

Supporting Information for
**Origin of Stereoselectivity in NHC-Catalyzed Desymmetrization of
Pseudo-Para-Substituted [2.2]Paracyclophane Dialdehydes Toward
Planar Chirality**

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Part 1: Computational details

All theoretical calculations were performed using density functional theory (DFT) as implemented in the Gaussian 16 software. Geometry optimizations were carried out in dichloromethane (DCM) using the IEF-PCM solvation model at the M06-2X/6-31G(d, p) level. Harmonic vibrational frequency calculations at the same level confirmed that all intermediates correspond to true local minima with no imaginary frequencies, whereas each transition state possesses one imaginary frequency. Based on the geometries optimized at the M06-2X/6-31G(d, p)/IEF-PCM_(DCM) level, single-point energy calculations were further performed at the M06-2X/6-311+G(d, p)/IEF-PCM_(DCM) level to refine the energies. Notably, several additional computational levels were also examined, including M06-2X/6-311++G(d, p)/IEF-PCM_(DCM)//M06-2X/6-31G(d, p)/IEF-PCM_(DCM) (L1), B3LYP-D3/6-311+G(d, p)/IEF-PCM_(DCM)//B3LYP-D3/6-31G(d, p)/IEF-PCM_(DCM) (L2), B3LYP-D3/6-311++G(d, p)/IEF-PCM_(DCM)//B3LYP-D3/6-31G(d, p)/IEF-PCM_(DCM) (L3), ω B97X-D/6-311+G(d, p)/IEF-PCM_(DCM)// ω B97X-D/6-31G(d, p)/IEF-PCM_(DCM) (L4), and ω B97X-D/6-311++G(d, p)/IEF-PCM_(DCM)// ω B97X-D/6-31G(d, p)/IEF-PCM_(DCM) (L5). As summarized in **Table S1**, only minor differences were observed among the relative Gibbs free energy barriers obtained at different computational levels, indicating that the selected methods are appropriate and reliable for this reaction system. Non-covalent interaction (NCI) and atoms-in-molecules (AIM) analyses were carried out using Multiwfn, the results were visualized with VMD, and the three-dimensional (3D) molecular structures were rendered using CYLView20 software¹.

Table S1. Comparisons of relative Gibbs free energies (GFE) for selected stationary points at different levels (L1–L5, unit: kcal/mol). $\Delta\Delta G^\ddagger_1$ is defined as the Gibbs free energy barrier of S_p -TS2 minus that of R_p -TS2.

Method	L1	L2	L3	L4	L5
$\Delta\Delta G^\ddagger_1$	1.5	1.3	1.3	0.9	1.5

In addition, the extent of enantioselectivity, in terms of enantiomeric excess (*ee*), was calculated by using the Boltzmann distribution of diastereomeric transition states with the following equation. (For convenient comparison with the experimental data, the calculated *ee* values were converted into enantiomeric ratio (*er*) according to Equation (3).)

$$\frac{[R_p]}{[S_p]} = \frac{\exp(-\Delta G^\ddagger_{[R_p]}/RT)}{\exp(-\Delta G^\ddagger_{[S_p]}/RT)} = \exp(\Delta\Delta G^\ddagger_{[S_p]-[R_p]}/RT) \quad (1)$$

$$ee = \frac{[S_p] - [R_p]}{[S_p] + [R_p]} \times 100\% = \frac{\frac{[R_p]}{[S_p]} - 1}{\frac{[R_p]}{[S_p]} + 1} \times 100\% \quad (2)$$

$$er = \frac{1 + ee}{1 - ee} \times 100\% \quad (3)$$

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

Part 2: Conformation search for key transition states

The conformational sampling of key transition states was performed at the GFN2-xTB level of theory using the CREST program (version 2.12) developed by Grimme and co-workers. Conformers and rotamers were generated through iterative metadynamics based on the genetic Z-matrix crossing algorithm (iMTD-GC) to comprehensively explore the low-energy conformational space. From each CREST sampling result, the lowest-energy conformers were selected and further optimized at the density functional theory (DFT) level. The conformer with the lowest DFT energy was then used as the representative transition state for full mechanistic investigations and for constructing the final Gibbs free energy profile on the potential energy surface (PES), ensuring the reliability and accuracy of the computational results.

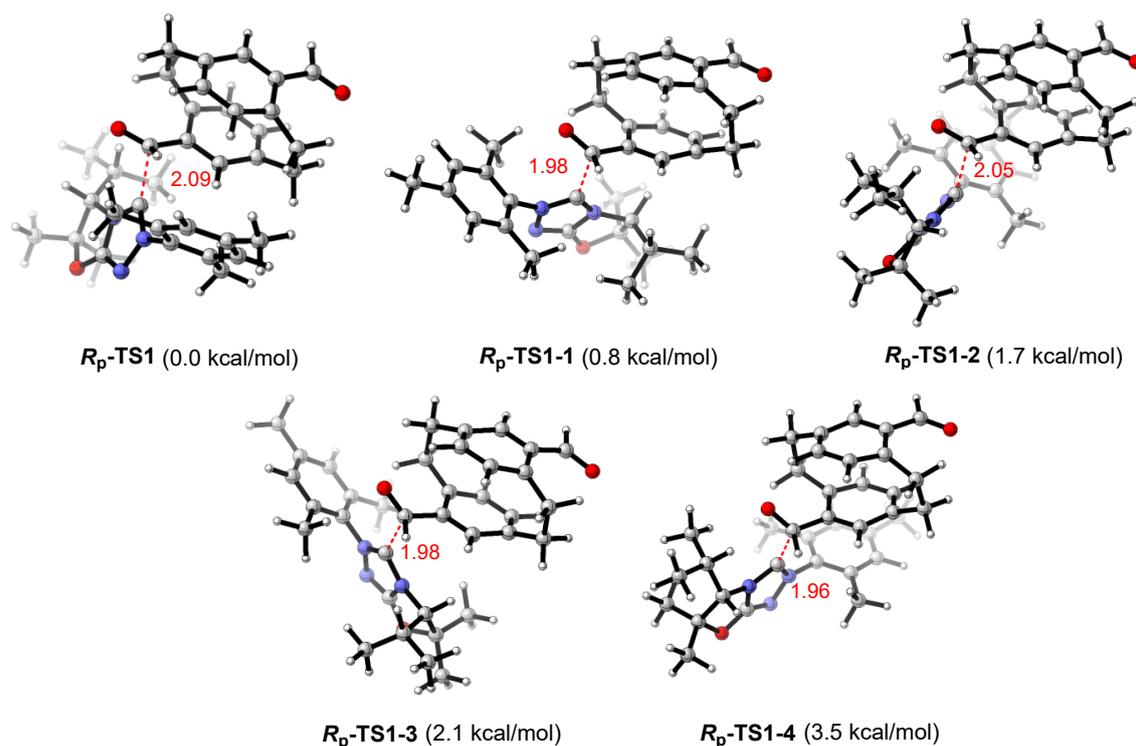


Figure S1. Conformational search for R_p -TS1s including R_p -TS1 and R_p -TS1- n ($n=4$) and relative energies. Blue, red, gray and white respectively represent nitrogen, oxygen, carbon and hydrogen atom.

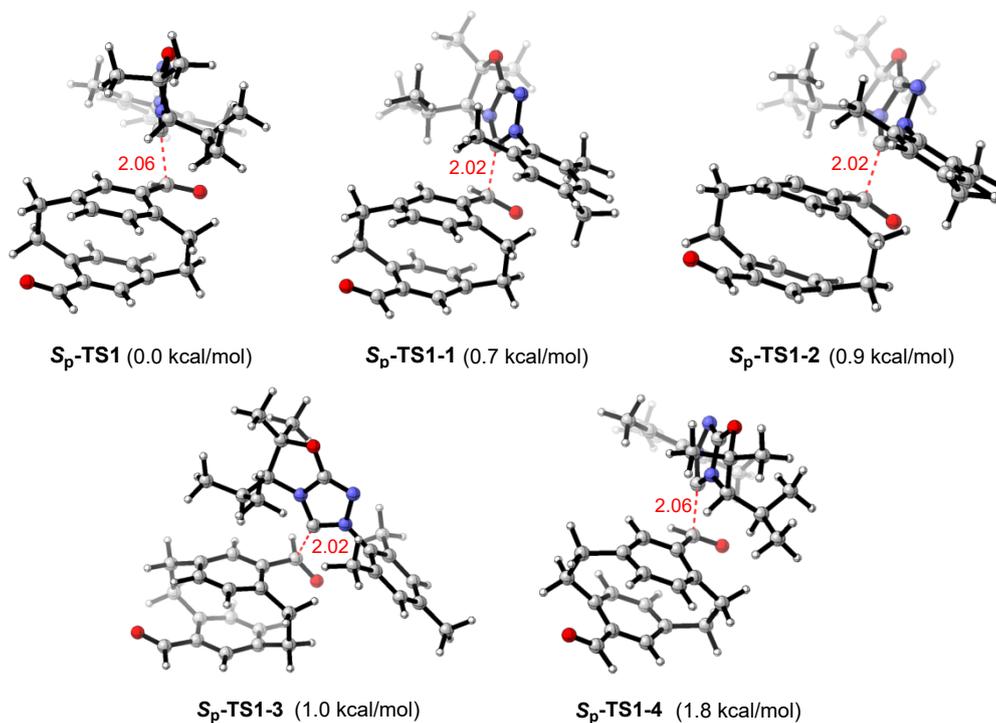


Figure S2. Conformational search for S_p -TS1s including S_p -TS1 and S_p -TS1- n ($n=4$) and relative energies. Blue, red, gray and white respectively represent nitrogen, oxygen, carbon and hydrogen atom.

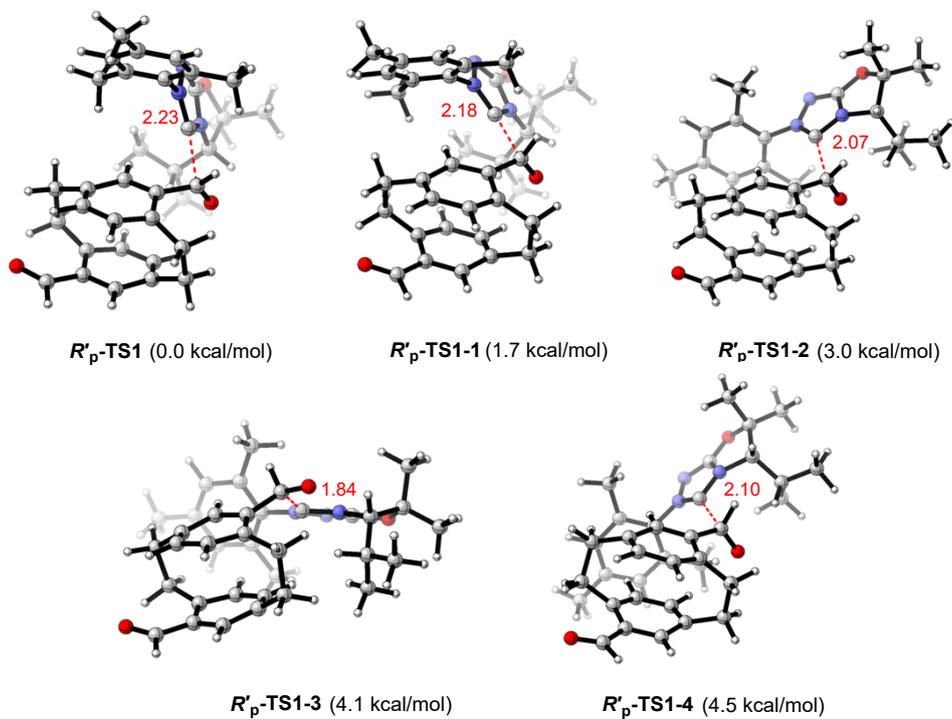


Figure S3. Conformational search for R'_p -TS1s including R'_p -TS1 and R'_p -TS1- n ($n=4$) and relative energies. Blue, red, gray and white respectively represent nitrogen, oxygen, carbon and hydrogen atom.

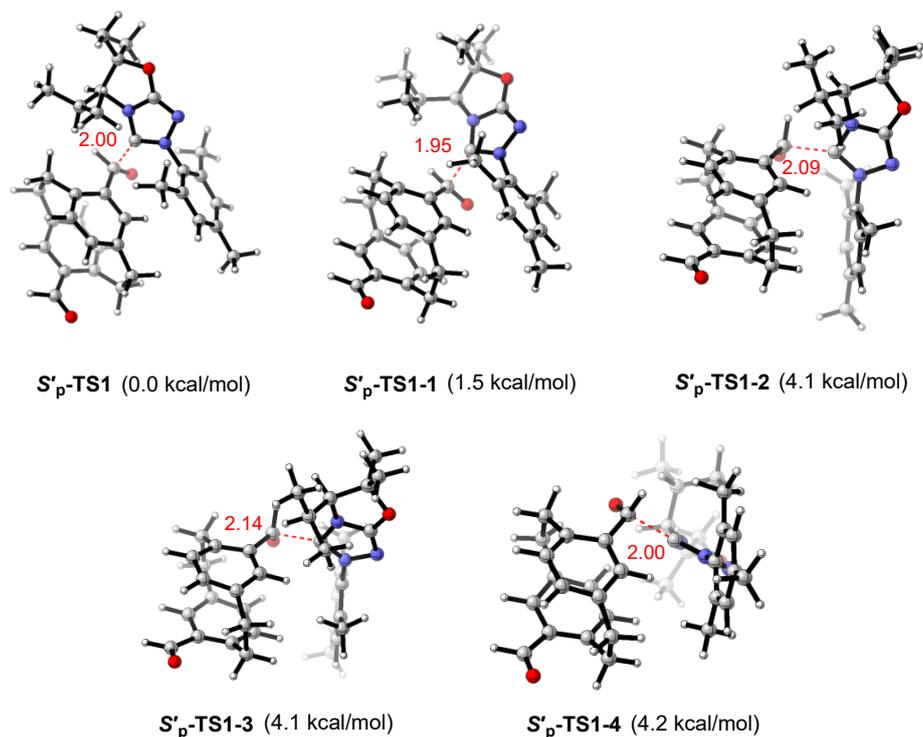


Figure S4. Conformational search for S'_p -TS1s including S'_p -TS1 and S'_p -TS1- n ($n=4$) and relative energies. Blue, red, gray and white respectively represent nitrogen, oxygen, carbon and hydrogen atom.

