962	79.0891
88.4112	88.6330	89.1246
103.9639	113.0980	124.9918
132.4364	135.7131	140.1209
163.5788	169.9505	170.9811
192.6901	202.1225	209.6939
220.5816	223.2938	226.7683
239.8465	248.1798	255.2155
271.8855	284.5059	295.5848
301.5641	308.4915	322.2042
325.4053	335.2567	342.1051
373.5195	392.1468	403.0742
415.4983	422.8511	428.8967
431.2615	437.2240	439.3748
444.2271	460.5249	483.0885
487.9780	507.4634	511.9709
517.4269	520.3221	540.4443
544.1117	548.7144	559.2264
580.7954	588.5015	611.0392
616.9544	626.8695	627.1858
632.8901	641.2903	658.2571
663.0054	668.0738	677.2708
700.4236	706.3793	713.8247
720.8496	721.2667	727.0191
727.3599	731.3854	745.8960
748.7556	751.5261	760.4139
769.4754	779.9783	788.6871
822.7971	834.3217	861.3403
865.5584	869.4242	873.9111
874.6582	880.0811	882.0630
904.8696	917.5224	929.6267
940.6375	950.5577	954.4354
964.3932	966.8874	968.1672
974.6910	1002.8697	1003.8684
1007.0974	1012.1360	1013.3804
1014.5495	1015.8108	1026.3800
1029.1875	1033.7465	1035.9585
1050.4374	1059.2553	1060.2690
1068.2929	1072.6379	1073.7055
1087.8029	1098.0710	1110.3281
1127.5012	1130.4982	1137.1531
1154.1995	1158.0849	1160.3505
1167.0734	1171.3279	1180.0728
1181.9301	1184.4212	1187.4455

1189.5073	1196.2894	1208.6726
1214.4681	1216.8404	1217.6614
1225.4419	1253.4643	1256.6408
1258.2019	1262.6170	1283.9744
1290.5018	1295.0842	1304.2763
1310.3984	1320.7753	1325.2283
1334.9155	1346.3916	1347.6602
1361.9469	1366.3090	1369.0196
1371.5861	1373.7520	1381.3185
1387.0980	1393.0932	1408.7720
1415.8833	1417.4865	1428.1383
1435.0016	1446.6180	1487.9780
1493.7472	1497.3872	1500.1296
1502.4470	1504.3562	1508.4284
1516.6534	1517.6064	1517.9692
1519.7597	1537.3436	1552.6176
1555.2264	1613.4034	1636.8015
1650.9918	1675.6508	1679.7920
1681.1726	1690.3389	1695.3904
1695.5651	1699.7233	1739.7786
1809.8500	3058.5149	3062.5270
3069.3759	3078.3979	3090.4453
3116.4103	3130.0581	3134.9458
3138.9247	3145.9644	3153.4115
3154.7577	3161.9471	3190.1620
3196.8931	3203.5740	3206.3616
3210.1998	3213.5533	3216.9811
3221.1937	3222.0199	3224.4488
3226.6055	3229.8587	3231.9096
3232.5147	3237.2204	3245.5011
3247.7517	3248.8835	3289.6853

TS3

Zero-point correction= 0.705014

Thermal correction to Energy= 0.755238

Thermal correction to Enthalpy= 0.756182

Thermal correction to Gibbs Free Energy= 0.618901

Sum of electronic and zero-point Energies= -4562.471775

Sum of electronic and thermal Energies= -4562.421550

Sum of electronic and thermal Enthalpies= -4562.420606

Sum of electronic and thermal Free Energies= -4562.557888

Cartesian coordinates

C	6.584453	3.246060	-1.312774
C	6.115795	4.279129	-0.490487

C	5.025265	4.086119	0.346012
C	4.409108	2.837002	0.333974
C	4.868744	1.817799	-0.495941
H	6.613898	5.241964	-0.504223
H	4.660899	4.879265	0.989177
C	3.089169	0.768149	0.511242
C	2.367705	-1.540376	0.031990
C	3.047654	-1.313104	-1.326009
C	4.349937	-0.555339	-1.151885
H	4.741308	-0.241090	-2.121234
S	3.039161	2.317129	1.290608
N	4.091691	0.658563	-0.367483
N	2.211852	-0.239151	0.734505
C	3.209248	-2.609731	-2.154537
C	4.503124	-3.383751	-1.876693
C	3.110709	-2.286437	-3.648422
H	2.361048	-3.258044	-1.895012
H	4.656066	-3.596964	-0.816035
H	4.474722	-4.336723	-2.411068
H	5.373971	-2.831724	-2.247764
H	2.158327	-1.807311	-3.892938
H	3.920037	-1.615790	-3.958507
H	3.195621	-3.200460	-4.241723
H	2.366420	-0.653425	-1.876302
H	1.359851	-1.874662	-0.208397
C	3.027181	-2.562582	0.930377
C	2.517234	-3.862231	0.960097
C	4.159690	-2.251672	1.687862
C	3.153941	-4.849470	1.706972
H	1.618361	-4.100614	0.396227
C	4.795435	-3.239189	2.435133
H	4.547459	-1.235454	1.709838
C	4.298722	-4.540997	2.438350
H	2.751256	-5.856621	1.722891
H	5.675373	-2.989516	3.018327
H	4.794864	-5.310059	3.020839
C	0.149213	-1.159792	1.803589
H	0.626777	-1.976704	2.357928
C	-1.134198	-0.702819	2.508545
C	-1.882881	-1.967818	2.997227
F	-3.177149	-2.016323	2.675458
F	-1.348298	-3.108701	2.503395
F	-1.798940	-2.074821	4.335284
O	1.182298	0.928079	2.392224

C	1.171631	-0.062489	1.696481
H	5.113751	-1.146154	-0.635919
C	0.119450	1.897053	-0.752196
C	-0.085163	3.119481	-0.080776
C	0.591602	4.279212	-0.463251
C	1.498575	4.196938	-1.512250
C	1.701231	2.988494	-2.197932
C	1.005901	1.843827	-1.836026
C	-1.311032	1.139743	0.775007
H	0.427537	5.216747	0.057192
H	2.053360	5.081064	-1.808808
H	2.399268	2.955135	-3.028316
H	1.111741	0.912144	-2.383348
N	-0.586202	0.814788	-0.255097
S	-1.214124	2.869469	1.213448
C	-3.161743	0.732873	2.392598
O	-3.323258	0.467982	3.584213
C	-4.180514	1.611216	1.707632
C	-5.045428	2.355840	2.513369
C	-4.316023	1.681732	0.317288
C	-6.022883	3.165029	1.943599
H	-4.936544	2.280958	3.590302
C	-5.298369	2.482866	-0.254659
H	-3.661875	1.096848	-0.323406
C	-6.151734	3.228678	0.557242
H	-6.685965	3.744039	2.578621
H	-5.401223	2.520108	-1.334680
H	-6.917133	3.855475	0.110142
C	5.972817	2.000372	-1.327685
H	6.350279	1.205120	-1.959183
H	7.443545	3.419320	-1.950978
C	-2.042681	0.177644	1.618723
H	-2.389637	-0.879898	0.655405
H	-0.878058	-0.158645	3.424196
C	-3.914134	-1.045451	-3.778675
C	-4.748596	-1.081890	-2.669161
C	-4.191808	-1.357261	-1.427898
C	-2.809110	-1.572101	-1.229041
C	-2.029218	-1.554812	-2.404879
C	-2.552970	-1.297536	-3.663536
H	-5.814553	-0.913131	-2.766231
H	-1.910461	-1.293017	-4.535940
O	-2.294181	-1.801448	-0.041289
H	-0.128363	-1.543893	0.819936

Cl	-0.327758	-1.926894	-2.278424
Cl	-4.592286	-0.701684	-5.352790
Cl	-5.237812	-1.489187	-0.042868

Vibrational frequencies

-937.3916	12.2984	19.5193
23.3592	24.3497	31.5184
33.8557	41.2847	47.6633
52.8833	57.4610	58.3051
61.4005	64.5092	67.2014
73.3402	78.7594	85.0446
85.4744	94.7767	99.1823
108.3680	117.0204	122.8288
131.4474	134.8639	143.1016
147.8851	165.8150	175.1842
181.0206	186.7186	189.4803
192.6663	197.6152	214.2658
216.7486	219.3708	225.9640
229.1982	231.3517	244.7352
247.2086	252.1477	272.8701
278.4529	287.8878	300.6635
303.4463	309.1604	315.2883
325.2073	335.6057	349.1456
360.4493	381.6293	383.9431
389.6550	392.2160	399.8901
405.0325	421.8015	423.0279
431.4126	436.7777	439.1199
443.2340	444.3957	447.3566
462.7894	487.8358	496.3971
514.4656	515.0488	515.4312
519.7385	522.6529	542.5645
551.0465	555.0082	568.3416
575.1436	582.4809	591.3436
600.6405	604.6821	621.2552
625.7774	627.0843	630.6071
643.6318	651.9252	663.7835
671.0390	683.7484	692.8397
702.4225	716.4362	718.7513
724.9250	727.2474	732.5031
733.8918	745.3257	748.7054
751.7762	756.4511	772.6041
774.1013	783.3120	790.4790
811.6577	826.2946	829.4864
857.3492	864.5980	866.5631
882.3921	883.6534	884.1208