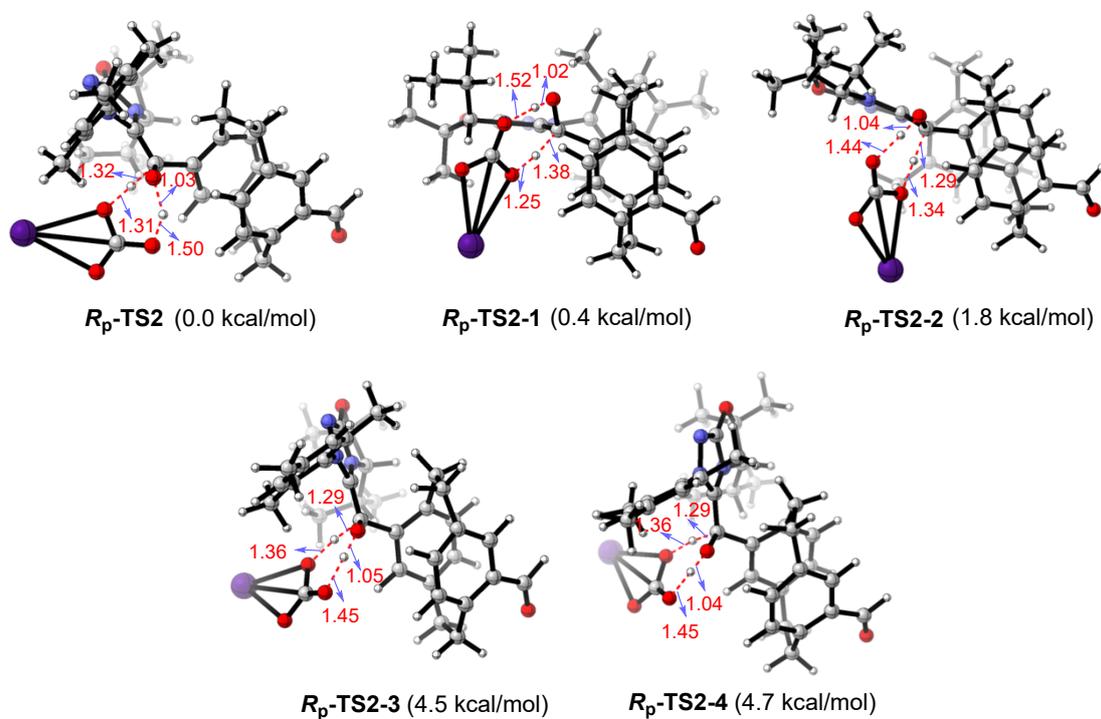


Figure S5. Conformational search for R_p -TS2s including R_p -TS2 and R_p -TS2- n ($n=4$) and relative energies. Blue, red, gray, white and purple respectively represent nitrogen, oxygen, carbon and hydrogen and cesium atom.

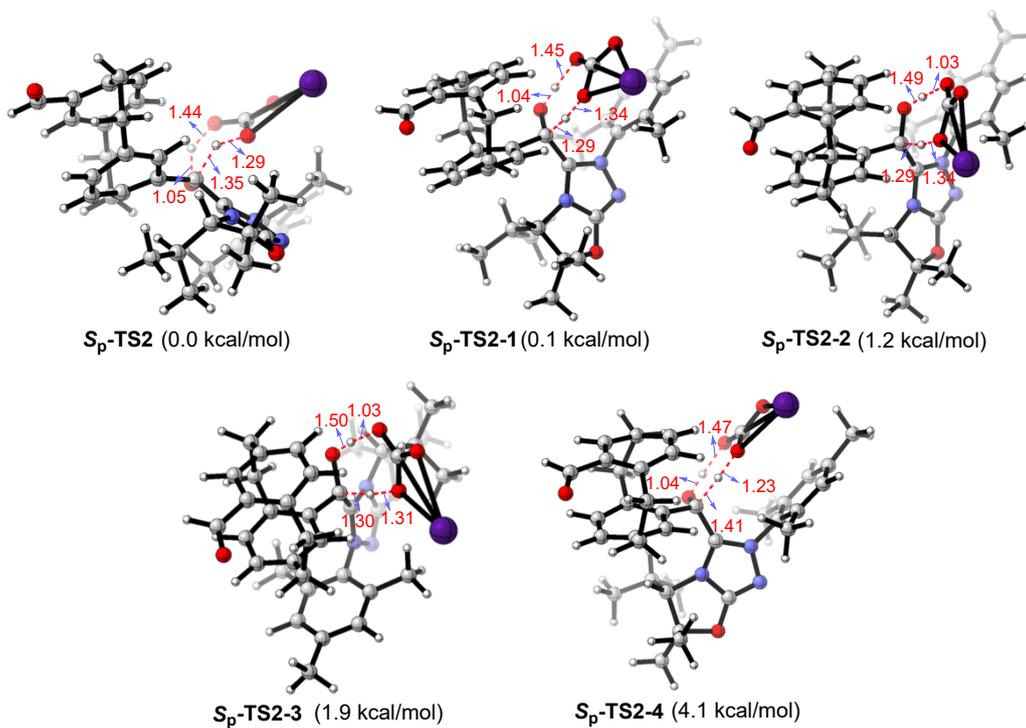


Figure S6. Conformational search for S_p -TS2s including S_p -TS2 and S_p -TS2- n ($n=4$) and relative energies. Blue, red, gray, white and purple respectively represent nitrogen, oxygen, carbon and hydrogen and cesium atom.

Part 3: Possible nucleophilic attack reaction pathways to **R1** by NHC

As shown in **Figure S7**, since planar chirality is established in the first bond-forming step, the NHC can nucleophilically attack either the *Re/Si*-face or the *Re'/Si'*-face of the given aldehyde of substrate **R1**, giving rise to four possible mechanistic pathways corresponding to transition states **R_p-TS1** ($\Delta G^\ddagger = 14.5$ kcal/mol), **S_p-TS1** ($\Delta G^\ddagger = 15.7$ kcal/mol), **R'_p-TS1** ($\Delta G^\ddagger = 16.2$ kcal/mol) and **S'_p-TS1** ($\Delta G^\ddagger = 17.5$ kcal/mol). The calculated results indicate that **R_p-TS1** and **S_p-TS1** feature relatively lower free energy barriers, rendering their associated reaction pathways thermodynamically more favorable. Therefore, subsequent mechanistic investigations mainly focus on these two pathways in the main text.

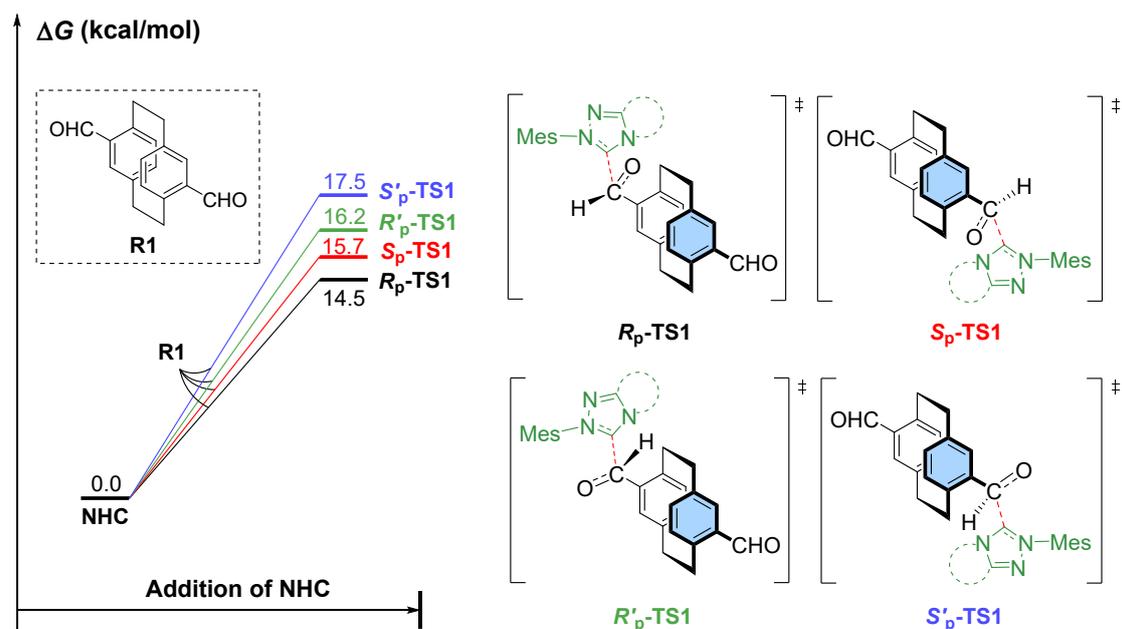


Figure S7. Possible nucleophilic attack pathways to **R1** by NHC.

As depicted in **Figure S8**, a two-dimensional (2D) representation of the transition-state structures along the R'_p -TS1 and S'_p -TS1 pathways is presented, illustrating the stereochemical differences in the nucleophilic attack of the NHC on the aldehyde carbonyl carbon. The green fragments correspond to the NHC catalyst, the gray moieties indicate the reactive sites of the [2.2]PCP dialdehyde substrate, and the red dashed lines denote the key directions of nucleophilic attack.

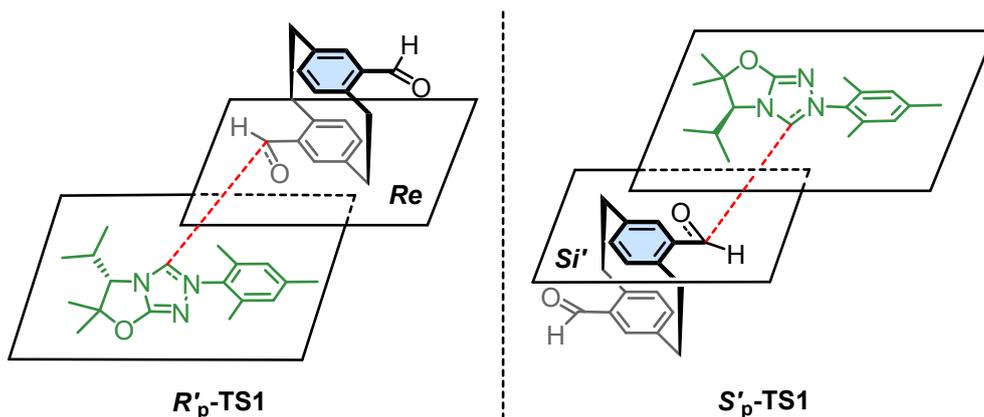


Figure S8. Stereochemical possibilities of the NHC nucleophilic attack on the carbonyl carbon in R'_p -TS1 and S'_p -TS1 from 2D structural perspective.

Part 4: Intrinsic reaction coordinate (IRC) results of key transition states

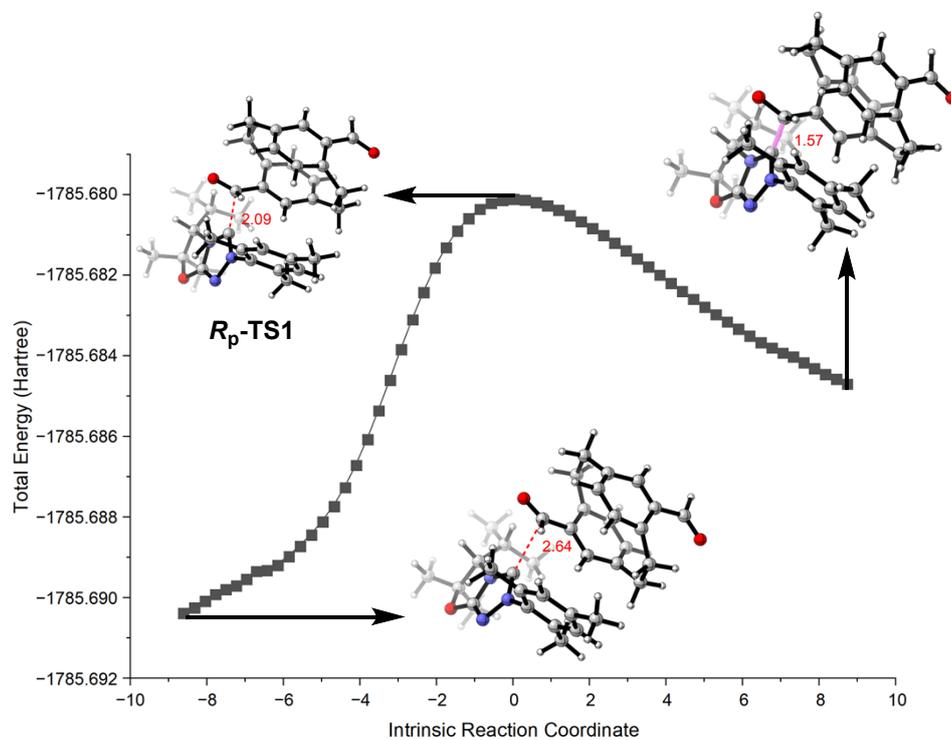


Figure S9. IRC results of R_p -TS1.

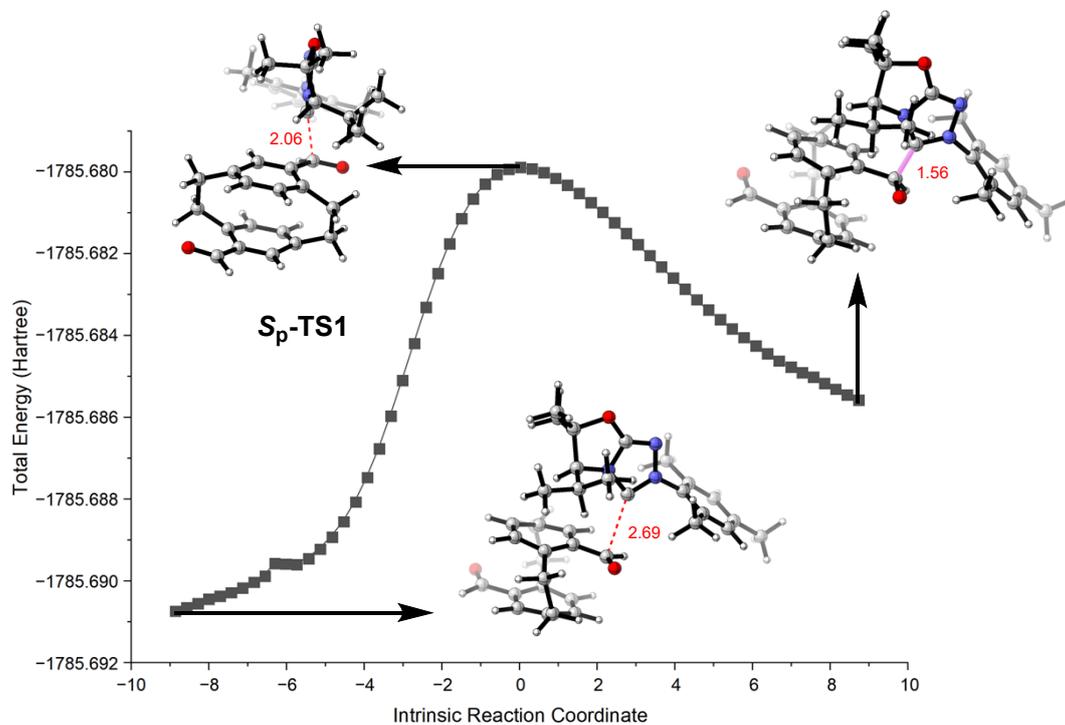


Figure S10. IRC results of S_p -TS1.

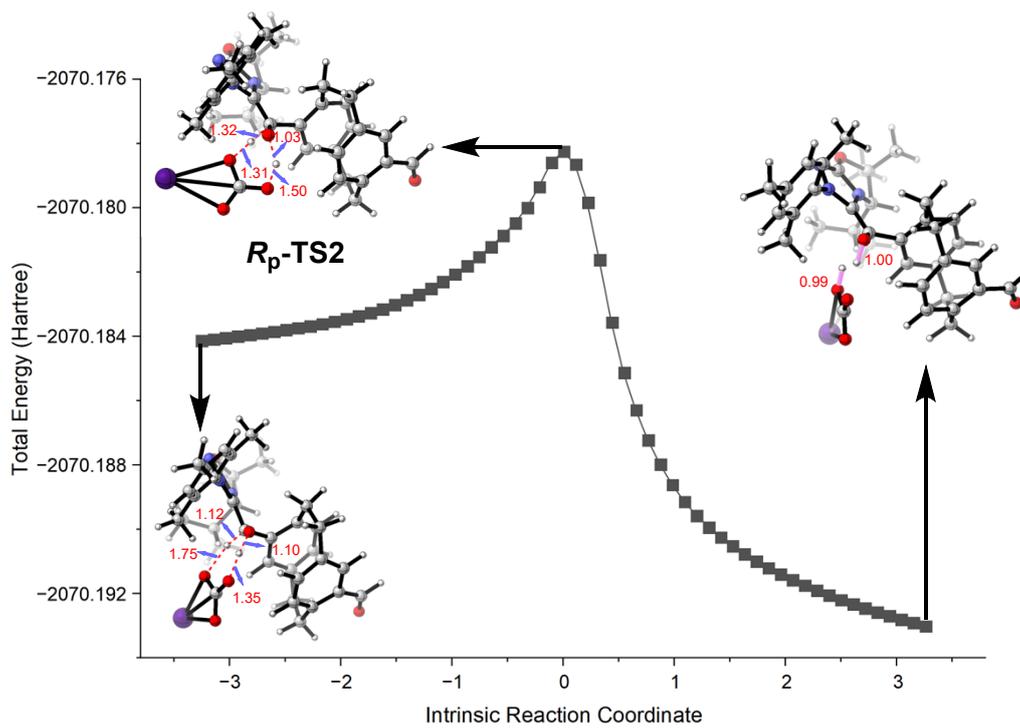


Figure S11. IRC results of R_p -TS2.

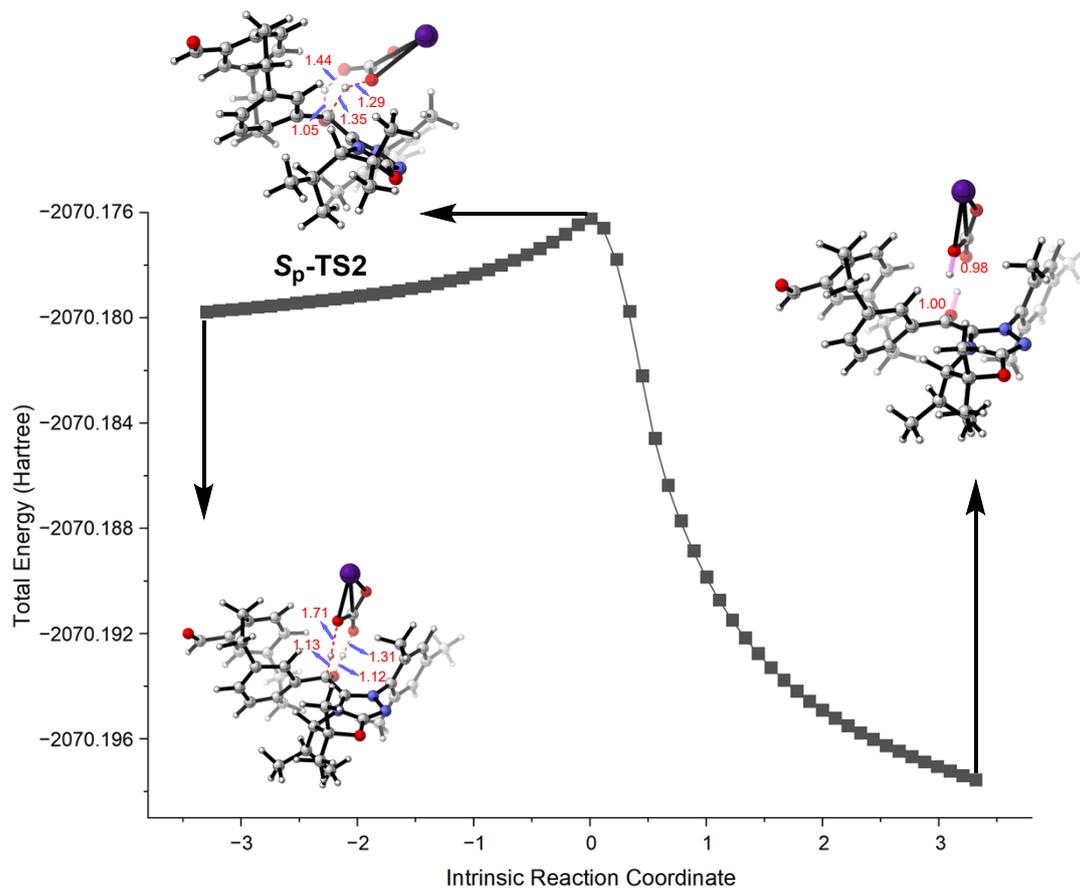


Figure S12. IRC results of S_p -TS2.

Part 5: Distortion-interaction analysis in the first step of the desymmetrization stage

Table S2. Distortion-interaction analysis in the first step of the desymmetrization stage. (unit: kcal/mol).

	R_p -TS1	S_p -TS1	R'_p -TS1	S'_p -TS1
$\Delta E_{\text{dist(R1)}}$	9.4	10.9	11.5	13.3
$\Delta E_{\text{dist(NHC)}}$	1.9	1.1	1.5	0.8
ΔE_{int}	-3.9	-3.7	-2	0.2

Part 6: Possible nucleophilic attack reaction pathways to **R2** by NHC

As shown in **Figure S13**, nucleophilic attack by NHC on the carbonyl carbon can occur from either the *Re*- or *Si*- face for substrate **R2**, leading to the formation of a new stereogenic center through transition states **TS1-Re** ($\Delta G^\ddagger = 10.2$ kcal/mol) and **TS2-Si** ($\Delta G^\ddagger = 12.2$ kcal/mol), respectively. The *Re*-face attack is kinetically favored. Based on this, we compared the most energetically favorable nucleophilic addition pathway for **R2** with the corresponding attack pathways by NHC for **R1**. More discussions can be found in the main text.

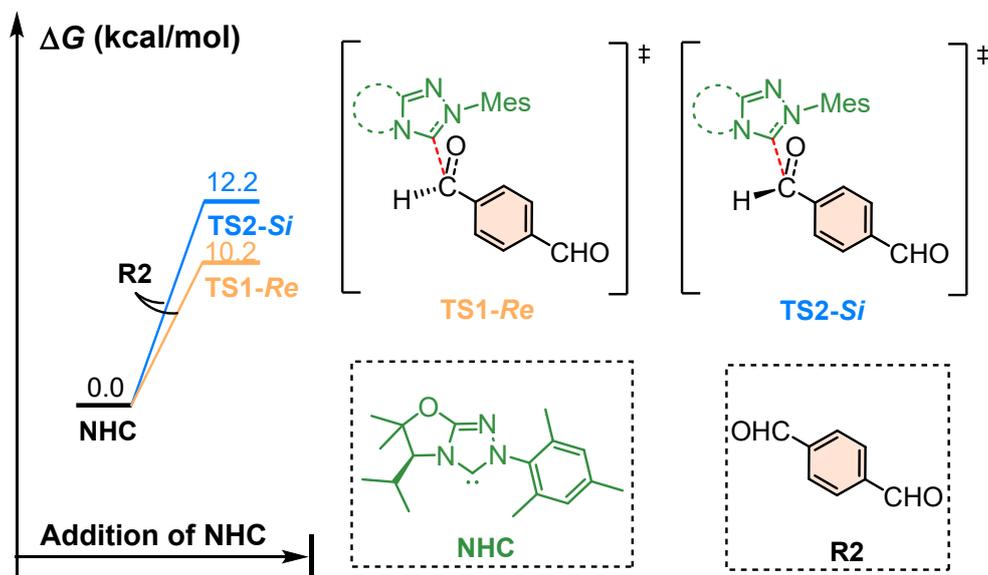


Figure S13. Possible nucleophilic attack pathways to **R2** by NHC.

Part 7: Global reactivity index (GRI), Fukui function, and Parr function analyses of substrates R1 and R2

Table S3. GRI analyses of substrates **R1** and **R2**.

Sub	E_H (a.u.)	E_L (a.u.)	μ (a.u.)	η (a.u.)	ω (a.u.)
R1	-0.28	-0.04	-0.16	0.24	0.11
R2	-0.32	-0.06	-0.19	0.27	0.14

Table S4. Fukui function analyses of substrates **R1-C1** and **R2-C2**.

Sub	f^+
R1-C1	0.07
R2-C2	0.10

Table S5. Parr function analyses of substrates **R1-C1** and **R2-C2**.