886.0463	889.2609	892.9225
895.8347	901.1497	912.1467
919.7469	935.1255	941.2343
960.9495	971.8152	974.2640
976.8701	977.6957	1004.9663
1008.8356	1009.6725	1012.5597
1012.7106	1017.9166	1019.3201
1021.8544	1027.4240	1033.4345
1040.7867	1052.3060	1058.6806
1063.6142	1065.6851	1067.7425
1070.7195	1093.4111	1096.0165
1102.5944	1109.7864	1119.7208
1125.1296	1128.9093	1147.6841
1151.8382	1153.4917	1161.8509
1170.9215	1173.7405	1174.9634
1177.7459	1182.9823	1185.6971
1186.3429	1191.2635	1194.2120
1209.0954	1211.0653	1212.7114
1220.2063	1223.5998	1228.9439
1251.3619	1253.8894	1266.2549
1272.4120	1280.3508	1292.7445
1294.7352	1305.3182	1312.3770
1316.3528	1326.4503	1331.2834
1333.5463	1340.0909	1351.2494
1361.1187	1361.9755	1364.3750
1364.9522	1366.8637	1370.3980
1375.1466	1381.8835	1382.9488
1388.3305	1404.3616	1416.9296
1428.6477	1433.2130	1437.7900
1448.7216	1453.1898	1470.8300
1488.9437	1489.5393	1495.5911
1499.0999	1506.2101	1509.4136
1512.0980	1513.7161	1514.7549
1518.5737	1527.0085	1542.3470
1546.9921	1554.3661	1574.0454
1586.3017	1595.9586	1629.3470
1644.5204	1670.0267	1679.7271
1680.1588	1682.0753	1684.7009
1689.0755	1694.6741	1699.0084
1747.9617	1851.5767	3057.4504
3061.5890	3067.0920	3088.2243
3096.7770	3098.6525	3108.3178
3135.7021	3140.1878	3154.6733
3159.2156	3166.3838	3170.3436

3190.3039	3190.5203	3200.2718
3201.0385	3205.6554	3213.4824
3216.2692	3217.0946	3217.5860
3220.6118	3220.8041	3226.7599
3227.5248	3228.0248	3233.6820
3235.6127	3239.2420	3240.6316
3241.4392	3244.1425	3257.5880

TS3'

Zero-point correction= 0.909034

Thermal correction to Energy= 0.961391

Thermal correction to Enthalpy= 0.962336

Thermal correction to Gibbs Free Energy= 0.823512

Sum of electronic and zero-point Energies= -3247.525101

Sum of electronic and thermal Energies= -3247.472743

Sum of electronic and thermal Enthalpies= -3247.471799

Sum of electronic and thermal Free Energies= -3247.610623

Cartesian coordinates

C	-7.737361	0.277262	-2.158393
C	-7.630011	-0.988918	-2.747670
C	-6.427292	-1.683068	-2.734856
C	-5.334796	-1.081495	-2.115411
C	-5.444441	0.181653	-1.540197
H	-8.498018	-1.435925	-3.218729
H	-6.339112	-2.664240	-3.187875
C	-3.238822	-0.291931	-1.077856
C	-1.803909	1.137196	0.281545
C	-2.591571	2.287093	-0.367215
C	-4.068740	1.937572	-0.384747
H	-4.630379	2.639942	-1.005122
S	-3.706401	-1.716561	-1.963202
N	-4.229506	0.604272	-0.982035
N	-2.032490	-0.101364	-0.505120
C	-2.287165	3.665677	0.263974
C	-3.190360	4.042685	1.442786
C	-2.350563	4.757247	-0.807457
H	-1.249778	3.622949	0.624244
H	-3.228798	3.271509	2.216027
H	-2.815950	4.960731	1.903462
H	-4.212409	4.244781	1.102909
H	-1.643060	4.560373	-1.618137
H	-3.356213	4.829774	-1.237064
H	-2.104547	5.730397	-0.372636
H	-2.249825	2.318683	-1.410313

H	-0.748232	1.384144	0.152041
C	-2.077052	0.921222	1.757260
C	-1.220430	1.508177	2.691088
C	-3.171927	0.180839	2.212572
C	-1.459596	1.376185	4.055415
H	-0.354864	2.066343	2.348580
C	-3.408598	0.041788	3.578545
H	-3.840096	-0.311980	1.509384
C	-2.556539	0.643323	4.502166
H	-0.779189	1.833344	4.766273
H	-4.259263	-0.539985	3.917653
H	-2.741784	0.531567	5.565245
C	0.266370	-0.942032	0.070619
C	1.419997	-0.257764	-0.701992
C	1.997677	-1.004060	-1.891472
F	2.657904	-2.126636	-1.581323
F	1.047597	-1.335409	-2.773709
F	2.865939	-0.208363	-2.553178
O	-1.209735	-1.958331	-1.519723
C	-0.963428	-1.073743	-0.717540
H	-4.504640	1.920780	0.619665
C	6.011802	-0.455474	-0.511110
C	6.198919	0.879984	-0.910103
C	7.434573	1.337654	-1.372518
C	8.479854	0.428100	-1.430815
C	8.304620	-0.908922	-1.035517
C	7.079357	-1.359339	-0.574656
C	3.955053	0.263874	-0.132545
H	7.572517	2.368937	-1.677892
H	9.449748	0.757017	-1.788392
H	9.142392	-1.595397	-1.093251
H	6.926323	-2.387424	-0.264798
N	4.735494	-0.761415	-0.066453
S	4.706257	1.752637	-0.715017
C	2.082166	1.344345	1.191629
O	1.969944	1.171285	2.390795
C	1.776354	2.693937	0.605788
C	1.459111	3.714435	1.514976
C	1.783839	2.986204	-0.766287
C	1.128054	4.986469	1.067302
H	1.484466	3.488515	2.575923
C	1.445631	4.260677	-1.213254
H	2.075484	2.242880	-1.500339
C	1.109941	5.258074	-0.301038

H	0.886034	5.765832	1.782073
H	1.451483	4.473439	-2.276692
H	0.843610	6.248616	-0.655605
C	-6.648332	0.883504	-1.546185
H	-6.740846	1.859237	-1.083881
H	-8.688531	0.797011	-2.176248
C	2.518286	0.144293	0.334302
H	1.041882	0.651633	-1.183713
H	0.363491	-2.340146	0.836767
H	2.564095	-0.676161	1.054379
H	0.082948	-0.304997	0.940402
N	0.264376	-3.398538	1.452627
C	1.423204	-4.242658	0.985431
H	1.410251	-5.155960	1.592832
C	2.742345	-3.509345	1.222259
H	3.564834	-4.209651	1.056888
H	2.866903	-2.690561	0.515096
H	2.846403	-3.117140	2.236636
C	1.276287	-4.599953	-0.493617
H	2.234820	-4.968612	-0.865432
H	0.529138	-5.376012	-0.668105
H	1.004367	-3.718066	-1.079635
C	-1.069889	-3.964544	1.024812
H	-1.050100	-3.924215	-0.065921
C	-1.290991	-5.404967	1.479334
H	-1.293332	-5.493835	2.569400
H	-2.271277	-5.731338	1.122973
H	-0.546538	-6.095898	1.079865
C	-2.211105	-3.068530	1.498168
H	-2.006037	-2.012700	1.314958
H	-3.120087	-3.339510	0.954313
H	-2.415952	-3.182762	2.567081
C	0.316857	-3.179696	2.938040
H	-0.501417	-3.737000	3.397042
H	1.236449	-3.625259	3.318108
C	0.236567	-1.715176	3.342459
H	-0.695998	-1.251608	3.006809
H	0.266452	-1.647043	4.433059
H	1.071053	-1.129987	2.945283

Vibrational frequencies

-898.5751	14.5493	19.8258
22.7438	32.9167	35.0246
38.9666	44.6899	47.3161
59.5255	64.0274	67.6295

68.9925	75.6559	82.3368
85.1225	91.3180	96.6437
101.9511	102.6208	107.3142
109.8019	116.9896	121.8298
127.8930	132.8808	137.4792
145.4082	150.0601	158.1050
165.9378	173.5874	191.7935
195.8896	201.2155	204.0930
210.0097	221.8366	224.6546
228.0938	237.5238	239.8474
244.5601	247.1534	253.3269
264.2384	270.4101	275.4304
284.4642	304.8889	307.7915
311.2840	316.6692	323.7447
326.7813	328.5092	334.6438
346.3640	368.6088	373.4087
379.3475	381.6523	394.2829
403.7258	419.3590	421.8142
429.4276	432.8712	437.8477
438.2669	441.9234	447.0116
449.2370	456.0833	473.3955
476.5437	478.9852	492.1387
507.3714	511.8113	517.4165
521.5223	537.3319	548.6475
551.4876	554.8897	559.9206
580.6061	598.7126	609.6244
618.4595	623.6930	625.7789
627.5662	636.2619	637.2142
647.5669	671.9315	677.3303
690.3259	708.5819	713.8613
719.2704	724.4677	726.2126
730.8884	734.7072	742.4027
749.7148	760.5854	778.2809
780.6482	783.0338	785.0894
790.0150	801.1332	820.7779
827.5973	832.7452	861.6090
866.8205	873.8269	874.9174
878.5057	884.8393	890.4148
897.2722	898.8608	907.6314
921.5901	934.7857	944.6764
954.2900	956.4565	965.0251
971.4959	973.3916	977.2941
981.2280	982.4487	993.1047
993.5079	1003.6648	1006.3064

1011.3316	1015.5363	1018.2960
1019.4173	1027.2946	1030.1690
1032.3543	1033.2656	1043.7521
1044.9924	1053.5185	1055.5824
1061.7610	1067.5118	1069.2062
1071.7477	1077.3513	1080.8649
1090.0155	1098.5541	1100.2042
1109.0773	1119.5168	1126.8652
1127.9530	1137.0825	1146.0499
1149.3861	1154.4307	1156.4428
1163.4863	1175.6767	1177.6021
1181.8185	1182.1592	1185.3382
1188.5892	1189.3426	1192.6957
1202.4941	1206.6485	1208.0881
1209.6102	1214.1606	1217.2660
1218.4866	1222.1116	1236.7490
1242.9536	1255.3979	1274.9986
1278.9608	1291.0549	1296.2362
1306.4820	1313.5248	1318.7450
1326.9306	1335.4478	1341.8497
1344.0444	1344.6112	1349.1420
1357.9440	1362.1807	1365.1264
1366.1930	1367.1749	1369.9220
1372.4572	1375.2141	1378.4305
1379.4565	1381.0844	1385.5799
1397.3777	1405.2294	1415.0707
1416.8746	1420.7839	1427.5947
1428.1919	1432.8597	1436.5529
1440.7101	1442.3821	1447.1775
1455.8229	1490.1885	1491.0905
1491.9540	1493.0702	1495.0728
1496.8652	1497.3281	1502.7105
1503.1818	1505.9590	1506.1201
1510.9597	1513.2801	1515.7524
1515.8907	1516.5955	1516.8210
1519.5563	1524.0259	1530.4852
1533.1791	1544.4254	1552.8166
1557.1698	1592.8260	1610.4162
1613.4419	1625.2472	1650.3749
1666.8678	1675.3986	1679.9158
1688.0393	1689.7960	1690.2355
1697.6645	1798.5235	1808.1270
3056.7538	3063.6335	3070.3803
3072.6352	3074.5251	3080.7966