Sub	P_k^+
R1-C1	0.13
R2-C2	0.24

Part 8: Energies, Cartesian coordinates, and vibrational frequencies of all the stationary points

NHC

Zero-point correction= 0.406728

Thermal correction to Energy= 0.429172

Thermal correction to Enthalpy= 0.430116

Thermal correction to Gibbs Free Energy= 0.354580

Sum of electronic and zero-point Energies= -939.632384

Sum of electronic and thermal Energies= -939.609941

Sum of electronic and thermal Enthalpies= -939.608996

Sum of electronic and thermal Free Energies= -939.684533

Cartesian coordinates

C	-1.160384	-0.703075	-0.721262
C	-0.124202	0.189730	1.063838
N	-1.327581	-0.194999	0.529288
N	0.686903	-0.182388	0.048296
N	0.078326	-0.746247	-1.086653
C	2.110616	-0.052675	0.043705
C	2.890066	-1.186209	0.289058
C	4.276695	-1.041254	0.268599
C	4.878957	0.192709	0.015860
C	4.063630	1.299330	-0.228525
C	2.672593	1.198522	-0.223216
H	4.900609	-1.911917	0.456545
H	4.521135	2.263892	-0.435428
C	2.234575	-2.511697	0.569292
H	1.520571	-2.420103	1.393756
H	1.673770	-2.860395	-0.302754

H	2.978523	-3.265521	0.831926
C	6.379752	0.332978	0.033001
H	6.734812	0.569253	1.041408
H	6.866923	-0.593724	-0.278797
H	6.709026	1.137039	-0.629065
C	1.792635	2.388436	-0.499194
H	1.126194	2.187711	-1.344407
H	1.158884	2.610090	0.364425
H	2.393047	3.269521	-0.731631
C	-2.745588	0.017103	0.803831
C	-3.331406	-0.981716	-0.260153
O	-2.305154	-1.018684	-1.324536
C	-4.644793	-0.626442	-0.924167
H	-4.884002	-1.395823	-1.662337
H	-5.443375	-0.607650	-0.179269
H	-4.605732	0.337985	-1.429125
C	-3.389536	-2.381828	0.342911
H	-4.173009	-2.426255	1.103529
H	-3.614810	-3.111101	-0.438017
H	-2.436606	-2.646093	0.810271
C	-3.052042	1.525724	0.747141
C	-2.610019	2.194208	-0.557093
H	-1.536193	2.065935	-0.724805
H	-3.137571	1.799505	-1.429592
H	-2.810250	3.267693	-0.505499
C	-4.499506	1.861033	1.114118
H	-4.575665	2.920804	1.370587
H	-5.189477	1.675369	0.288534
H	-4.837716	1.281923	1.979301
H	-2.999831	-0.355918	1.800655

H -2.413817 1.933435 1.543100

Vibrational frequencies

15.7597	28.6817	34.1413
51.5813	80.2348	85.0438
109.7012	118.5774	147.1485
164.0532	172.8572	190.2200
196.9340	214.8026	223.3655
235.9158	247.8786	264.0687
276.2424	283.5371	299.1154
307.4033	314.5317	325.8549
344.6910	369.0584	400.3985
415.7872	445.2416	462.7460
505.8046	525.0937	532.9938
556.7829	571.4200	587.5864
602.4153	628.7256	652.3025
670.1532	743.8566	759.4122
777.9708	810.6085	854.8244
874.3319	885.7539	915.1316
916.6332	938.9267	949.1149
961.4354	966.7687	979.5877
982.1717	993.8438	1000.6507
1035.1549	1035.7346	1037.6449
1061.4329	1063.1755	1066.1893
1068.6504	1076.8027	1109.7143
1159.2977	1170.3500	1198.9407
1214.4337	1229.0628	1246.8824
1265.1923	1278.8830	1291.6568
1315.3847	1332.2748	1344.4264
1350.7154	1359.7094	1381.4287

1398.6339	1413.4285	1415.9892
1417.7632	1418.7618	1426.6278
1428.1104	1436.5073	1443.3551
1464.0298	1480.6351	1483.1125
1483.5736	1486.9851	1489.3294
1493.6006	1495.5498	1497.4316
1499.7629	1504.9421	1506.2688
1509.2339	1521.1716	1522.4703
1524.7274	1566.3101	1680.5310
1694.9128	1734.4432	3056.3631
3073.3064	3074.9480	3076.3547
3077.1316	3079.4937	3081.1405
3096.2575	3113.5963	3140.1570
3143.4381	3144.4442	3151.4336
3151.9885	3161.2121	3164.7995
3168.2467	3168.9227	3173.5812
3174.0445	3174.4292	3178.5578
3200.4759	3202.5720	3204.8644

R1

Zero-point correction= 0.296348

Thermal correction to Energy= 0.312012

Thermal correction to Enthalpy= 0.312956

Thermal correction to Gibbs Free Energy= 0.254860

Sum of electronic and zero-point Energies= -845.338483

Sum of electronic and thermal Energies= -845.322819

Sum of electronic and thermal Enthalpies= -845.321875

Sum of electronic and thermal Free Energies= -845.379970

Cartesian coordinates

C	1.460407	1.210303	-0.462358
C	1.450020	0.096419	-1.328121
C	0.331891	-0.034553	-2.152534
H	0.312154	-0.830278	-2.893060
C	-0.837810	0.685491	-1.904314
H	-1.740828	0.435794	-2.456678
C	-0.917941	1.574857	-0.830118
C	0.289687	1.937916	-0.233681
H	0.296743	2.699999	0.545378
C	2.607414	1.550710	0.403105
C	2.417972	-1.060062	-1.198618
H	3.456844	-0.730443	-1.248665
H	2.236211	-1.738613	-2.036813
C	2.238039	-1.870978	0.156079
H	2.336544	-2.934826	-0.079339
H	3.052612	-1.599506	0.830647
C	0.917921	-1.574760	0.830432
C	-0.289605	-1.937994	0.233901
H	-0.296533	-2.700121	-0.545115
C	-1.460399	-1.210435	0.462445
C	-1.450216	-0.096554	1.328201
C	-0.332206	0.034535	2.152766
H	-0.312673	0.830222	2.893335
C	0.837583	-0.685355	1.904600
H	1.740547	-0.435561	2.457032
C	-2.607187	-1.550900	-0.403297
H	-2.480320	-2.499371	-0.965324
C	-2.418444	1.059640	1.198648
H	-2.237663	1.737852	2.037320
H	-3.457178	0.729477	1.247699

C	-2.237897	1.871350	-0.155609
H	-3.052664	1.600851	-0.830326
H	-2.335624	2.935111	0.080497
O	3.618096	0.891249	0.543187
O	-3.617312	-0.890860	-0.544677
H	2.480181	2.498513	0.966171

Vibrational frequencies

59.6900	86.2340	91.5267
128.6747	150.6968	160.3448
212.8406	222.3686	242.0088
246.0835	277.5863	290.6867
315.1576	330.0134	368.5342
376.3476	411.2605	425.8110
435.9766	461.6568	464.6257
493.2739	537.0108	551.4432
619.1469	658.0928	665.7840
681.6531	736.0685	736.8580
745.9094	753.8778	766.7225
806.2845	807.9060	833.8234
858.8571	889.1940	906.2090
921.7926	928.1061	938.0236
953.9603	973.6047	990.4955
998.0005	1008.7225	1012.7722
1042.6091	1043.8595	1134.5553
1153.6843	1177.8071	1179.4414
1195.5847	1199.3172	1219.9814
1221.4982	1223.8411	1231.6415
1271.0797	1275.8149	1288.1913
1291.1610	1314.7936	1330.8432

1343.2713	1346.6752	1362.7171
1364.6611	1434.6073	1436.7672
1469.8564	1471.1854	1480.2025
1484.0674	1499.5108	1501.9899
1550.3336	1550.7343	1639.7400
1642.7699	1683.4654	1685.9304
1828.4480	1829.5378	2969.7713
2970.1288	3093.2711	3093.3612
3100.7522	3101.4986	3154.3403
3154.3886	3167.3600	3167.4450
3177.5946	3177.6069	3197.6098
3197.7603	3212.3439	3212.4849

R_p-TS1

Zero-point correction= 0.704831

Thermal correction to Energy= 0.743485

Thermal correction to Enthalpy= 0.744429

Thermal correction to Gibbs Free Energy= 0.633838

Sum of electronic and zero-point Energies= -1784.975285

Sum of electronic and thermal Energies= -1784.936632

Sum of electronic and thermal Enthalpies= -1784.935688

Sum of electronic and thermal Free Energies= -1785.046279

Cartesian coordinates

C	-4.275028	-1.536751	0.104232
C	-3.952532	-0.163735	0.157649
C	-3.318725	0.276544	1.319834
H	-3.104101	1.337302	1.436625
C	-2.750018	-0.628296	2.220211
H	-2.125681	-0.249672	3.026469

C	-2.795351	-2.003728	1.980657
C	-3.699390	-2.431633	1.008227
H	-3.845933	-3.499044	0.843751
C	-5.047133	-2.143648	-0.997906
C	-3.989995	0.730091	-1.064919
H	-4.990586	0.794465	-1.496267
H	-3.690690	1.734564	-0.747171
C	-3.000611	0.249221	-2.209575
H	-2.548282	1.146980	-2.646429
H	-3.581312	-0.247112	-2.990134
C	-1.941728	-0.697625	-1.689066
C	-1.069830	-0.262566	-0.698361
H	-0.982158	0.806665	-0.500818
C	-0.462109	-1.134878	0.202592
C	-0.757933	-2.504193	0.140181
C	-1.401053	-2.957841	-1.022804
H	-1.583271	-4.024504	-1.136663
C	-1.981287	-2.076153	-1.931684
H	-2.596319	-2.465322	-2.740057
C	0.257175	-0.495506	1.374075
H	-0.222168	0.468310	1.650129
C	-0.724736	-3.406284	1.361956
H	-1.016829	-4.410776	1.039914
H	0.269967	-3.467821	1.804945
C	-1.720709	-2.932858	2.502642
H	-1.140399	-2.404417	3.262217
H	-2.150793	-3.826217	2.966642
O	-5.490237	-1.562775	-1.968579
O	0.882501	-1.147528	2.226183
H	-5.209570	-3.235745	-0.882915

C	3.737458	1.279090	-0.144881
C	1.676173	0.609451	0.307328
N	2.956961	0.207051	0.151991
N	1.781460	1.925794	0.078661
N	3.069066	2.388465	-0.217210
C	0.660086	2.815491	0.100105
C	-0.002864	3.083650	-1.101393
C	-1.174717	3.836168	-1.038139
C	-1.673429	4.312617	0.177834
C	-0.966435	4.037333	1.350204
C	0.211281	3.288764	1.335660
H	-1.717317	4.045790	-1.957167
H	-1.342347	4.409136	2.300174
C	0.506020	2.513089	-2.397679
H	0.403842	1.420795	-2.398291
H	1.565457	2.742131	-2.540356
H	-0.057979	2.910781	-3.243100
C	-2.938084	5.131259	0.216707
H	-3.640796	4.806767	-0.554482
H	-2.718627	6.188940	0.039095
H	-3.429406	5.052871	1.188877
C	0.973028	2.981190	2.598456
H	2.015630	3.299454	2.506972
H	0.982983	1.906123	2.808617
H	0.526071	3.493708	3.451568
C	3.755450	-1.003853	0.289101
C	5.077225	-0.517447	-0.410862
O	5.018946	0.967495	-0.289945
C	6.317848	-0.965060	0.332784
H	7.209816	-0.538179	-0.130855

H	6.394460	-2.054878	0.295408
H	6.273187	-0.651450	1.377857
C	5.163849	-0.791230	-1.903181
H	5.263210	-1.860913	-2.097976
H	6.046042	-0.283526	-2.299382
H	4.280526	-0.416256	-2.425657
C	3.002038	-2.264221	-0.166892
C	3.868250	-3.511002	0.018241
H	4.294249	-3.559706	1.025295
H	4.691500	-3.544587	-0.703463
H	3.263422	-4.408382	-0.135257
C	2.365920	-2.217226	-1.559138
H	1.611283	-3.006003	-1.622041
H	3.090872	-2.384396	-2.358595
H	1.849559	-1.268638	-1.739611
H	3.974896	-1.133679	1.356808
H	2.176889	-2.319607	0.556770

Vibrational frequencies

-117.4939	10.0753	18.8993
26.5775	29.4957	33.9732
44.2725	49.2570	58.7634
69.1090	79.6492	95.4762
97.6999	107.1345	116.1180
124.3834	133.4800	144.4402
145.8137	155.9602	169.9420
194.4164	197.0799	203.4458
212.4818	220.2105	222.9227
234.6799	241.5023	244.4492
253.5790	260.1336	264.9064

269.3528	279.5192	285.2318
289.0162	302.6899	308.3438
315.9463	323.5547	328.8444
330.9479	352.6625	363.1406
368.9099	370.0721	387.0942
412.1444	417.1771	426.1812
435.1849	446.8232	458.3778
465.8938	475.3987	491.9054
505.7868	524.0396	528.9284
541.2765	550.0083	561.0355
563.5920	571.3002	587.2655
597.4985	619.1716	641.3064
657.0829	657.7758	666.5218
679.7959	684.0350	733.0819
733.1775	737.7953	741.8119
752.0353	757.8777	768.3285
780.3251	801.9918	805.1743
809.8967	830.9665	852.3181
858.8363	878.3921	884.8762
888.2774	907.0482	912.4924
916.4946	924.8377	938.3555
946.2309	949.1694	953.9763
956.9924	962.8170	970.3062
978.4788	980.4918	981.0527
991.0669	992.3743	1001.2109
1009.0279	1012.0502	1020.1381
1023.4448	1036.4769	1039.0251
1043.1176	1060.5893	1063.1662
1066.4569	1068.7030	1084.2623
1116.2574	1127.6140	1131.2288

1147.5182	1154.4546	1172.3709
1172.7676	1177.7699	1192.4348
1199.8595	1200.0483	1217.3691
1220.3417	1223.1873	1232.2842
1233.5169	1236.3181	1261.0882
1262.7713	1271.2096	1278.0513
1283.7887	1286.8881	1293.4003
1311.3937	1320.5130	1331.5793
1333.7918	1342.1590	1345.6223
1347.0544	1353.1346	1361.1493
1363.4553	1368.2031	1390.1660
1403.2924	1406.5804	1415.4506
1416.1185	1419.7600	1421.6130
1426.1520	1429.5821	1434.1902
1438.5228	1440.3283	1454.4380
1461.1304	1464.0746	1469.5245
1474.9765	1480.6916	1480.8366
1485.8717	1487.3211	1488.2564
1492.3877	1493.8090	1495.0915
1495.3651	1496.6146	1498.0798
1498.9505	1505.4905	1512.7569
1514.9435	1515.7560	1519.1449
1524.6945	1546.9294	1548.8855
1563.3370	1639.0928	1641.8705
1666.7352	1677.2476	1683.0283
1689.8231	1693.8598	1723.1923
1830.0925	2925.7664	2965.2078
3064.4302	3064.6632	3069.0008
3072.7627	3074.0991	3074.6549
3076.7000	3079.4520	3085.6231

3085.8408	3086.4034	3090.6625
3094.4494	3137.0275	3138.4305
3140.2959	3146.7886	3148.0912
3151.2124	3152.2982	3155.0862
3159.2616	3167.4181	3168.1500
3169.8054	3173.5123	3175.5580
3175.6752	3176.7467	3176.8008
3178.0028	3181.0633	3184.2810
3186.4919	3187.4650	3200.0658
3204.1249	3204.2748	3204.6806

S_p-TS1

Zero-point correction= 0.704997

Thermal correction to Energy= 0.743638

Thermal correction to Enthalpy= 0.744582

Thermal correction to Gibbs Free Energy= 0.634818

Sum of electronic and zero-point Energies= -1784.974895

Sum of electronic and thermal Energies= -1784.936254

Sum of electronic and thermal Enthalpies= -1784.935310

Sum of electronic and thermal Free Energies= -1785.045074

Cartesian coordinates

C	-4.528620	-1.762407	0.007470
C	-3.520865	-2.538471	-0.602830
C	-2.545173	-3.062430	0.245840
H	-1.788717	-3.726801	-0.164897
C	-2.385028	-2.581726	1.546964
H	-1.510825	-2.883876	2.119465
C	-3.210918	-1.571539	2.045178
C	-4.368848	-1.301144	1.316132

H	-5.093868	-0.586199	1.704955
C	-5.687222	-1.217864	-0.727636
C	-3.307115	-2.573376	-2.100926
H	-4.201471	-2.902667	-2.632157
H	-2.507906	-3.291812	-2.304419
C	-2.885421	-1.163178	-2.700629
H	-2.107322	-1.344105	-3.448703
H	-3.748870	-0.734207	-3.213657
C	-2.413219	-0.202369	-1.632413
C	-1.270140	-0.481421	-0.886095
H	-0.547233	-1.208615	-1.261596
C	-1.100029	-0.013243	0.416171
C	-2.110006	0.764053	1.010575
C	-3.087602	1.285943	0.150822
H	-3.841376	1.954862	0.561359
C	-3.241649	0.817778	-1.152382
H	-4.105649	1.128317	-1.735289
C	0.096478	-0.542180	1.191823
H	0.415953	-1.538148	0.820698
C	-2.366398	0.807135	2.507895
H	-3.214736	1.479414	2.673567
H	-1.513461	1.190666	3.068904
C	-2.723841	-0.613692	3.109210
H	-1.820753	-1.024004	3.565507
H	-3.470060	-0.469410	3.897069
O	-5.893125	-1.319258	-1.920775
O	0.293356	-0.226444	2.382071
H	-6.404963	-0.664943	-0.086242
C	2.540158	2.129678	-0.886876
C	1.494899	0.398901	0.015657

N	1.361182	1.689881	-0.370664
N	2.763103	0.142778	-0.330112
N	3.455674	1.212707	-0.909275
C	3.422408	-1.121030	-0.193597
C	3.599785	-1.905018	-1.336891
C	4.237037	-3.135076	-1.183946
C	4.684353	-3.576095	0.063425
C	4.480928	-2.760622	1.177920
C	3.853091	-1.519031	1.074726
H	4.381932	-3.765644	-2.057734
H	4.822394	-3.096085	2.154122
C	3.106684	-1.428893	-2.677083
H	2.053942	-1.132366	-2.622340
H	3.669603	-0.552467	-3.010513
H	3.208028	-2.214699	-3.427108
C	5.397856	-4.896679	0.199138
H	5.060614	-5.607701	-0.558347
H	6.477417	-4.765891	0.072343
H	5.232400	-5.335687	1.185482
C	3.639628	-0.636415	2.275817
H	4.041187	0.365569	2.092004
H	2.572530	-0.528624	2.503153
H	4.145199	-1.053890	3.148495
C	0.429098	2.802892	-0.190066
C	1.077241	3.789631	-1.225567
O	2.513539	3.410364	-1.235822
C	1.006990	5.272059	-0.930894
H	1.549408	5.812202	-1.710556
H	-0.034786	5.599536	-0.951218
H	1.440168	5.525813	0.035354

C	0.533424	3.482661	-2.617251
H	-0.513177	3.791269	-2.678976
H	1.108048	4.027593	-3.368990
H	0.588742	2.411573	-2.833724
C	0.344191	3.134370	1.310870
C	1.690046	3.474980	1.955955
H	2.412458	2.663349	1.820734
H	2.135034	4.393197	1.564968
H	1.550692	3.606654	3.032150
C	-0.746247	4.160078	1.619288
H	-0.935502	4.179465	2.696146
H	-0.469458	5.172487	1.315494
H	-1.683277	3.891662	1.119168
H	-0.565605	2.520344	-0.549077
H	0.027668	2.181445	1.756217

Vibrational frequencies

-145.6176	14.4509	24.7143
30.2261	35.1345	41.7940
47.9250	50.8211	67.6271
69.8097	82.1248	86.9850
91.0298	99.9712	112.5485
116.9783	122.5766	133.7422
160.1320	165.7349	171.1036
187.2544	190.9789	196.8373
201.6807	215.6189	220.3443
231.1760	237.8850	242.9070
244.6028	259.2764	266.7445
276.0794	283.7738	287.0001
293.6862	302.7359	306.5136

312.5563	320.7340	329.2848
330.8866	348.6158	368.7668
371.9478	375.2267	396.6451
414.8090	418.0056	424.7680
433.2589	442.3931	461.5095
467.8131	476.8297	494.9999
510.2662	524.9644	527.9627
539.3552	548.9772	558.3085
561.6594	583.1788	588.4378
605.2566	622.7082	636.5805
653.4565	658.8514	668.8384
680.7709	701.4683	732.5948
734.6930	742.9970	748.4797
757.9570	758.8075	775.3432
782.4898	803.5255	807.6610
817.2955	829.7460	849.5562
858.7640	879.4443	886.7502
890.2765	903.0629	917.0832
919.2915	920.8620	931.8789
940.2329	941.5747	952.7704
954.3492	963.5136	968.7107
979.4735	981.1486	982.2584
988.9321	989.3776	996.1831
1002.3940	1008.0669	1012.5524
1036.6402	1037.8294	1040.4103
1042.7815	1061.6668	1063.3561
1070.3360	1075.2104	1081.6509
1109.7081	1117.2833	1127.5541
1146.6641	1167.6548	1169.7470
1175.3165	1178.2068	1193.5010

1200.5064	1201.8451	1217.1608
1220.0074	1220.9793	1225.4590
1232.1782	1238.2384	1257.4679
1262.9887	1272.5970	1278.0185
1281.0569	1286.2677	1293.0610
1303.6457	1310.0811	1325.8115
1332.0689	1334.4421	1343.4769
1346.8452	1353.5708	1358.1473
1362.5782	1364.6247	1388.2919
1396.3160	1407.7301	1416.7531
1417.6882	1421.2088	1421.6410
1424.6938	1432.2270	1433.0187
1436.8652	1438.4868	1451.9104
1463.9760	1467.5641	1469.5975
1476.8946	1482.2524	1482.5100
1485.5982	1488.4157	1490.0530
1492.4713	1495.4752	1495.7854
1496.7856	1498.9367	1500.5322
1502.5379	1507.6052	1510.0408
1511.2341	1520.5289	1521.8003
1523.3438	1542.5147	1549.9354
1563.6035	1626.8771	1640.2635
1644.6201	1681.5425	1683.9903
1687.7317	1692.3349	1727.2954
1829.0086	2928.3657	2962.5059
3057.6045	3071.7721	3074.4788
3075.7316	3076.5891	3080.1676
3080.5947	3083.2711	3088.1325
3091.9072	3099.1588	3099.4043
3120.1205	3129.0207	3141.3591

3145.4034	3145.7110	3148.3669
3150.3434	3153.6742	3155.4206
3162.9081	3164.3403	3166.1253
3166.2346	3167.4005	3168.9646
3169.8946	3174.6480	3176.7319
3176.8492	3179.5209	3189.2592
3196.5544	3203.5610	3205.3201
3208.0775	3211.2127	3211.2152

R'_p -TS1

Zero-point correction= 0.704189

Thermal correction to Energy= 0.743224

Thermal correction to Enthalpy= 0.744169

Thermal correction to Gibbs Free Energy= 0.632889

Sum of electronic and zero-point Energies= -1784.969455

Sum of electronic and thermal Energies= -1784.930420

Sum of electronic and thermal Enthalpies= -1784.929476

Sum of electronic and thermal Free Energies= -1785.040756

Cartesian coordinates

C	-4.654139	-0.377205	-0.298478
C	-3.710028	-1.122111	-1.034392
C	-2.957184	-2.048313	-0.314692
H	-2.274774	-2.701557	-0.854431
C	-2.887576	-2.000234	1.076990
H	-2.141593	-2.600827	1.587676
C	-3.600727	-1.035563	1.794951
C	-4.598385	-0.354640	1.099059
H	-5.248713	0.339712	1.631075
C	-5.587593	0.581046	-0.919079

C	-3.279850	-0.760503	-2.436820
H	-4.128778	-0.659935	-3.113501
H	-2.640663	-1.566571	-2.808924
C	-2.457014	0.600862	-2.484227
H	-1.582012	0.435326	-3.121841
H	-3.079761	1.358957	-2.965039
C	-2.045885	1.095447	-1.114752
C	-1.056478	0.437763	-0.374842
H	-0.385501	-0.256722	-0.877129
C	-0.993401	0.535111	1.011974
C	-1.994825	1.251573	1.692115
C	-2.792101	2.118707	0.942799
H	-3.518179	2.745895	1.455525
C	-2.803851	2.060902	-0.449130
H	-3.524524	2.654253	-1.006603
C	-0.004154	-0.231122	1.869308
H	0.545023	0.427485	2.568967
C	-2.409616	0.862328	3.095524
H	-3.104198	1.617348	3.474488
H	-1.561058	0.833541	3.787248
C	-3.119900	-0.560645	3.149389
H	-2.400592	-1.288131	3.532536
H	-3.943259	-0.494135	3.867300
O	-5.604958	0.912912	-2.088391
O	-0.117333	-1.434436	2.119450
H	-6.313628	1.025738	-0.206433
C	3.377517	-1.214793	-0.571412
C	1.750122	-0.136840	0.491584
N	2.281642	-1.359258	0.222871
N	2.608205	0.664416	-0.159121

N	3.654096	0.022287	-0.835466
C	2.546544	2.094415	-0.183494
C	2.061798	2.725941	-1.332749
C	2.015103	4.118782	-1.333997
C	2.431658	4.867555	-0.231051
C	2.917481	4.195572	0.891158
C	2.988251	2.803092	0.936088
H	1.643299	4.631539	-2.217799
H	3.258297	4.767712	1.750584
C	1.599146	1.919974	-2.516854
H	0.716162	1.328643	-2.251064
H	1.334596	2.574435	-3.349053
H	2.374748	1.223794	-2.847460
C	2.337496	6.371619	-0.247686
H	1.336234	6.698223	0.051231
H	3.052996	6.820514	0.444620
H	2.527147	6.767925	-1.247955
C	3.528145	2.081097	2.142357
H	4.289419	1.350946	1.851848
H	3.972381	2.787048	2.845829
H	2.735661	1.532039	2.660297
C	1.914019	-2.773767	0.334051
C	3.309744	-3.388345	-0.045134
O	3.924765	-2.370004	-0.931010
C	3.328645	-4.697467	-0.804188
H	4.365636	-4.955312	-1.032417
H	2.907969	-5.491352	-0.183403
H	2.771402	-4.641143	-1.738391
C	4.182791	-3.468521	1.202676
H	3.798220	-4.241320	1.872795