3084.6200	3085.2367	3085.5893
3092.7886	3095.8044	3096.6835
3124.9561	3129.2732	3135.3750
3136.0090	3140.7224	3143.5804
3144.0790	3148.3684	3155.8808
3156.1726	3159.5931	3159.7115
3161.3993	3163.8909	3170.3926
3175.8858	3179.1031	3181.0097
3183.5262	3185.2098	3196.1508
3210.9545	3213.5995	3216.7292
3217.8628	3218.6607	3219.2495
3222.0727	3223.5275	3227.7030
3228.0747	3233.2767	3234.4302
3235.6268	3237.1818	3237.8210
3242.9712	3245.4938	3254.0210

M3

Zero-point correction= 0.631241

Thermal correction to Energy= 0.671767

Thermal correction to Enthalpy= 0.672711

Thermal correction to Gibbs Free Energy= 0.555804

Sum of electronic and zero-point Energies= -2876.485172

Sum of electronic and thermal Energies= -2876.444645

Sum of electronic and thermal Enthalpies= -2876.443701

Sum of electronic and thermal Free Energies= -2876.560608

Cartesian coordinates

C	7.771161	-2.180616	-0.719296
C	7.285347	-3.493930	-0.765900
C	5.964869	-3.780585	-0.446483
C	5.140371	-2.720219	-0.077842
C	5.631592	-1.418621	-0.023104
H	7.948125	-4.299929	-1.059515
H	5.584025	-4.794748	-0.486231
C	3.444716	-1.058849	0.581276
C	2.473634	1.170965	0.920863
C	3.869761	1.540115	1.457541
C	4.938634	0.916630	0.575950
H	5.914266	0.964054	1.061241
S	3.444634	-2.782824	0.367223
N	4.643372	-0.507840	0.375620
N	2.354342	-0.313350	0.873850
C	4.068749	3.060663	1.605233
C	5.510477	3.392022	2.004506
C	3.106943	3.643722	2.643784

H	3.862838	3.523537	0.631522
H	5.793649	2.856150	2.917889
H	6.231568	3.144381	1.220989
H	5.603051	4.462367	2.203420
H	3.261432	3.167483	3.618306
H	3.289422	4.714649	2.760939
H	2.056469	3.522730	2.370596
H	3.955985	1.087406	2.455578
H	1.754246	1.493763	1.673354
C	2.114378	1.791221	-0.416331
C	1.288126	2.916358	-0.440264
C	2.588680	1.269756	-1.623768
C	0.966530	3.530683	-1.646335
H	0.856091	3.292408	0.482567
C	2.267283	1.884398	-2.829363
H	3.188149	0.363031	-1.641721
C	1.462502	3.021052	-2.842305
H	0.312644	4.396046	-1.648468
H	2.638109	1.467477	-3.759823
H	1.207127	3.495312	-3.784223
C	-0.148215	-0.097348	1.046742
H	-0.579401	-0.203919	2.047092
C	-1.201158	-0.602449	0.034110
C	-0.688800	-0.424323	-1.385022
F	-0.586481	0.853521	-1.760720
F	0.546972	-0.968220	-1.547126
F	-1.490942	-1.039979	-2.268790
O	1.055484	-2.164281	1.073241
C	1.089773	-0.955585	1.010595
H	5.000660	1.406738	-0.402645
C	-5.735192	-1.593857	0.833311
C	-5.262101	-2.779720	0.225668
C	-6.048800	-3.924378	0.140648
C	-7.341428	-3.882347	0.656832
C	-7.828533	-2.713341	1.254431
C	-7.038509	-1.575303	1.349291
C	-3.698274	-0.826470	0.332568
H	-5.665967	-4.828181	-0.322625
H	-7.972787	-4.762540	0.594328
H	-8.838886	-2.696869	1.651293
H	-7.408214	-0.666901	1.813733
N	-4.845361	-0.548432	0.901988
S	-3.634420	-2.512902	-0.341597
C	-2.668080	1.448559	0.293717

O	-1.702548	2.209048	0.525253
C	6.954122	-1.121911	-0.347449
H	7.331057	-0.106239	-0.322872
H	8.804619	-1.982731	-0.980102
C	-2.566229	0.026541	0.204631
H	-1.272272	-1.687716	0.166558
C	-3.981478	2.138477	0.001076
C	-4.318012	3.277909	0.731610
C	-4.791294	1.754445	-1.070673
C	-5.469134	4.000779	0.427627
H	-3.661894	3.590382	1.538114
C	-5.929607	2.485985	-1.391528
H	-4.515230	0.880022	-1.653740
C	-6.277310	3.606475	-0.636231
H	-5.731170	4.876384	1.013961
H	-6.547036	2.184980	-2.232374
H	-7.169988	4.173270	-0.882419
H	0.017046	0.958724	0.866141

Vibrational frequencies

14.1219	16.7025	18.8848
27.8259	34.3251	41.1199
47.7198	55.4713	59.0145
65.4895	70.6950	76.1608
82.3630	92.5661	99.8510
102.3940	106.1322	115.5293
127.5962	132.8631	140.4495
152.1611	171.5815	175.1896
184.4477	206.6339	209.0634
226.3688	230.2797	233.9445
242.9994	251.3657	256.3967
261.1472	288.3573	292.2644
297.2963	302.8364	327.8455
333.6383	348.9593	367.7815
378.6781	382.4728	392.9269
400.9858	417.4168	418.6021
424.1162	431.3918	438.1110
441.2578	453.6433	454.1064
485.5646	504.9752	505.6997
511.4904	519.4770	535.7046
547.3243	548.9626	557.6692
574.5137	583.2959	586.1769
611.3996	618.8605	625.6706
632.1520	635.8796	641.3921
648.9982	667.7580	675.7751

686.0619	703.5437	717.1455
717.7824	720.1483	724.7451
732.2449	734.0567	741.2102
748.5493	772.3581	775.5687
776.9577	793.9841	813.2617
824.4857	827.3577	843.5931
862.1091	872.9386	875.4982
877.2010	882.1178	882.6956
916.9342	926.7005	933.9541
951.0525	953.2194	958.5189
975.7585	977.4734	980.0553
983.4879	997.1132	999.6650
1005.4512	1009.8543	1011.8208
1017.9807	1020.3377	1026.8299
1027.2412	1029.3254	1040.8107
1057.1248	1064.6629	1067.1655
1074.0476	1075.2344	1079.9505
1093.2063	1108.6182	1114.7139
1119.7042	1135.2599	1149.2618
1154.1664	1165.0086	1167.8759
1175.2558	1177.1497	1183.3976
1184.2805	1184.9394	1188.3010
1190.4233	1199.7165	1201.8471
1217.4097	1224.7401	1229.6468
1248.9136	1256.4638	1262.4076
1269.0907	1283.0206	1285.9231
1297.2405	1305.9588	1330.4827
1332.1591	1338.2133	1341.8025
1346.9463	1349.2134	1359.6907
1361.3090	1362.8713	1368.8263
1375.0416	1376.9109	1393.9108
1402.2037	1405.6097	1414.2035
1418.7612	1425.4832	1428.3211
1435.5329	1446.1244	1478.3982
1493.5680	1494.5669	1494.7023
1504.6438	1506.8964	1508.5344
1510.4393	1513.6054	1514.8125
1527.0624	1530.6565	1549.7782
1556.0186	1557.3899	1603.4744
1643.3086	1646.2491	1677.8188
1680.4981	1682.6841	1683.3173
1686.7159	1699.1671	1702.0610
1843.0966	3058.9778	3068.0920
3070.8405	3084.6861	3097.9596

3110.3120	3116.4700	3138.7850
3148.1731	3151.1223	3157.3058
3166.5286	3172.4293	3198.9718
3205.5792	3206.9580	3208.2580
3209.8432	3212.1050	3218.4549
3219.4498	3222.9588	3223.2913
3226.0083	3227.8483	3233.7208
3235.3784	3236.8262	3236.9161
3241.8422	3243.5083	3248.4123

M3'

Zero-point correction= 0.635449

Thermal correction to Energy= 0.674940

Thermal correction to Enthalpy= 0.675884

Thermal correction to Gibbs Free Energy= 0.562233

Sum of electronic and zero-point Energies= -2553.524019

Sum of electronic and thermal Energies= -2553.484529

Sum of electronic and thermal Enthalpies= -2553.483585

Sum of electronic and thermal Free Energies= -2553.597236

Cartesian coordinates

C	-7.525843	0.700373	-1.360815
C	-7.588968	-0.416205	-2.203653
C	-6.486113	-1.242115	-2.378421
C	-5.318432	-0.924744	-1.690088
C	-5.258451	0.192106	-0.860957
H	-8.511706	-0.642096	-2.725904
H	-6.529444	-2.109597	-3.027237
C	-3.127182	-0.632628	-0.594626
C	-1.466340	0.327902	0.932692
C	-2.133092	1.669706	0.571810
C	-3.642947	1.497674	0.546377
H	-4.121842	2.359419	0.079897
S	-3.786386	-1.779088	-1.729491
N	-3.993833	0.334369	-0.274608
N	-1.906416	-0.706145	-0.037542
C	-1.717875	2.823320	1.505209
C	-2.525020	4.093002	1.212842
C	-0.227299	3.134730	1.366614
H	-1.926095	2.514237	2.538341
H	-2.445187	4.367356	0.154566
H	-3.584010	3.989104	1.463979
H	-2.131983	4.924802	1.802813
H	0.004111	3.463575	0.346854
H	0.055067	3.936658	2.054367