H	5.207309	-3.721840	0.922440
H	4.187371	-2.516069	1.740461
C	0.656525	-3.041644	-0.514143
C	0.778515	-2.621280	-1.980632
H	1.110233	-1.581689	-2.083366
H	1.472658	-3.249794	-2.544908
H	-0.200385	-2.699100	-2.465135
C	0.137048	-4.472802	-0.359213
H	-0.890727	-4.536725	-0.728677
H	0.726886	-5.197141	-0.924798
H	0.131375	-4.778527	0.691855
H	1.684956	-3.013145	1.374953
H	-0.086082	-2.385869	-0.040118

Vibrational frequencies

-86.5169	13.9859	16.7605
27.4206	37.2083	40.6345
43.9849	52.4573	60.4905
70.2258	76.1488	84.5356
93.5990	97.5449	104.3551
121.8743	124.4176	130.8640
139.6923	149.0122	161.3225
173.1734	182.9588	190.5538
204.8064	207.8147	214.7947
219.1424	233.2738	240.2181
240.8920	252.2443	262.6971
269.7529	274.9879	281.2356
286.7754	305.4718	310.1086
313.6238	315.9088	326.1032
329.1596	348.1327	358.3201

372.5508	375.9125	386.0193
399.2011	418.4192	422.5448
431.5984	447.6927	458.7926
462.3039	473.7672	490.6632
508.2977	524.0837	526.0286
532.5775	544.5999	555.8182
568.0893	570.5671	586.6590
603.9642	606.3948	634.5654
651.5754	656.2664	668.7541
685.2679	699.3800	713.2125
738.1305	746.0007	750.7103
756.4348	762.0658	780.0845
791.0092	797.1739	810.5685
815.5423	829.0504	850.0839
851.2013	879.7649	882.7363
885.3525	906.9869	914.3453
916.5798	921.6993	927.3752
935.0942	940.6408	951.3987
953.4634	962.1541	972.5441
978.1894	978.9951	980.3909
985.6475	986.8437	994.0714
1001.4670	1006.4299	1009.9881
1034.1778	1035.9357	1037.2776
1039.0289	1042.1642	1060.7714
1063.8390	1064.9903	1068.3740
1081.2596	1110.2041	1115.5243
1149.3894	1162.3486	1172.3112
1174.8391	1181.4619	1190.5387
1198.8529	1200.8306	1217.2111
1218.2695	1222.6935	1227.0847

1232.0294	1233.6699	1251.3193
1259.8671	1274.2094	1277.0050
1279.8191	1287.8875	1294.2792
1298.2111	1308.5246	1324.1072
1327.0411	1331.8628	1336.5722
1347.3852	1353.0916	1359.0091
1361.6042	1364.2415	1388.8715
1396.6930	1399.0017	1407.3001
1411.9431	1417.1201	1419.7903
1421.0940	1426.4127	1431.6422
1437.7002	1439.3359	1459.2197
1463.9222	1468.1984	1472.6286
1479.7827	1482.4113	1483.8381
1485.0977	1485.5571	1488.5386
1490.0417	1493.0948	1495.1174
1496.5873	1497.5727	1500.1141
1502.1745	1504.0823	1507.4995
1508.1662	1520.3413	1520.9523
1525.4579	1533.1936	1551.9592
1565.2467	1639.0360	1642.9950
1680.7560	1683.8344	1686.5777
1693.1766	1699.0984	1731.7771
1825.4642	2962.9564	2967.3186
3065.4791	3075.3562	3076.1367
3076.4815	3076.6819	3080.3619
3081.3722	3082.0669	3082.4471
3091.9023	3095.5577	3098.6729
3129.1345	3132.2668	3141.3487
3144.5280	3144.9143	3146.1321
3146.2304	3146.3871	3153.7429

3155.4291	3165.4510	3168.7714
3169.3043	3169.5275	3174.1060
3174.9841	3175.5394	3176.6712
3179.8585	3192.5959	3196.2837
3198.7085	3202.8701	3205.3242
3207.1749	3210.9519	3236.3792

S'_p -TS1

Zero-point correction= 0.704713

Thermal correction to Energy= 0.743270

Thermal correction to Enthalpy= 0.744214

Thermal correction to Gibbs Free Energy= 0.635231

Sum of electronic and zero-point Energies= -1784.972379

Sum of electronic and thermal Energies= -1784.933821

Sum of electronic and thermal Enthalpies= -1784.932877

Sum of electronic and thermal Free Energies= -1785.041860

Cartesian coordinates

C	-0.685126	-0.631969	0.247380
C	-0.714219	-1.871934	-0.417349
C	-1.473671	-1.946869	-1.589261
H	-1.473657	-2.872753	-2.160907
C	-2.383114	-0.943254	-1.928845
H	-3.060741	-1.096627	-2.765863
C	-2.571060	0.148442	-1.077658
C	-1.623809	0.342767	-0.070623
H	-1.683360	1.208327	0.587156
C	0.212231	-0.374351	1.442843
C	-0.274658	-3.161455	0.260007
H	0.777338	-3.163244	0.563354
H	-0.387449	-3.973035	-0.465152

C	-1.135047	-3.510837	1.548132
H	-1.280084	-4.595524	1.567318
H	-0.559415	-3.246986	2.440653
C	-2.452356	-2.769779	1.587969
C	-3.425674	-2.990594	0.613556
H	-3.383705	-3.893959	0.005187
C	-4.335851	-1.992654	0.258446
C	-4.301019	-0.735937	0.900499
C	-3.547651	-0.657725	2.070347
H	-3.530751	0.275319	2.627679
C	-2.625949	-1.651145	2.404151
H	-1.916648	-1.454540	3.203436
C	-5.151922	-2.266700	-0.939547
H	-5.081681	-3.314969	-1.298803
C	-4.760959	0.539259	0.227580
H	-4.677605	1.348747	0.958531
H	-5.801017	0.479807	-0.096630
C	-3.878701	0.907011	-1.041649
H	-4.455060	0.677951	-1.941121
H	-3.701826	1.988265	-1.020196
O	-0.136415	0.430427	2.335312
O	-5.849110	-1.468075	-1.533642
H	0.815193	-1.268043	1.715378
C	3.801072	0.990337	-0.157860
C	1.752044	0.408318	0.442100
N	3.033112	-0.021447	0.334782
N	1.854160	1.680804	0.045532
N	3.135180	2.085592	-0.344446
C	0.756481	2.592962	-0.088554
C	0.404989	3.392929	1.001269

C	-0.705596	4.221152	0.853977
C	-1.440082	4.259620	-0.335403
C	-1.033911	3.461178	-1.404770
C	0.067553	2.610956	-1.301796
H	-1.007512	4.850232	1.688087
H	-1.595461	3.485545	-2.335633
C	1.192164	3.326372	2.280521
H	1.055385	2.338383	2.731284
H	2.259451	3.474883	2.090587
H	0.853399	4.090705	2.982231
C	-2.661240	5.136496	-0.445162
H	-3.486699	4.721822	0.142675
H	-2.461528	6.140730	-0.062126
H	-2.996313	5.221860	-1.480908
C	0.469202	1.697385	-2.427617
H	1.527199	1.822495	-2.679070
H	0.310886	0.650695	-2.138507
H	-0.127668	1.897763	-3.318989
C	3.756648	-1.289580	0.249220
C	5.213307	-0.701208	0.248432
O	5.057015	0.629118	-0.390153
C	6.273535	-1.449723	-0.529923
H	7.212856	-0.895528	-0.466832
H	6.428058	-2.435177	-0.084832
H	6.011175	-1.570304	-1.579840
C	5.664065	-0.450688	1.683396
H	5.845046	-1.404118	2.185629
H	6.590350	0.127188	1.681257
H	4.904720	0.099554	2.245862
C	3.211305	-2.081719	-0.955703

C	3.280225	-1.327741	-2.286391
H	2.752163	-0.370228	-2.233751
H	4.304688	-1.132280	-2.612028
H	2.792438	-1.923118	-3.062498
C	3.788377	-3.494937	-1.048653
H	3.172727	-4.095683	-1.723051
H	4.807215	-3.501755	-1.441660
H	3.794494	-3.988246	-0.071543
H	3.612413	-1.873884	1.163241
H	2.142413	-2.182982	-0.721157

Vibrational frequencies

-167.5649	13.2472	24.9623
33.6082	38.0402	48.1932
58.7495	63.8831	70.3611
70.8383	73.5417	77.5935
94.0631	100.3025	108.2280
120.7666	130.7996	156.7775
166.0465	172.2627	178.7628
181.1391	196.1369	198.8446
206.5735	209.6306	217.8315
221.2942	234.0513	242.8292
247.8137	248.7061	261.4316
273.1933	281.3990	285.5250
288.0268	298.4242	309.0473
315.5361	326.8897	331.7235
337.9905	342.4747	361.8605
372.8907	377.2643	393.4601
407.8230	420.5235	432.0749
433.5244	448.8976	458.6427

472.2957	480.7458	500.0653
507.8489	520.0294	528.0239
535.0446	553.0428	564.7941
566.6272	579.3222	588.2964
602.0208	621.9745	630.3683
649.0528	659.7521	667.1777
677.8169	700.9285	715.2717
736.3047	745.1754	754.6915
755.2317	760.1373	777.6790
785.6449	789.3189	808.7514
818.1291	828.9072	850.4610
855.1234	879.5273	881.8219
887.8160	910.7658	911.3766
916.0882	926.6114	936.0437
940.6929	952.3909	953.7435
956.9217	961.7273	963.7786
976.1129	979.2465	980.6690
982.1084	989.3315	997.1349
1002.4114	1007.3586	1013.0843
1035.0166	1035.8205	1042.4398
1042.9448	1062.7848	1064.8850
1069.6752	1072.1889	1080.3905
1105.0026	1107.4070	1139.1943
1149.4520	1163.4205	1169.0504
1173.8242	1181.5707	1188.4610
1198.3647	1199.3367	1211.7186
1217.4325	1221.5784	1223.3532
1231.0492	1235.2926	1255.3263
1259.4290	1275.2550	1276.3109
1278.4081	1284.7532	1292.0822

1302.4913	1307.2083	1321.9643
1330.7628	1333.6904	1340.1093
1345.6782	1347.5926	1357.3293
1362.8422	1365.9422	1374.9039
1390.3367	1396.1718	1407.0468
1415.1581	1418.8236	1419.8485
1423.2008	1425.4637	1432.7295
1439.5087	1440.6676	1462.6259
1464.9580	1470.4651	1473.5759
1480.2784	1482.6200	1484.9211
1486.8223	1488.4960	1490.0759
1490.7852	1491.7289	1493.5992
1498.3557	1500.4477	1502.4670
1504.6292	1507.7623	1510.3224
1511.9735	1520.7415	1522.5805
1525.6706	1534.1260	1550.5669
1562.6000	1607.4525	1642.1274
1650.6511	1679.8892	1684.7195
1688.3122	1690.0912	1728.0024
1828.5805	2901.7106	2961.8725
3060.8988	3063.4188	3072.5624
3073.1852	3076.8322	3078.2976
3079.8883	3080.8663	3084.5137
3087.7324	3097.6596	3100.2596
3118.7174	3122.6997	3129.6947
3140.1457	3141.6841	3144.7101
3148.9693	3151.9169	3152.4209
3165.2208	3167.7662	3168.3393
3168.5224	3171.4934	3171.7999
3172.9256	3176.7499	3178.4499

3181.2346	3186.6432	3196.7809
3200.7473	3202.8290	3203.7796
3204.0809	3211.6306	3220.4354

R_p -INT1

Zero-point correction= 0.707315

Thermal correction to Energy= 0.745605

Thermal correction to Enthalpy= 0.746550

Thermal correction to Gibbs Free Energy= 0.639513

Sum of electronic and zero-point Energies= -1784.986349

Sum of electronic and thermal Energies= -1784.948058

Sum of electronic and thermal Enthalpies= -1784.947114

Sum of electronic and thermal Free Energies= -1785.054151

Cartesian coordinates

C	-3.953865	-1.689500	0.075639
C	-3.656073	-0.405416	-0.427627
C	-3.156420	0.517123	0.491742
H	-2.973260	1.542677	0.175026
C	-2.678587	0.106249	1.738749
H	-2.172924	0.832831	2.371891
C	-2.655554	-1.247078	2.088182
C	-3.450564	-2.092081	1.314695
H	-3.554795	-3.139459	1.597669
C	-4.611366	-2.738197	-0.726527
C	-3.574361	-0.112848	-1.911125
H	-4.530505	-0.269075	-2.414321
H	-3.300800	0.942124	-2.021008
C	-2.489075	-0.999463	-2.657251
H	-1.993042	-0.356743	-3.392394