H	0.414714	2.277601	1.582877
H	-1.789401	1.902465	-0.446571
H	-0.401803	0.453378	0.740072
C	-1.693983	-0.140602	2.357025
C	-0.717757	0.115592	3.323580
C	-2.861260	-0.809661	2.736041
C	-0.912896	-0.267558	4.647414
H	0.207891	0.608253	3.036813
C	-3.056711	-1.194483	4.059737
H	-3.622271	-1.053398	1.998756
C	-2.085678	-0.920025	5.019135
H	-0.143096	-0.065910	5.384791
H	-3.966195	-1.716404	4.338121
H	-2.237384	-1.224031	6.049491
C	0.251620	-1.998195	0.307629
H	0.433687	-1.313948	1.132893
C	1.476074	-2.019905	-0.650637
C	2.309660	-3.237659	-0.320035
F	2.658447	-3.314045	0.972418
F	1.597296	-4.359872	-0.575329
F	3.422755	-3.321608	-1.059824
O	-1.361829	-2.465536	-1.365027
C	-1.011494	-1.731361	-0.467122
H	-4.054545	1.362767	1.553860
C	5.601098	-0.562285	0.322052
C	5.593593	0.260741	-0.809403
C	6.707387	0.930924	-1.284630
C	7.886623	0.738069	-0.564346
C	7.923107	-0.083196	0.572420
C	6.787262	-0.743804	1.033987
C	3.601239	-0.541408	-0.437280
H	6.663326	1.561814	-2.164784
H	8.794536	1.233500	-0.891996
H	8.861675	-0.204505	1.103607
H	6.814486	-1.376140	1.914830
N	4.315729	-1.041908	0.534723
C	1.395199	0.353751	-1.180158
O	0.195860	0.152931	-1.553295
C	-6.361396	1.022985	-0.675825
H	-6.321428	1.882131	-0.016417
H	-8.401977	1.326743	-1.236076
C	2.200412	-0.693697	-0.722660
H	1.075065	-2.240984	-1.649341
C	1.841353	1.794477	-1.153347

C	1.289682	2.663237	-2.098884
C	2.677594	2.321734	-0.163198
C	1.590438	4.022555	-2.079625
H	0.613750	2.251951	-2.841752
C	2.970066	3.681786	-0.133186
H	3.081933	1.669827	0.607126
C	2.432160	4.536207	-1.094792
H	1.164406	4.683118	-2.828751
H	3.612975	4.077227	0.647140
H	2.662971	5.596730	-1.072136
H	0.091669	-2.993849	0.735344
O	4.329526	0.248990	-1.310725

Vibrational frequencies

16.2525	21.1911	26.5057
31.5967	34.0732	40.0937
47.9070	52.0264	59.0686
71.5309	76.2722	84.3834
89.9406	96.1324	98.6859
110.1948	113.4023	128.3327
135.2791	142.6895	156.3861
165.3205	175.2859	193.0038
197.9806	217.3261	222.1297
232.0249	241.8163	245.0213
262.0107	268.0958	272.9937
277.1025	287.3995	291.5800
300.7305	325.4957	334.0483
349.8590	362.3624	370.5381
386.9842	394.4330	411.3438
416.0467	421.9470	427.6882
433.4468	442.1559	446.4580
455.0879	462.4070	475.6364
493.2215	509.5409	520.1611
539.5108	546.7655	547.9821
562.1212	564.8707	582.3259
591.4878	595.2735	611.0870
627.4459	628.2643	633.7529
637.2441	639.6283	661.0381
671.5279	683.7792	694.1153
716.8739	721.2534	722.5975
729.3172	735.5198	741.8786
753.6796	763.9579	768.5961
775.3397	784.7306	786.7924
818.8225	829.0596	831.0020
850.5011	868.8306	874.6382

879.2748 883.6343 888.7197
888.8999 907.3979 921.3268
938.7020 942.7643 943.6135
956.1004 958.3183 968.2059
976.7144 979.0255 987.9670
996.0071 996.5192 1003.3449
1010.1529 1012.1572 1018.6659
1019.3161 1023.2867 1025.3678
1030.2733 1042.7557 1045.8025
1058.3369 1067.3068 1069.5156
1071.4432 1074.1267 1104.5239
1114.6674 1118.3266 1121.7012
1131.7822 1142.3608 1156.9544
1161.3953 1165.2812 1172.1934
1173.4511 1176.4950 1181.3550
1183.3046 1186.5182 1197.6701
1201.5094 1206.7758 1211.7923
1217.6904 1244.4266 1253.1475
1259.4684 1263.5654 1278.3339
1284.6402 1297.7160 1303.8256
1305.4463 1322.4725 1331.9063
1333.2167 1336.2148 1341.0472
1350.2666 1360.6129 1360.9875
1364.1983 1367.2589 1372.6806
1380.9301 1386.2169 1393.9051
1402.9414 1408.0532 1416.1373
1421.3288 1426.9194 1436.5050
1448.7760 1474.2165 1489.5752
1491.9663 1497.2903 1500.6218
1505.5344 1508.4513 1511.6969
1514.7731 1516.4565 1527.3156
1531.9470 1534.9302 1545.6841
1555.2119 1573.7817 1609.1438
1634.0575 1676.4003 1679.4808
1681.0080 1689.9796 1693.2281
1694.2846 1699.6043 1710.1503
1834.6868 3058.0654 3063.0180
3067.4519 3076.9361 3077.6024
3092.8836 3107.9959 3137.8743
3143.2459 3147.7660 3162.0528
3172.6140 3180.3288 3193.5338
3196.1854 3198.3278 3202.5334
3203.9263 3204.4317 3210.2869
3210.5356 3218.2071 3218.9872

3224.5527	3225.0847	3231.4893
3233.7308	3234.3855	3240.5190
3243.5166	3246.6614	3247.6606

TS4-A

Zero-point correction= 0.631715

Thermal correction to Energy= 0.670814

Thermal correction to Enthalpy= 0.671759

Thermal correction to Gibbs Free Energy= 0.560916

Sum of electronic and zero-point Energies= -2876.487741

Sum of electronic and thermal Energies= -2876.448642

Sum of electronic and thermal Enthalpies= -2876.447697

Sum of electronic and thermal Free Energies= -2876.558540

Cartesian coordinates

C	-6.936089	-1.667101	-0.161067
C	-7.025515	-1.631999	-1.556046
C	-5.919990	-1.301651	-2.333333
C	-4.725292	-1.010218	-1.683661
C	-4.646405	-1.033910	-0.293879
H	-7.966421	-1.867226	-2.040660
H	-5.983774	-1.275602	-3.415560
C	-2.467439	-0.464250	-0.813944
C	-0.692489	-0.300309	0.831266
C	-1.793914	0.251572	1.757742
C	-3.053233	-0.580846	1.589908
H	-3.905144	-0.094706	2.072530
S	-3.188307	-0.554828	-2.410694
N	-3.364869	-0.695523	0.161827
N	-1.178796	-0.258739	-0.566560
C	-1.353309	0.395013	3.233381
C	-1.588022	-0.849986	4.097029
C	-2.051787	1.602349	3.865419
H	-0.275315	0.605342	3.220219
H	-1.133908	-0.700307	5.080028
H	-2.659324	-1.016352	4.258155
H	-1.160545	-1.758359	3.664866
H	-1.732800	1.730668	4.903346
H	-1.824997	2.520634	3.316404
H	-3.139620	1.466921	3.866982
H	-2.014902	1.258405	1.377899
H	0.139928	0.402878	0.878400
C	-0.161653	-1.662816	1.227959
C	1.024340	-1.718424	1.965478
C	-0.821303	-2.851186	0.907155

C	1.529363	-2.939712	2.403205
H	1.560364	-0.797251	2.187658
C	-0.317929	-4.073245	1.347401
H	-1.722341	-2.833763	0.298756
C	0.853492	-4.119802	2.100446
H	2.454578	-2.966879	2.969983
H	-0.838712	-4.990619	1.093814
H	1.244369	-5.073487	2.439087
C	1.071038	-0.638460	-1.662192
H	1.210273	-1.196265	-0.735619
C	2.263987	0.307167	-1.877048
C	3.391462	-0.422789	-2.577841
F	4.548783	0.249832	-2.540044
F	3.618739	-1.661548	-2.111285
F	3.073183	-0.581524	-3.879259
C	-0.256111	0.125566	-1.703119
H	-2.942683	-1.587978	2.004767
C	-0.706069	2.643447	-0.540070
C	-0.327514	3.412932	0.572366
C	-1.236566	4.252789	1.208776
C	-2.542569	4.308879	0.725824
C	-2.918484	3.559608	-0.394816
C	-2.007628	2.734174	-1.045025
C	1.451350	1.935345	-0.341169
H	-0.936778	4.846530	2.066765
H	-3.266414	4.952981	1.213508
H	-3.933153	3.633055	-0.772812
H	-2.276186	2.172060	-1.932756
N	0.292548	1.811339	-1.020033
S	1.366634	3.135775	0.962905
C	3.686985	1.197909	0.244197
O	3.829694	2.151212	1.028143
C	4.708822	0.101006	0.334278
C	4.325610	-1.230825	0.478383
C	6.060392	0.442891	0.434038
C	5.283785	-2.218090	0.701861
H	3.273656	-1.498140	0.429152
C	7.019350	-0.542845	0.631374
H	6.344461	1.487797	0.356776
C	6.631198	-1.876611	0.768889
H	4.973901	-3.251383	0.824232
H	8.069353	-0.274025	0.688958
H	7.379570	-2.645345	0.933613
C	-5.745302	-1.368942	0.492384

H	-5.678463	-1.406507	1.573543
H	-7.807941	-1.933113	0.425905
C	2.544755	1.124900	-0.630913
H	1.938681	1.028514	-2.640856
H	0.983869	-1.356275	-2.482790
O	-0.822602	0.312924	-2.782999

Vibrational frequencies

-180.0661	18.2499	27.2120
32.9892	35.7488	42.4662
56.2287	62.0282	63.9622
69.0965	76.6754	83.3707
84.9081	88.3032	98.9082
101.6691	116.4966	127.3107
132.5597	138.5372	159.1238
174.0185	182.8657	188.6153
209.5667	217.2553	221.3943
225.3004	238.2446	243.7847
248.7109	261.8206	262.9272
274.3035	277.6994	281.7936
307.1134	310.2999	315.7889
327.4533	351.8153	360.8705
384.8483	390.8408	404.1576
412.6248	421.7944	425.0518
427.3810	433.4681	439.5107
452.3214	456.9793	472.3095
492.0474	508.6509	510.3058
513.2283	518.0111	533.0431
539.4271	551.3038	564.9559
570.8845	578.3658	591.2529
604.7891	621.8494	626.2178
626.7425	641.1279	644.4649
658.1217	671.8327	677.2304
701.2880	705.9420	718.0759
719.5837	721.1865	729.2241
732.8445	733.0451	750.1772
756.4634	759.6791	775.7300
778.3498	788.3608	796.1669
816.2355	823.1561	841.9580
870.0750	881.5493	882.3054
886.5275	897.8911	904.0253
922.4785	932.3093	939.8622
950.1784	960.7246	966.2938
972.3527	977.1795	977.9783
1001.1808	1003.2413	1007.9881

1009.3844	1014.9747	1016.8460
1019.9713	1021.8615	1027.3637
1032.1530	1036.9897	1041.0005
1060.2267	1062.7093	1065.0144
1067.5169	1072.1102	1083.0831
1088.5986	1101.4865	1110.3034
1114.4939	1122.8502	1133.3738
1142.4951	1157.7103	1157.9474
1170.9108	1177.8497	1179.9331
1181.3566	1184.3247	1187.9323
1193.5417	1194.8339	1213.6910
1216.7818	1223.4914	1241.5908
1246.2829	1260.4634	1266.2683
1286.1665	1292.7039	1296.0835
1310.9293	1317.1146	1322.9544
1328.4983	1333.6259	1346.0599
1349.4816	1352.2682	1357.5098
1362.4876	1367.2465	1371.1186
1373.2759	1377.9790	1383.6539
1397.4236	1412.7425	1418.3905
1428.0796	1433.2559	1436.7754
1448.6879	1450.5729	1476.5507
1492.9933	1495.7421	1499.4738
1501.4470	1505.1240	1509.1597
1510.2850	1514.0932	1518.4056
1519.7450	1520.0885	1533.2623
1548.8485	1553.6219	1602.6540
1658.3976	1671.6705	1675.5184
1678.0405	1684.0964	1688.3314
1691.5748	1695.3680	1696.2560
1701.0141	3054.9340	3058.5422
3059.4347	3067.6489	3084.2949
3098.4389	3107.2213	3134.0761
3142.3131	3152.4185	3153.8576
3163.4705	3173.6656	3179.8464
3183.9466	3200.0634	3207.4888
3207.7747	3209.9623	3219.0319
3219.4577	3220.0343	3221.3641
3222.3388	3223.7318	3232.8279
3234.3628	3234.8942	3235.7310
3240.2424	3251.9933	3254.5126

TS4-B

Zero-point correction= 0.631022

Thermal correction to Energy= 0.670363
Thermal correction to Enthalpy= 0.671307
Thermal correction to Gibbs Free Energy= 0.557966
Sum of electronic and zero-point Energies= -2876.485606
Sum of electronic and thermal Energies= -2876.446265
Sum of electronic and thermal Enthalpies= -2876.445321
Sum of electronic and thermal Free Energies= -2876.558662
Cartesian coordinates

C	-7.485400	1.230428	-0.728643
C	-7.688841	0.356707	-1.801444
C	-6.659747	-0.456723	-2.263866
C	-5.425742	-0.380281	-1.626646
C	-5.227322	0.498873	-0.564817
H	-8.661144	0.308986	-2.278910
H	-6.813732	-1.136336	-3.094844
C	-3.139498	-0.479254	-0.685837
C	-1.328355	-0.012043	0.863370
C	-1.893347	1.416435	0.848261
C	-3.409571	1.360141	0.942582
H	-3.849809	2.340494	0.741634
S	-3.959250	-1.274263	-2.013161
N	-3.915687	0.435574	-0.076942
N	-1.912089	-0.762696	-0.269094
C	-1.255083	2.356776	1.894340
C	-1.935518	2.346441	3.267607
C	-1.212089	3.782215	1.339483
H	-0.215714	2.023414	2.019888
H	-2.929166	2.805916	3.213700
H	-2.042681	1.341629	3.684216
H	-1.344387	2.940282	3.969945
H	-2.225002	4.165762	1.169129
H	-0.717626	4.455886	2.045551
H	-0.664298	3.816984	0.393636
H	-1.627601	1.798410	-0.147704
H	-0.264763	0.083181	0.640367
C	-1.472558	-0.756410	2.173116
C	-0.388829	-0.768663	3.055404
C	-2.658780	-1.394481	2.542804
C	-0.497941	-1.377759	4.302097
H	0.546975	-0.297801	2.759372
C	-2.768178	-2.005699	3.789541
H	-3.500794	-1.429341	1.855662
C	-1.691984	-1.991578	4.673822
H	0.351019	-1.379518	4.977575

H	-3.694139	-2.498433	4.067288
H	-1.780085	-2.469317	5.643980
C	0.101291	-2.282275	-0.434594
H	0.239913	-1.975979	0.602708
C	1.422892	-2.114948	-1.201731
C	2.342091	-3.254569	-0.840114
F	2.533306	-3.351230	0.490280
F	1.821690	-4.430776	-1.233429
F	3.548987	-3.152140	-1.415023
O	-1.537426	-2.051255	-2.149465
C	-1.012777	-1.544021	-1.161372
H	-3.746786	1.017684	1.926366
C	5.324812	0.652991	-0.800925
C	5.532872	0.026836	0.443994
C	6.727063	0.189393	1.148341
C	7.706970	1.002503	0.595492
C	7.508727	1.635713	-0.642119
C	6.327548	1.465113	-1.345179
C	3.367982	-0.389573	-0.683963
H	6.883062	-0.300457	2.103444
H	8.640356	1.149590	1.128786
H	8.292229	2.264613	-1.051579
H	6.159732	1.943515	-2.304167
N	4.108367	0.390248	-1.406228
S	4.124648	-0.908870	0.850883
C	1.072864	0.270320	-1.301638
O	-0.130779	-0.015293	-1.730089
C	-6.251455	1.315368	-0.093120
H	-6.098821	1.987820	0.743251
H	-8.302450	1.853071	-0.381681
C	1.979060	-0.717310	-1.011167
H	1.195829	-2.261069	-2.268053
C	1.321201	1.735440	-1.106249
C	2.001167	2.240054	0.007972
C	0.795099	2.632296	-2.041140
C	2.193067	3.610346	0.157308
H	2.382731	1.554568	0.760721
C	0.999944	4.002586	-1.900088
H	0.237052	2.239234	-2.885002
C	1.706760	4.494783	-0.804809
H	2.721856	3.987782	1.027009
H	0.605584	4.686872	-2.644733
H	1.864899	5.562706	-0.692025
H	-0.213342	-3.329227	-0.439697

Vibrational frequencies

-137.0595	12.7879	15.9801
26.6553	30.6673	33.3849
48.9046	54.0149	61.8039
63.4944	64.5413	72.0607
77.6523	89.7982	95.2608
101.3186	110.1823	128.5860
133.0690	137.6556	151.0763
166.2131	176.1337	185.6996
203.7914	206.5728	216.0894
222.7010	234.8620	248.7569
251.4522	254.5350	270.7746
277.1181	285.2142	291.9296
304.7742	313.3471	327.1496
330.4188	346.6490	366.9327
377.8713	397.7713	412.2849
418.5606	419.0405	423.7481
426.1073	435.3219	439.9343
447.4358	457.7587	469.9924
489.4865	508.9787	512.0080
515.3582	517.8152	523.6630
551.4461	556.8263	559.0760
567.2695	584.0375	594.3317
614.9139	625.0885	626.3029
628.3009	629.9032	647.2429
657.0638	664.7278	672.6398
681.5681	707.1803	718.5654
723.2021	724.9003	728.0997
729.0365	735.3104	747.3147
748.8285	753.8663	772.0443
782.1867	790.5399	809.0549
823.4272	836.4021	853.6405
866.3435	871.3265	874.8605
879.5178	887.1603	888.1575
923.2181	932.4856	935.7951
946.0876	956.5756	967.5555
969.0782	973.6585	977.8627
1002.4909	1004.9687	1006.0634
1010.2718	1015.3220	1016.5257
1017.9501	1018.4669	1027.6689
1030.7880	1036.5553	1046.8489
1056.6420	1061.4763	1065.4734
1070.0044	1072.9847	1081.0180
1094.3534	1105.3846	1108.0945

1118.6801	1127.0131	1140.5784
1147.2124	1157.0266	1158.5162
1167.2879	1172.1832	1177.2942
1183.6427	1185.3927	1186.4966
1189.3034	1206.4048	1210.1860
1214.3607	1216.5504	1222.5606
1254.2867	1260.3072	1264.5885
1285.5585	1290.2616	1296.0866
1305.3418	1308.6919	1318.3689
1321.7616	1331.3984	1335.1670
1343.5885	1349.9242	1356.8699
1360.3551	1363.9673	1365.6009
1367.8449	1375.5234	1381.8580
1393.1216	1410.4767	1412.4656
1417.1112	1423.8168	1436.9442
1437.2893	1446.0178	1486.5934
1494.0796	1494.6287	1497.4386
1499.1585	1504.1329	1509.5639
1515.7037	1517.6748	1519.3344
1520.8613	1531.9048	1544.7507
1556.0992	1601.5312	1610.3695
1624.1296	1649.0630	1672.5778
1680.7617	1681.6776	1691.4354
1693.4876	1693.9203	1699.1238
1731.3185	3055.1703	3060.1578
3060.4657	3064.8002	3067.0552
3096.6550	3117.1048	3132.6164
3139.0777	3153.9185	3158.4262
3160.6072	3165.8074	3176.4279
3182.6997	3193.3999	3200.5596
3206.4003	3211.0803	3214.0538
3215.8990	3215.9907	3218.6953
3221.3031	3221.8391	3223.4224
3230.4345	3232.8650	3233.4341
3235.7636	3238.3065	3239.2769