H	-3.003062	-1.793157	-3.203846
C	-1.490395	-1.616790	-1.702837
C	-0.688955	-0.793418	-0.913961
H	-0.611393	0.262050	-1.177608
C	-0.165708	-1.202681	0.312267
C	-0.496956	-2.477192	0.798973
C	-1.047233	-3.383951	-0.116398
H	-1.246227	-4.402543	0.211570
C	-1.531882	-2.970384	-1.357617
H	-2.086741	-3.670067	-1.978586
C	0.522031	-0.139970	1.190292
H	-0.298527	0.584007	1.403712
C	-0.585112	-2.766287	2.286704
H	-0.917236	-3.802854	2.409252
H	0.379440	-2.637420	2.777979
C	-1.602394	-1.807981	3.023875
H	-1.021710	-0.975348	3.431269
H	-2.044653	-2.357945	3.861581
O	-4.995551	-2.629515	-1.874414
O	1.242726	-0.513167	2.249554
H	-4.747409	-3.697788	-0.184648
C	3.339968	1.451258	-0.510997
C	1.470981	0.688193	0.306358
N	2.737751	0.351051	0.010329
N	1.363928	1.953627	-0.102059
N	2.542921	2.470934	-0.627389
C	0.176287	2.754192	-0.027094
C	-0.524463	3.023437	-1.204892
C	-1.709995	3.752332	-1.091198
C	-2.182481	4.193736	0.145435

C	-1.430534	3.919648	1.292219
C	-0.234757	3.206277	1.233408
H	-2.277845	3.973751	-1.991446
H	-1.779915	4.278644	2.256980
C	-0.008067	2.581278	-2.549105
H	0.427865	1.578684	-2.512575
H	0.777993	3.258345	-2.896868
H	-0.813448	2.582119	-3.285935
C	-3.495338	4.924784	0.250597
H	-4.303606	4.222436	0.480015
H	-3.746082	5.425838	-0.686522
H	-3.469776	5.669683	1.048999
C	0.600690	2.959237	2.464788
H	1.583604	3.428407	2.350013
H	0.774079	1.893377	2.657169
H	0.116571	3.395905	3.339748
C	3.719794	-0.685188	0.330569
C	4.928414	-0.160621	-0.529145
O	4.629653	1.287280	-0.735986
C	6.234017	-0.227901	0.235829
H	7.040364	0.212123	-0.354692
H	6.483041	-1.272420	0.440750
H	6.151772	0.305677	1.184894
C	5.045261	-0.741785	-1.927847
H	5.323207	-1.796648	-1.887296
H	5.826589	-0.198874	-2.464148
H	4.107973	-0.642727	-2.479503
C	3.176457	-2.111781	0.170867
C	4.230782	-3.138522	0.587633
H	4.648392	-2.910968	1.573298

H	5.055702	-3.192426	-0.130967
H	3.777039	-4.131596	0.635803
C	2.549174	-2.461206	-1.182360
H	1.844451	-3.285184	-1.038557
H	3.292512	-2.779261	-1.917013
H	1.977132	-1.627122	-1.600446
H	3.960110	-0.553961	1.392210
H	2.375978	-2.126175	0.922102

Vibrational frequencies

21.6541	30.2975	38.1791
43.1755	49.5957	51.5792
60.9176	64.8778	75.4321
82.8503	97.2889	108.6564
115.7881	129.3282	137.7662
145.3279	150.2103	163.3743
169.2598	178.3185	195.7100
203.7027	206.2854	215.9687
220.5889	226.2840	236.6369
242.6348	246.1323	252.4787
261.5122	273.0459	274.6608
283.2345	285.9870	292.3501
298.1752	318.8263	320.6571
322.6797	327.5320	329.8401
337.8412	353.0075	367.4142
373.1055	381.7095	404.9748
419.0167	424.5387	437.5416
455.1540	460.5471	467.5267
479.8262	483.1064	496.5514
510.1751	528.7289	535.3897

543.3509	552.0905	563.3486
586.3230	592.2553	600.4548
607.9141	631.6219	656.2235
658.0551	662.1586	673.7755
714.3982	719.0035	729.9201
735.6632	745.9208	747.5331
755.7611	759.5910	774.2585
792.4496	801.2351	817.0675
833.3379	838.9348	857.2875
864.5005	883.1730	884.7126
898.2813	904.4627	914.6057
918.9014	922.9689	935.0915
944.2754	952.5940	956.4236
958.2317	964.3226	968.8736
978.1859	982.4364	982.9844
996.1182	999.6792	1007.9743
1014.0254	1019.1231	1023.2062
1039.6340	1042.0648	1042.8116
1059.4699	1063.8294	1066.7903
1076.0559	1091.8262	1108.3306
1111.5424	1128.5967	1142.9581
1155.6161	1164.9669	1175.2986
1177.6868	1190.7091	1200.2097
1204.5126	1216.3074	1219.8958
1220.8870	1225.6579	1234.9477
1236.3434	1245.0992	1260.7351
1267.3829	1271.2952	1281.7015
1284.7609	1289.3581	1297.5260
1303.0016	1320.2998	1328.4328
1329.4368	1333.8461	1345.0621

1346.1357	1350.4458	1359.9199
1363.2338	1367.0887	1370.4393
1378.8669	1397.1272	1402.7593
1417.7805	1419.0019	1422.3636
1424.3734	1430.6286	1435.8075
1438.8604	1439.9052	1454.9071
1461.2865	1465.4704	1470.9148
1471.7750	1478.3393	1480.4006
1482.2322	1486.6545	1492.2292
1493.7234	1494.9731	1495.9827
1496.5041	1498.1052	1498.9701
1504.9762	1506.4568	1513.7821
1516.3997	1518.5411	1523.3707
1535.4015	1546.8317	1547.5823
1555.6015	1574.3156	1636.7564
1642.3823	1677.2123	1680.3214
1683.4026	1686.6626	1730.6859
1827.9327	2887.6751	2963.0754
3059.4403	3065.9937	3075.7765
3076.1719	3077.4776	3077.8901
3078.6512	3082.7210	3084.6197
3087.4158	3088.4309	3092.2970
3094.9437	3125.7431	3139.2896
3140.8058	3145.8406	3147.0042
3147.1548	3152.5012	3156.0249
3158.6484	3164.7953	3171.5429
3172.5104	3173.5533	3174.1830
3175.7198	3176.7584	3178.5422
3179.6692	3180.6762	3185.4303
3187.8633	3188.1969	3201.3879

3205.0253

3205.5846

3207.4746

S_p-INT1

Zero-point correction= 0.706554

Thermal correction to Energy= 0.745081

Thermal correction to Enthalpy= 0.746025

Thermal correction to Gibbs Free Energy= 0.636855

Sum of electronic and zero-point Energies= -1784.981620

Sum of electronic and thermal Energies= -1784.943093

Sum of electronic and thermal Enthalpies= -1784.942149

Sum of electronic and thermal Free Energies= -1785.051319

Cartesian coordinates

C	-4.416917	-1.635557	0.632781
C	-3.412845	-2.625694	0.668833
C	-2.470325	-2.513979	1.692132
H	-1.714305	-3.289095	1.797255
C	-2.327957	-1.332990	2.422534
H	-1.454228	-1.192906	3.054441
C	-3.153724	-0.234256	2.172567
C	-4.283776	-0.467994	1.390191
H	-5.004831	0.334520	1.234865
C	-5.536241	-1.653173	-0.326839
C	-3.152893	-3.576021	-0.480952
H	-4.037668	-4.160881	-0.738085
H	-2.368666	-4.270290	-0.164248
C	-2.668508	-2.832990	-1.798330
H	-1.911131	-3.466367	-2.271932
H	-3.516539	-2.758740	-2.482969
C	-2.138583	-1.445382	-1.511410

C	-1.019304	-1.275739	-0.695883
H	-0.373950	-2.137566	-0.520258
C	-0.827050	-0.138219	0.091625
C	-1.787983	0.886836	0.048619
C	-2.724415	0.837997	-0.992171
H	-3.425857	1.663378	-1.098903
C	-2.910963	-0.308821	-1.760565
H	-3.759493	-0.370456	-2.438633
C	0.352399	-0.167674	1.095207
H	0.527973	-1.266428	1.273287
C	-2.026426	1.858239	1.186296
H	-2.700379	2.641766	0.821778
H	-1.094592	2.314761	1.512942
C	-2.682220	1.171122	2.459695
H	-1.918200	1.138538	3.236784
H	-3.513493	1.796038	2.802785
O	-5.715037	-2.467374	-1.211831
O	0.292182	0.573229	2.189783
H	-6.254519	-0.817369	-0.191567
C	3.703609	0.303929	-0.397089
C	1.632290	0.217205	0.295585
N	2.793687	-0.466998	0.260376
N	1.916312	1.368880	-0.317039
N	3.229572	1.452638	-0.761722
C	1.071339	2.522117	-0.458709
C	0.314437	2.659982	-1.622988
C	-0.483072	3.798375	-1.731187
C	-0.511382	4.771107	-0.730042
C	0.296076	4.604858	0.397248
C	1.103329	3.480299	0.558066

H	-1.094795	3.927472	-2.620648
H	0.294122	5.365376	1.174167
C	0.344310	1.611483	-2.700753
H	-0.166223	0.701081	-2.365842
H	-0.156811	1.973990	-3.599866
H	1.373130	1.344036	-2.960350
C	-1.415420	5.970358	-0.852580
H	-1.593000	6.228019	-1.898984
H	-2.387547	5.763838	-0.392648
H	-0.990060	6.840158	-0.346973
C	1.953122	3.268907	1.779582
H	1.611884	2.356483	2.284160
H	3.006151	3.143114	1.506255
H	1.871411	4.120258	2.457576
C	3.336430	-1.810110	0.512045
C	4.863992	-1.444610	0.376008
O	4.877610	-0.284443	-0.548269
C	5.789816	-2.482206	-0.219560
H	6.793787	-2.056044	-0.280121
H	5.829442	-3.360444	0.427833
H	5.480174	-2.785276	-1.219098
C	5.384793	-0.942960	1.717650
H	5.445449	-1.775105	2.423070
H	6.381387	-0.516717	1.588417
H	4.724326	-0.179280	2.138787
C	2.664864	-2.826803	-0.429506
C	2.687978	-2.413187	-1.902454
H	2.157890	-1.468847	-2.066175
H	3.705477	-2.302675	-2.287812
H	2.185051	-3.175562	-2.502677

C	3.160817	-4.259558	-0.211691
H	2.425018	-4.958191	-0.616774
H	4.107307	-4.453633	-0.718408
H	3.286026	-4.485067	0.851880
H	3.141426	-2.096767	1.549191
H	1.616249	-2.811424	-0.104999

Vibrational frequencies

15.5669	22.4740	25.9423
30.1952	35.0123	45.5098
60.2606	68.5754	76.3635
85.5342	93.3284	100.0493
109.0527	119.1449	127.6964
144.8893	161.1700	168.4563
172.2870	177.1544	193.3839
199.2531	205.6486	209.1939
216.6493	220.0645	236.1475
244.7520	249.9685	252.4942
257.5969	266.9389	279.8617
280.7008	283.7987	286.0577
290.4331	311.1770	312.4606
318.8656	328.8315	332.4355
345.4073	363.4607	369.9162
372.2197	382.4076	409.2986
420.9653	421.5166	431.9846
437.2340	449.8897	461.4777
470.1322	488.1109	503.9300
519.2602	528.0416	536.1342
542.9378	553.5405	569.7677
588.2751	590.4123	599.6420

616.7504	629.9951	652.6630
657.6040	670.3023	680.1528
711.8549	727.2599	736.8035
739.2389	744.7392	751.9894
759.5705	774.8634	783.0914
791.5304	803.0101	804.6616
827.4737	838.1986	852.8850
854.8239	879.5436	885.0281
898.5737	905.7119	910.8091
913.0900	918.1173	924.6685
936.7498	943.0375	952.9900
954.7586	964.1617	966.2878
976.2370	980.8995	983.5027
994.4970	995.1718	1000.6899
1008.3976	1010.7180	1036.6606
1038.1256	1043.2258	1043.6528
1061.3643	1063.0951	1072.0638
1073.8743	1075.6351	1102.4849
1112.2912	1125.5428	1147.7442
1163.5637	1166.2033	1175.6849
1181.8760	1193.1400	1200.0919
1201.4745	1215.9219	1216.7031
1219.2957	1228.2876	1231.6698
1239.2435	1251.3647	1255.5835
1268.8291	1274.3827	1278.7569
1282.1427	1284.5231	1288.2985
1297.0052	1304.4300	1318.9641
1327.6344	1331.6253	1336.0171
1336.3913	1346.1566	1347.9098
1361.2805	1363.3610	1367.0789

1373.3843	1392.1211	1397.2909
1411.1046	1416.2385	1419.8265
1421.6576	1425.5878	1432.0299
1439.1593	1440.8067	1454.0928
1462.3575	1463.8405	1472.4973
1475.1669	1480.9218	1481.5953
1482.5749	1486.9804	1488.0981
1490.0137	1493.5891	1494.8300
1495.1818	1498.6489	1501.7855
1506.4286	1508.6353	1509.3727
1519.6878	1523.6723	1524.1950
1532.3966	1539.9495	1547.4164
1551.4200	1571.1440	1638.7838
1642.8971	1679.8747	1680.7157
1685.4086	1689.3643	1740.6158
1825.8876	2727.5381	2961.0049
3054.3294	3068.0490	3071.0626
3072.9556	3075.2495	3076.0846
3082.3184	3082.6763	3083.1733
3086.7402	3093.4817	3100.9608
3126.6373	3129.5660	3140.4371
3145.0561	3145.6714	3148.8521
3156.3757	3161.0116	3163.7818
3164.9234	3166.2613	3169.1981
3169.5007	3170.5656	3172.0388
3176.4087	3176.6698	3182.2108
3183.4105	3184.5896	3192.1376
3201.0107	3201.9056	3203.7708
3205.8815	3208.6409	3214.8048