PA

Zero-point correction= 0.276076

Thermal correction to Energy= 0.296654

Thermal correction to Enthalpy= 0.297598

Thermal correction to Gibbs Free Energy= 0.225053

Sum of electronic and zero-point Energies= -1633.444751

Sum of electronic and thermal Energies= -1633.424173

Sum of electronic and thermal Enthalpies= -1633.423229

Sum of electronic and thermal Free Energies= -1633.495773

Cartesian coordinates

C	1.064508	2.594672	-1.110025
H	1.148678	2.438626	-2.191401
C	-0.363808	2.297255	-0.681048
C	-0.628958	2.827045	0.715428
F	-0.472504	4.155560	0.787158
F	0.212581	2.277903	1.613372
F	-1.875724	2.541374	1.117776
C	2.091265	1.691344	-0.469245
C	2.598929	-0.705574	-0.046323
C	1.979288	-1.951794	-0.161665
C	2.681958	-3.134572	0.017611
C	4.039576	-3.057095	0.319132
C	4.660610	-1.816536	0.441969
C	3.955133	-0.626869	0.265105
C	0.361269	-0.052878	-0.503899
H	2.182511	-4.092537	-0.076955
H	4.608738	-3.968923	0.462249
H	5.716297	-1.764857	0.685000
H	4.441194	0.330389	0.369654
N	1.691457	0.356589	-0.293225
S	0.261937	-1.815485	-0.526687
C	-2.060033	0.443214	-0.991104
O	-2.731897	1.136195	-1.740742
C	-2.672895	-0.739346	-0.314458
C	-3.599643	-1.518509	-1.010567
C	-2.406541	-1.000276	1.032906
C	-4.230474	-2.579950	-0.371668
H	-3.812735	-1.283634	-2.048667
C	-3.058350	-2.046993	1.676320
H	-1.701299	-0.372371	1.571466
C	-3.961008	-2.841742	0.971820
H	-4.937805	-3.197324	-0.915307
H	-2.862298	-2.243630	2.724991
H	-4.460986	-3.664610	1.472549
C	-0.657586	0.818989	-0.698038
H	-1.070392	2.799908	-1.346847
H	1.354497	3.624142	-0.895689
O	3.209870	2.060132	-0.195474

Vibrational frequencies

24.6871	36.7790	41.9940
54.1292	62.6663	78.9648
89.2188	99.1080	117.3731

169.1924	181.2385	197.5171
230.4380	246.5179	259.0374
283.5531	293.3321	328.0248
362.3793	392.3154	403.0776
413.8704	419.4626	436.6354
444.3399	478.5357	505.5465
525.3701	536.1914	553.1315
555.5143	567.2971	622.7913
626.1013	631.8708	651.1155
683.9786	687.7863	717.0831
724.9839	732.0549	757.8654
759.2946	773.7798	809.8223
827.6150	838.7202	881.2048
895.6469	930.8719	936.8437
972.3883	974.0658	981.0484
1009.2842	1017.4528	1019.8910
1036.5079	1043.7425	1065.7196
1076.2066	1094.4548	1116.6734
1118.6727	1155.4646	1171.8214
1184.8888	1186.2825	1189.6881
1200.3277	1212.3863	1250.4106
1264.1564	1268.1812	1306.4906
1323.9302	1333.9802	1339.2994
1346.1268	1362.1976	1364.9743
1375.3059	1399.7821	1420.4608
1466.7011	1502.7822	1510.7695
1524.4104	1548.2649	1664.9532
1675.1615	1680.0675	1688.6964
1694.0338	1784.6515	1856.2168
3096.0871	3139.7641	3176.9877
3202.4360	3213.2165	3214.6078
3227.6928	3229.3850	3235.4973
3237.8839	3243.8831	3309.8669

PB

Zero-point correction= 0.275853

Thermal correction to Energy= 0.296361

Thermal correction to Enthalpy= 0.297305

Thermal correction to Gibbs Free Energy= 0.224263

Sum of electronic and zero-point Energies= -1633.442102

Sum of electronic and thermal Energies= -1633.421594

Sum of electronic and thermal Enthalpies= -1633.420650

Sum of electronic and thermal Free Energies= -1633.493692

Cartesian coordinates

C	-2.548506	-1.795578	-1.338922
H	-3.012372	-2.781243	-1.377322
C	-1.179545	-1.819347	-0.666324
C	-1.252389	-2.573204	0.648593
F	-1.611258	-3.850503	0.462547
F	-2.168309	-2.018810	1.467021
F	-0.082847	-2.567957	1.297595
O	-4.663010	-1.037527	-0.457393
C	-3.492978	-0.857495	-0.635315
C	2.896446	-0.760689	-0.592827
C	3.063430	0.218313	0.406305
C	4.330337	0.575386	0.870950
C	5.428789	-0.071181	0.323194
C	5.274381	-1.050843	-0.672082
C	4.017619	-1.400966	-1.135606
C	0.764123	-0.251637	-0.303341
H	4.452856	1.331795	1.638069
H	6.423849	0.185870	0.670528
H	6.153110	-1.537272	-1.081685
H	3.880709	-2.154371	-1.903622
N	1.585178	-1.008721	-0.959206
S	1.504803	0.830751	0.878976
C	-1.592909	0.579614	-0.284770
O	-2.948755	0.329890	-0.223720
C	-0.692117	-0.410100	-0.425330
H	-0.455428	-2.345068	-1.293938
C	-1.326415	2.027607	-0.167210
C	-1.993825	2.776096	0.807494
C	-0.444802	2.660218	-1.049069
C	-1.751315	4.140684	0.920114
H	-2.693332	2.283377	1.475001
C	-0.211507	4.025920	-0.937232
H	0.049933	2.079637	-1.822276
C	-0.859152	4.765667	0.050796
H	-2.261037	4.716388	1.685267
H	0.470944	4.513291	-1.625327
H	-0.674464	5.831394	0.138080
H	-2.429992	-1.429039	-2.364019

Vibrational frequencies

20.8497	30.9382	35.9839
48.0753	65.8389	71.2470
97.7385	106.8420	122.2493
137.0232	196.9086	203.1342
205.8219	240.1183	245.0139

278.7438	299.8080	319.0552
352.5995	380.9447	415.3233
430.9706	438.7476	464.5775
487.0080	511.1190	516.9814
527.2264	552.6350	563.0232
578.3222	604.7220	622.3019
628.9752	652.3417	663.0779
677.8654	708.2955	715.2770
724.9684	738.1275	750.9256
770.1364	786.3256	797.6699
829.2118	870.8078	880.4376
888.9229	897.2553	954.4107
966.1196	976.8127	984.9772
1010.4414	1016.0529	1018.9413
1029.9279	1034.4707	1060.0047
1063.0491	1081.0663	1096.7758
1115.0021	1157.5267	1163.9170
1177.7228	1186.0444	1190.6152
1198.4986	1205.1716	1245.0987
1276.6373	1279.6215	1289.8625
1304.5634	1324.4687	1327.3031
1337.4266	1357.1566	1363.1439
1368.0291	1398.0421	1416.7430
1458.7540	1496.0347	1497.5125
1515.7462	1548.1056	1601.3922
1649.4428	1668.9608	1692.7382
1697.2528	1748.9415	1925.3384
3100.4145	3140.1730	3177.6379
3208.7925	3211.2131	3214.9573
3219.9935	3224.0521	3228.0889
3235.2618	3247.1084	3249.4285

TS4-A'

Zero-point correction= 0.634602

Thermal correction to Energy= 0.673216

Thermal correction to Enthalpy= 0.674160

Thermal correction to Gibbs Free Energy= 0.564338

Sum of electronic and zero-point Energies= -2553.507885

Sum of electronic and thermal Energies= -2553.469271

Sum of electronic and thermal Enthalpies= -2553.468326

Sum of electronic and thermal Free Energies= -2553.578148

Cartesian coordinates

C	-6.964148	-1.287297	-0.474976
C	-7.074184	-0.848792	-1.798461

C	-5.966382	-0.357805	-2.481414
C	-4.747901	-0.317654	-1.811841
C	-4.647912	-0.745857	-0.491328
H	-8.033650	-0.894482	-2.301345
H	-6.046494	-0.018749	-3.508424
C	-2.450298	-0.150888	-0.893256
C	-0.644287	-0.506069	0.693873
C	-1.716652	-0.208690	1.763215
C	-3.002372	-0.927005	1.390875
H	-3.830322	-0.583929	2.016694
S	-3.200147	0.253165	-2.426521
N	-3.343071	-0.612215	0.001623
N	-1.149312	-0.073612	-0.630969
C	-1.269395	-0.504813	3.214698
C	-1.542249	-1.937258	3.690301
C	-1.939377	0.486693	4.171022
H	-0.186955	-0.325458	3.257342
H	-1.073445	-2.091221	4.665721
H	-2.617937	-2.102647	3.819008
H	-1.157124	-2.699025	3.008192
H	-1.686305	1.518908	3.914015
H	-3.030313	0.385296	4.135404
H	-1.624234	0.297407	5.200826
H	-1.911809	0.869329	1.692500
H	0.214917	0.133550	0.911731
C	-0.164584	-1.944458	0.688998
C	0.981978	-2.266384	1.420823
C	-0.848316	-2.957355	0.013645
C	1.425962	-3.583156	1.499232
H	1.531978	-1.478011	1.930029
C	-0.406498	-4.276251	0.094350
H	-1.721557	-2.722607	-0.590022
C	0.726976	-4.592485	0.839943
H	2.319144	-3.816874	2.069723
H	-0.945378	-5.056434	-0.432909
H	1.070548	-5.619904	0.897319
C	1.124483	-0.152984	-1.760749
H	1.273083	-0.907187	-0.987904
C	2.294151	0.849122	-1.743777
C	3.455472	0.314969	-2.556415
F	4.581495	1.014603	-2.361763
F	3.734389	-0.980520	-2.339988
F	3.159805	0.404560	-3.869630
C	-0.229884	0.557856	-1.650925

H	-2.912820	-2.013816	1.491331
C	-0.654457	2.708969	0.188168
C	-0.016510	3.063033	1.380462
C	-0.655770	3.689614	2.429085
C	-2.019655	3.957168	2.247250
C	-2.674583	3.620048	1.059867
C	-2.002761	2.997079	0.003016
C	1.434537	2.056997	0.088749
H	-0.131242	3.951417	3.340697
H	-2.571152	4.445593	3.043212
H	-3.728065	3.855496	0.950714
H	-2.501447	2.754131	-0.929559
N	0.275758	2.065864	-0.613398
C	3.755461	1.357460	0.479333
O	4.010766	2.246341	1.293979
C	4.678351	0.169298	0.440253
C	6.044514	0.367246	0.659311
C	4.185032	-1.129744	0.332422
C	6.907494	-0.719278	0.734848
H	6.412666	1.382221	0.771333
C	5.043460	-2.222269	0.429733
H	3.121909	-1.290602	0.181428
C	6.406546	-2.017802	0.623575
H	7.969851	-0.558645	0.888802
H	4.645226	-3.229459	0.352701
H	7.079518	-2.866809	0.691875
C	-5.749148	-1.243389	0.199572
H	-5.665939	-1.594446	1.221530
H	-7.838980	-1.671906	0.037301
C	2.563493	1.397562	-0.352756
H	1.958826	1.704024	-2.349243
H	1.069708	-0.665582	-2.725333
O	-0.792465	0.965988	-2.668448
O	1.299422	2.672563	1.304088

Vibrational frequencies

-190.7380	23.5153	24.9471
30.8254	37.5780	40.8560
50.2367	57.6840	64.9986
71.8355	78.2862	84.9583
91.5544	95.1021	102.0278
108.0704	116.0056	123.7256
131.3177	137.6899	157.9787
166.9075	184.0995	193.3570
213.4430	214.2937	226.8198

228.1149	232.6505	246.9148
255.7167	260.3161	277.3660
280.6050	293.0437	297.7339
309.2590	315.7211	316.9577
331.4739	350.7018	366.4286
390.6275	399.4333	406.2727
417.1525	419.6836	430.5124
435.5869	437.4514	448.7983
461.3425	473.6310	491.8979
504.5747	511.2672	517.1414
520.0078	540.3686	549.2769
559.2907	566.1757	572.5492
587.7732	592.5581	609.7428
623.7453	626.9817	628.3856
637.7265	642.3414	665.1591
671.3140	680.7794	705.3190
712.5268	717.3760	727.2140
727.8826	733.8339	735.6190
747.7799	753.6622	765.7094
769.9249	775.7919	781.7195
790.1707	813.3304	828.5098
838.6917	868.2555	878.5447
879.1788	880.8425	892.2035
893.4461	905.6860	920.9068
932.4013	936.1439	953.4935
954.2971	961.4297	963.1259
968.5232	969.2768	978.1776
1000.9032	1001.7818	1006.8748
1011.6271	1015.3548	1016.6998
1018.3715	1022.1448	1026.9208
1035.2862	1039.0399	1043.4677
1046.7384	1064.6260	1067.4851
1069.5611	1073.3642	1087.5615
1097.3052	1111.9380	1121.9733
1124.5200	1132.9781	1136.2554
1146.0413	1155.9421	1170.2473
1174.3382	1174.6172	1182.0863
1183.1865	1185.9103	1193.0424
1195.0427	1213.8990	1218.7542
1222.3709	1233.0304	1240.8290
1245.4331	1259.9443	1266.5992
1293.5884	1295.7156	1305.0531
1307.7259	1314.2670	1324.3931
1330.6914	1333.1452	1343.3498

1345.7572	1358.4321	1360.3407
1364.2295	1366.6772	1375.5788
1378.1426	1384.1610	1390.4924
1408.9700	1410.6315	1416.9340
1418.5482	1427.6538	1439.3935
1444.6773	1447.7376	1484.3758
1495.2512	1496.7071	1501.4919
1504.9445	1509.8537	1518.1982
1519.2593	1522.1767	1523.7823
1524.5949	1535.9088	1547.3967
1553.4372	1588.3214	1602.9103
1674.1262	1676.0022	1679.5643
1686.5555	1692.2039	1696.3422
1696.6912	1703.9294	1706.9344
1742.8209	3055.5500	3060.0139
3064.2640	3070.6515	3083.5631
3102.5185	3115.1347	3137.8755
3143.6694	3145.7351	3157.6524
3162.9810	3170.4191	3193.6187
3201.1380	3205.3694	3210.1084
3210.2209	3211.3234	3216.5947
3218.1735	3218.5501	3224.4327
3224.5637	3225.0556	3228.9578
3232.4230	3233.3203	3233.3576
3239.2355	3241.4713	3244.2476

TS4-B'

Zero-point correction= 0.634299

Thermal correction to Energy= 0.672162

Thermal correction to Enthalpy= 0.673106

Thermal correction to Gibbs Free Energy= 0.563916

Sum of electronic and zero-point Energies= -2553.520219

Sum of electronic and thermal Energies= -2553.482356

Sum of electronic and thermal Enthalpies= -2553.481412

Sum of electronic and thermal Free Energies= -2553.590601

Cartesian coordinates

C	-7.443929	0.907019	-0.665549
C	-7.616132	0.004394	-1.719684
C	-6.551470	-0.760220	-2.185113
C	-5.313723	-0.605498	-1.569675
C	-5.147236	0.301328	-0.525508
H	-8.591865	-0.104387	-2.179767
H	-6.681071	-1.463038	-3.000831
C	-3.011431	-0.564927	-0.663741

C	-1.214422	0.008507	0.861817
C	-1.844401	1.409087	0.835164
C	-3.356356	1.283616	0.940994
H	-3.842886	2.238761	0.725654
S	-3.805897	-1.423563	-1.967238
N	-3.826792	0.317606	-0.057574
N	-1.766733	-0.778687	-0.260331
C	-1.240111	2.386882	1.867405
C	-1.920947	2.370988	3.240287
C	-1.243246	3.804231	1.291069
H	-0.190318	2.090794	2.000298
H	-1.997047	1.366934	3.666013
H	-1.348623	2.989256	3.937034
H	-2.928277	2.798845	3.181284
H	-0.685540	3.843819	0.351004
H	-2.267556	4.146520	1.101925
H	-0.783136	4.506936	1.991935
H	-1.603764	1.791602	-0.166909
H	-0.156777	0.149831	0.634964
C	-1.322078	-0.727920	2.179914
C	-0.239917	-0.681735	3.062940
C	-2.478205	-1.415732	2.556181
C	-0.323182	-1.281197	4.316375
H	0.674226	-0.173496	2.762476
C	-2.561875	-2.017080	3.809320
H	-3.315978	-1.496757	1.868181
C	-1.488650	-1.943985	4.694436
H	0.524110	-1.237425	4.992588
H	-3.464675	-2.548689	4.091415
H	-1.556295	-2.414169	5.669929
C	0.318286	-2.191415	-0.440639
H	0.449499	-1.865981	0.591920
C	1.630402	-1.982561	-1.209269
C	2.623929	-3.036464	-0.778789
F	3.837971	-2.851246	-1.322311
F	2.779256	-3.086450	0.553686
F	2.209079	-4.258802	-1.161662
O	-1.343132	-2.048354	-2.146763
C	-0.829310	-1.504796	-1.170218
H	-3.671429	0.943801	1.933034
C	5.455327	0.614288	-0.770439
C	5.305954	-0.168862	0.375916
C	6.304453	-0.359898	1.317642
C	7.506902	0.294433	1.061250

C	7.683627	1.089312	-0.083387
C	6.666372	1.262642	-1.016038
C	3.480445	-0.183287	-0.797385
H	6.154776	-0.978141	2.194985
H	8.326831	0.186112	1.763246
H	8.639709	1.577249	-0.241302
H	6.800808	1.873092	-1.902265
N	4.270476	0.565559	-1.500922
C	1.144443	0.390696	-1.350096
O	-0.058812	0.047983	-1.739570
C	-6.206741	1.069652	-0.051357
H	-6.077838	1.765017	0.770156
H	-8.288157	1.491143	-0.316574
C	2.098767	-0.548433	-1.073566
H	1.427453	-2.195257	-2.268863
C	1.341178	1.863713	-1.177275
C	2.044197	2.396655	-0.090986
C	0.749433	2.734376	-2.097520
C	2.191125	3.773904	0.045746
H	2.472988	1.727921	0.651552
C	0.909001	4.111350	-1.968826
H	0.177016	2.315602	-2.919105
C	1.636524	4.633927	-0.901022
H	2.736645	4.175952	0.893628
H	0.464321	4.777670	-2.701247
H	1.758082	5.707562	-0.797674
H	0.046877	-3.250477	-0.431085
O	4.038795	-0.667680	0.365124

Vibrational frequencies

-122.0724	-3.6457	11.9388
24.1795	30.8677	34.0840
40.0383	50.9117	58.8252
63.0263	63.6760	77.4216
79.1836	85.6544	99.0858
100.3088	109.9366	121.3259
133.8599	141.6733	163.1237
167.5682	183.9889	187.1807
209.6097	217.8964	222.6944
238.8562	251.1316	253.5739
259.8567	271.9790	274.3214
281.2085	285.9244	291.3713
306.4324	314.0616	328.1999
337.6059	356.6419	369.5107
382.8219	410.7897	414.6989

419.0216	420.4278	425.6395
434.1558	443.9954	445.4785
467.0314	475.7394	483.3983
492.1571	508.7629	514.9370
519.7095	550.6282	553.9211
560.0721	566.8438	586.1004
594.7457	597.5372	615.8906
625.6431	627.6671	629.2265
635.1078	638.2982	649.5166
671.8909	679.5490	683.7411
713.2920	721.0035	723.0168
727.2691	734.1537	743.5558
752.1648	767.2030	771.7395
776.1060	788.9176	789.6931
808.2444	822.8358	831.7996
843.0605	863.3851	872.0905
875.2565	879.1961	881.3211
886.2365	904.6793	923.5868
933.9966	944.2990	950.8537
955.8132	962.6217	966.0969
970.2939	978.8501	1002.7005
1003.6779	1007.6317	1009.1152
1012.3873	1014.1230	1018.4805
1020.8242	1021.3431	1026.7636
1029.4607	1034.7519	1038.5659
1051.0710	1066.1848	1067.1769
1070.7017	1074.7551	1092.2682
1107.2710	1118.1206	1124.0005
1126.6880	1135.8887	1139.9395
1147.1297	1157.5826	1161.8773
1170.1052	1175.5317	1178.0522
1185.7650	1187.6437	1190.7557
1203.7566	1212.6279	1215.6168
1218.9883	1223.3407	1248.9863
1251.2706	1260.6809	1265.6863
1292.6924	1300.1701	1305.9227
1308.1066	1314.9335	1322.4945
1323.9961	1331.2226	1334.5053
1347.3603	1357.7836	1358.2751
1362.4621	1365.0994	1368.1982
1374.6165	1382.1065	1393.4854
1395.7423	1410.0352	1414.0142
1416.1840	1423.2081	1434.8221
1435.5435	1447.3253	1489.9868

1494.2288	1495.3696	1499.8677
1505.2011	1506.1190	1509.9068
1518.1001	1519.4691	1521.0338
1533.1913	1533.5489	1544.5086
1557.8269	1609.2748	1644.9841
1650.6271	1675.7601	1680.0641
1681.2238	1691.9068	1692.3746
1692.8876	1700.5318	1706.2623
1726.6074	3055.2787	3059.8237
3064.3632	3065.5784	3068.9995
3093.5346	3117.8395	3134.6012
3139.0011	3150.0911	3157.2016
3160.1911	3161.0052	3178.2334
3184.6231	3199.2032	3199.5956
3209.6444	3211.7647	3214.2597
3214.6509	3218.1150	3221.0860
3222.1307	3223.9043	3226.3228
3229.3398	3230.9703	3234.2191
3235.5973	3237.3521	3249.3929

PA'

Zero-point correction= 0.279079

Thermal correction to Energy= 0.299175

Thermal correction to Enthalpy= 0.300119

Thermal correction to Gibbs Free Energy= 0.228675

Sum of electronic and zero-point Energies= -1310.469012

Sum of electronic and thermal Energies= -1310.448916

Sum of electronic and thermal Enthalpies= -1310.447972

Sum of electronic and thermal Free Energies= -1310.519416

Cartesian coordinates

C	0.518514	2.883357	0.005724
H	0.419165	3.064878	1.083602
C	-0.731848	2.125692	-0.491673
C	-1.889984	2.617317	0.366959
F	-3.076099	2.142626	-0.020718
F	-1.725335	2.264397	1.654464
F	-1.965682	3.958477	0.332040
C	1.852620	2.190015	-0.122875
C	2.861443	-0.103207	-0.017349
C	2.277863	-1.361487	-0.097547
C	3.004279	-2.529955	-0.068062
C	4.392086	-2.384335	0.046721
C	4.988223	-1.126213	0.125990
C	4.232093	0.051186	0.096715

C	0.599988	0.083098	-0.202966
H	2.523042	-3.497978	-0.133605
H	5.013063	-3.272656	0.071609
H	6.066649	-1.053310	0.211765
H	4.682091	1.032711	0.154486
N	1.788176	0.805891	-0.062971
C	-1.740769	-0.201764	-0.931095
O	-2.414734	0.224272	-1.856683
C	-2.047958	-1.525813	-0.312311
C	-2.728185	-2.476458	-1.077727
C	-1.744114	-1.794040	1.024689
C	-3.079479	-3.698236	-0.517242
H	-2.971061	-2.240389	-2.108717
C	-2.112283	-3.010669	1.589683
H	-1.240794	-1.038685	1.621265
C	-2.772768	-3.964488	0.817529
H	-3.596675	-4.441751	-1.114682
H	-1.887385	-3.214411	2.631325
H	-3.054343	-4.915933	1.257698
C	-0.619725	0.619214	-0.407709
H	-0.975120	2.410012	-1.521442
H	0.607645	3.857279	-0.474167
O	2.915558	2.766923	-0.173806
O	0.904245	-1.238669	-0.206403

Vibrational frequencies

25.0340	33.7757	44.3294
53.8561	66.2296	91.1941
99.0657	102.6308	148.8076
154.2788	171.2558	205.6131
227.4666	257.6593	268.4069
284.2093	301.0965	327.1850
345.5652	406.0192	420.3005
426.6168	433.1470	445.9840
470.7713	506.0282	537.1843
555.7317	562.9851	571.3732
588.4020	624.6474	629.5344
647.8906	672.7968	686.7470
701.8904	708.8983	715.1824
730.0994	737.9600	765.5939
777.4201	824.2813	835.8923
868.6373	885.1222	888.6215
893.3502	937.3650	964.9506
966.4500	972.1235	1013.9112
1015.5780	1018.7258	1033.8361

1040.6056	1046.1538	1065.6201
1076.7241	1118.4688	1127.3399
1170.9452	1176.0953	1176.5013
1189.1575	1198.1986	1202.2717
1221.0420	1246.8430	1268.2474
1280.1822	1300.4232	1313.5793
1331.4307	1340.8188	1343.9231
1353.0873	1363.3053	1378.9307
1411.5222	1419.8092	1429.8992
1465.4029	1502.2268	1531.2978
1536.8777	1546.3038	1674.9500
1695.1163	1698.0287	1716.0584
1755.1880	1786.0013	1850.1089
3085.4391	3112.7044	3184.3754
3204.9155	3210.2007	3219.8053
3232.1920	3235.9663	3244.0636
3245.2979	3254.3050	3273.9605

PB'

Zero-point correction= 0.279487

Thermal correction to Energy= 0.299367

Thermal correction to Enthalpy= 0.300312

Thermal correction to Gibbs Free Energy= 0.229366

Sum of electronic and zero-point Energies= -1310.466297

Sum of electronic and thermal Energies= -1310.446416

Sum of electronic and thermal Enthalpies= -1310.445472

Sum of electronic and thermal Free Energies= -1310.516417

Cartesian coordinates

C	-2.864961	-1.771277	0.202024
H	-2.750962	-1.756744	1.293175
C	-1.479441	-1.741475	-0.441588
C	-0.650450	-2.880785	0.119779
F	0.551721	-2.958074	-0.468297
F	-0.454000	-2.753203	1.438652
F	-1.269256	-4.053071	-0.082842
O	-4.856916	-0.555578	-0.384667
C	-3.678627	-0.563556	-0.172312
C	2.624220	0.111103	-0.874972
C	2.639714	-0.418409	0.415590
C	3.796563	-0.654487	1.141934
C	4.983914	-0.327245	0.494951
C	4.996438	0.207178	-0.805632
C	3.822375	0.435476	-1.512323
C	0.612992	-0.233588	-0.301675

H	3.772795	-1.067646	2.143062
H	5.925930	-0.489771	1.007484
H	5.949516	0.444111	-1.266145
H	3.827042	0.845771	-2.515780
N	1.297479	0.208795	-1.300108
C	-1.633157	0.698660	-0.089448
O	-3.005794	0.625690	-0.210576
C	-0.849278	-0.384316	-0.215961
H	-1.550994	-1.937048	-1.519606
C	-1.195576	2.095258	0.119161
C	-0.092029	2.394675	0.926429
C	-1.909287	3.134002	-0.488635
C	0.306618	3.715154	1.098697
H	0.438307	1.599119	1.440404
C	-1.503815	4.452495	-0.314904
H	-2.774410	2.901885	-1.099865
C	-0.394187	4.745374	0.475019
H	1.160040	3.940227	1.729368
H	-2.055115	5.252317	-0.797845
H	-0.080621	5.775188	0.611414
H	-3.431835	-2.658342	-0.076152
O	1.342660	-0.634728	0.783596

Vibrational frequencies

30.7689	33.3204	49.6999
51.8505	65.8995	82.2984
95.2475	111.4696	135.6000
157.9839	184.5156	196.0817
232.2897	239.2554	277.9257
282.3320	306.8302	348.4566
375.5917	382.4596	416.0384
419.8338	458.5781	477.4310
495.7278	514.8638	552.2086
559.7979	571.9933	594.8032
626.3784	627.5752	636.0531
648.9301	663.6798	681.6322
713.0853	717.7869	738.9134
768.2953	775.8036	789.3483
803.3855	834.8514	858.8402
887.0174	887.5634	898.1264
905.8405	958.5566	963.4547
971.4978	973.8928	1013.0801
1014.7185	1016.7844	1034.4235
1036.2497	1040.4016	1070.2157
1075.0199	1116.5742	1127.3106

1136.6582	1167.2252	1182.9714
1185.2223	1196.6058	1206.7325
1212.7884	1242.7758	1257.6959
1289.0501	1300.0117	1312.3282
1315.0734	1330.7948	1337.3647
1346.9128	1349.7989	1366.0090
1382.8454	1402.5243	1432.0224
1472.9970	1502.1895	1506.4380
1538.7952	1552.3672	1667.8541
1672.3241	1698.2940	1700.8046
1713.5305	1760.5854	1924.9544
3078.7138	3091.6022	3199.4393
3209.1848	3212.0269	3224.4765
3227.9674	3231.6856	3232.7072
3240.3793	3243.8676	3247.4208

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