[Cs]HCO₃

Zero-point correction= 0.028035

Thermal correction to Energy= 0.033660

Thermal correction to Enthalpy= 0.034604

Thermal correction to Gibbs Free Energy= -0.004272

Sum of electronic and zero-point Energies= -284.462558

Sum of electronic and thermal Energies= -284.456933

Sum of electronic and thermal Enthalpies= -284.455989

Sum of electronic and thermal Free Energies= -284.494865

Cartesian coordinates

C	2.064756	0.037542	0.000336
O	1.543127	-1.102621	0.000837
O	1.511796	1.154095	0.000745
Cs	-1.239398	-0.006279	-0.000106
O	3.451928	0.070516	-0.000966
H	3.723570	-0.855803	-0.001094

Vibrational frequencies

50.3611	129.6144	137.8110
536.3421	584.2283	683.8699
831.6748	1016.3212	1231.8260
1424.8366	1799.6488	3879.3215

R_p-TS2

Zero-point correction= 0.732685

Thermal correction to Energy= 0.777319

Thermal correction to Enthalpy= 0.778263

Thermal correction to Gibbs Free Energy= 0.654598

Sum of electronic and zero-point Energies= -2069.445568

Sum of electronic and thermal Energies= -2069.400934

Sum of electronic and thermal Enthalpies= -2069.399990

Sum of electronic and thermal Free Energies= -2069.523654

Cartesian coordinates

C	-0.377627	1.079811	0.486246
C	-0.128651	2.332782	1.085797
C	-1.088207	2.829170	1.968010
H	-0.884449	3.751001	2.509148
C	-2.369435	2.273561	2.027592
H	-3.140041	2.766657	2.616359
C	-2.716324	1.225532	1.175448
C	-1.672335	0.564810	0.515551
H	-1.885121	-0.306080	-0.102376
C	0.729354	0.324756	-0.240309
C	0.985399	3.220394	0.583144
H	1.884731	2.635853	0.371103
H	1.232316	3.962382	1.348460
C	0.599809	3.988203	-0.764613
H	0.755692	5.058657	-0.598447
H	1.293021	3.657453	-1.539835
C	-0.818542	3.728617	-1.217979
C	-1.899841	4.343571	-0.588725
H	-1.733988	5.227765	0.026785
C	-3.166107	3.748955	-0.569286
C	-3.371891	2.501375	-1.196578
C	-2.377746	2.074899	-2.076653
H	-2.501435	1.142368	-2.625175
C	-1.121038	2.681400	-2.092391
H	-0.336475	2.207505	-2.669776

C	-4.162310	4.388436	0.305351
H	-3.848634	5.382389	0.689250
C	-4.418597	1.512923	-0.730586
H	-4.382623	0.654079	-1.407915
H	-5.427148	1.929317	-0.759819
C	-4.150505	1.005682	0.747482
H	-4.814329	1.548815	1.424108
H	-4.424957	-0.054218	0.789386
O	1.319307	0.986087	-1.325346
O	-5.242321	3.930071	0.627807
H	0.150433	-0.740487	-0.762108
C	-0.847985	-1.035416	-2.649411
O	-0.563371	-1.585072	-1.463809
O	-1.869239	-1.435862	-3.267373
Cs	-2.725805	-3.614485	-1.495419
O	-0.058976	-0.129639	-3.105143
H	0.843901	0.558104	-2.129306
C	2.589394	-1.021749	2.520483
C	1.708621	-0.146488	0.710769
N	1.432271	-0.555339	1.978293
N	3.036029	-0.362406	0.586221
N	3.608660	-0.923548	1.734432
C	3.910089	-0.047239	-0.505869
C	4.850064	0.970162	-0.319379
C	5.726682	1.241238	-1.369715
C	5.677228	0.527801	-2.567456
C	4.728963	-0.487655	-2.702519
C	3.832176	-0.798795	-1.681995
H	6.463908	2.030958	-1.247169
H	4.686522	-1.058280	-3.627183

C	4.928659	1.739122	0.973213
H	3.933121	2.007115	1.340252
H	5.407101	1.140902	1.753995
H	5.505355	2.655569	0.837162
C	6.611762	0.859103	-3.702248
H	6.888587	-0.038673	-4.260071
H	6.134500	1.548759	-4.405899
H	7.524294	1.335919	-3.337789
C	2.807090	-1.883985	-1.855151
H	2.676125	-2.460308	-0.934076
H	1.833734	-1.457651	-2.122855
H	3.111919	-2.569327	-2.649023
C	0.287119	-0.924108	2.816117
C	1.074349	-1.062713	4.167032
O	2.425483	-1.507072	3.743354
C	0.571418	-2.064303	5.183705
H	1.258444	-2.075550	6.033073
H	-0.411824	-1.755904	5.545692
H	0.501997	-3.072852	4.779238
C	1.236134	0.317893	4.795820
H	0.271630	0.662240	5.177033
H	1.945587	0.265962	5.624016
H	1.594555	1.046931	4.063075
C	-0.437225	-2.126957	2.183274
C	0.450249	-3.356769	1.975856
H	1.318936	-3.122135	1.351568
H	0.814664	-3.788381	2.910764
H	-0.120442	-4.130488	1.454862
C	-1.751811	-2.441110	2.898766
H	-2.329979	-3.157174	2.307853

H	-1.600320	-2.882621	3.885980
H	-2.354967	-1.534083	3.012615
H	-0.406956	-0.081766	2.894399
H	-0.704193	-1.770522	1.179375

Vibrational frequencies

-1310.3837	16.3644	22.5300
30.2082	34.1312	37.5543
42.6444	48.2613	52.1488
58.8943	65.4405	67.0383
71.1954	75.7890	87.8944
91.7202	102.4238	110.1340
124.3404	131.1146	138.2387
142.7748	147.5608	149.4822
157.0111	168.6683	173.9335
181.2682	190.7666	198.0071
202.2285	211.2656	212.6036
222.0054	227.2286	243.3346
245.1624	249.7378	255.5520
273.4220	275.6423	283.6756
289.0937	291.8511	293.4478
302.4838	308.8163	318.0763
323.8591	331.4370	341.6731
346.6851	358.0503	367.2743
374.7288	382.2823	402.4380
412.4843	418.4153	421.5894
435.8833	448.5456	460.4279
469.9628	471.9650	484.8685
507.9281	518.3141	528.5724
537.0913	552.6648	562.3001

576.1989	584.9430	589.7816
607.2151	627.5579	644.8561
651.6714	664.8446	682.0659
684.9792	692.6482	705.3130
714.5699	728.9741	741.5863
743.9143	751.0540	758.0541
773.5380	784.9408	788.3017
808.4340	809.8232	824.8200
844.2883	848.2068	851.5660
864.9844	871.0871	885.3460
896.8467	901.6043	907.4031
916.5447	917.3095	927.3293
934.3467	939.3401	951.6684
954.0493	966.3052	969.5490
977.8888	981.6508	985.2748
991.6025	997.8086	1001.0699
1002.5627	1008.6185	1027.6253
1036.3852	1039.0437	1043.1743
1044.5093	1057.1876	1063.0341
1063.8370	1067.1919	1077.2501
1084.6431	1099.0287	1109.4371
1111.4446	1132.4069	1147.4595
1166.5786	1171.5183	1179.5740
1184.7375	1191.6700	1197.7845
1201.2293	1217.7337	1219.4558
1222.1412	1226.2001	1233.5086
1235.7863	1236.2588	1250.2949
1269.4252	1275.8224	1281.8953
1283.7288	1284.7235	1285.7391
1301.3858	1317.0421	1325.3685

1334.2376	1336.8752	1345.1505
1349.5991	1353.5622	1355.2570
1364.0806	1382.0037	1390.0943
1399.2230	1412.6059	1418.1472
1418.9516	1420.7721	1421.2634
1428.9906	1431.3724	1438.1425
1442.0687	1457.2512	1461.6842
1465.2493	1467.4473	1471.7514
1473.6278	1479.2813	1482.0386
1486.3079	1487.8305	1490.5844
1491.7802	1493.3099	1494.9482
1495.6742	1498.3397	1501.2478
1503.4626	1507.4864	1512.1309
1518.1459	1521.3868	1523.7830
1529.4877	1544.2505	1549.6924
1550.2381	1566.5740	1583.7661
1637.8707	1643.1202	1644.9173
1680.9520	1683.3562	1684.2409
1693.6506	1708.6861	1755.1585
1823.8679	2661.9534	2958.6308
3073.0882	3075.2902	3077.1464
3077.7859	3078.1383	3079.2942
3080.6500	3082.1714	3082.3940
3091.6462	3093.5981	3101.6794
3127.2963	3139.0304	3145.9561
3146.5689	3146.7226	3148.1048
3150.9815	3151.7756	3160.9151
3164.1875	3165.9382	3166.3192
3169.5206	3169.8535	3171.9207
3174.9751	3177.4408	3178.2736

3182.8105	3188.3300	3190.7991
3193.6133	3203.4625	3205.1607
3205.5499	3215.1768	3270.1202

S_p -TS2

Zero-point correction= 0.732328

Thermal correction to Energy= 0.776741

Thermal correction to Enthalpy= 0.777686

Thermal correction to Gibbs Free Energy= 0.654691

Sum of electronic and zero-point Energies= -2069.443891

Sum of electronic and thermal Energies= -2069.399477

Sum of electronic and thermal Enthalpies= -2069.398533

Sum of electronic and thermal Free Energies= -2069.521528

Cartesian coordinates

C	-1.430969	0.575755	0.602792
C	-2.348952	1.059724	1.558044
C	-3.689517	1.149342	1.168860
H	-4.402718	1.598612	1.857014
C	-4.165535	0.520599	0.019563
H	-5.236398	0.478236	-0.165819
C	-3.295277	-0.237023	-0.766477
C	-1.927262	-0.077782	-0.531667
H	-1.212372	-0.616884	-1.153404
C	0.072161	0.581233	0.769950
C	-2.005502	1.235199	3.022450
H	-1.067387	1.775424	3.154237
H	-2.806417	1.816272	3.490233
C	-1.872983	-0.151355	3.793877
H	-2.447248	-0.080362	4.723026

H	-0.820882	-0.289606	4.047294
C	-2.340957	-1.321755	2.960187
C	-3.697991	-1.541858	2.722980
H	-4.440559	-1.072824	3.368650
C	-4.139190	-2.182497	1.560102
C	-3.206670	-2.650113	0.609111
C	-1.875312	-2.699983	1.018000
H	-1.114491	-3.067599	0.334612
C	-1.440533	-2.036049	2.166291
H	-0.369526	-1.936985	2.331567
C	-5.589342	-2.131118	1.309827
H	-6.184001	-1.789165	2.183138
C	-3.524804	-2.797847	-0.863383
H	-2.655299	-3.260312	-1.340945
H	-4.389025	-3.440941	-1.037402
C	-3.808828	-1.407448	-1.574647
H	-4.888520	-1.304119	-1.705738
H	-3.352832	-1.444767	-2.569499
O	0.577554	0.493867	2.068980
O	-6.151226	-2.407315	0.266669
H	0.482656	-0.501724	0.209009
C	1.816620	-2.186098	0.735307
O	0.965632	-1.703276	-0.170883
O	2.530083	-3.175425	0.425076
Cs	1.586061	-3.710804	-2.280657
O	1.866817	-1.624262	1.893545
H	1.142556	-0.386314	2.062239
C	1.205242	3.026086	-1.643401
C	0.719538	1.611769	-0.037601
N	0.179265	2.356085	-1.042672

N	2.040299	1.876338	-0.114782
N	2.363914	2.775655	-1.132284
C	3.107028	1.327639	0.672225
C	3.896515	0.321443	0.112250
C	4.953191	-0.167534	0.879230
C	5.217579	0.321886	2.157929
C	4.415359	1.346609	2.666015
C	3.353545	1.873800	1.934834
H	5.578097	-0.956753	0.468466
H	4.624940	1.749453	3.653899
C	3.616899	-0.201479	-1.270843
H	2.596905	-0.597760	-1.313540
H	3.714666	0.594216	-2.015788
H	4.315110	-1.003108	-1.520578
C	6.335954	-0.257517	2.984801
H	5.975330	-1.108022	3.572164
H	7.151257	-0.616277	2.352254
H	6.736811	0.480953	3.682965
C	2.494915	2.984802	2.472041
H	2.459843	3.825912	1.771673
H	1.475495	2.614473	2.618543
H	2.883343	3.347116	3.425507
C	-1.095627	2.998045	-1.411564
C	-0.635188	3.554727	-2.801361
O	0.801000	3.856463	-2.593683
C	-1.292111	4.821297	-3.305871
H	-0.835716	5.097450	-4.259278
H	-2.355590	4.639515	-3.476201
H	-1.179597	5.653131	-2.612532
C	-0.715165	2.447644	-3.848244

H	-1.762062	2.230783	-4.073995
H	-0.217107	2.770904	-4.764521
H	-0.241316	1.528930	-3.490781
C	-1.526571	3.955851	-0.283494
C	-0.500368	5.039532	0.058037
H	0.467145	4.607357	0.334958
H	-0.331461	5.744026	-0.759679
H	-0.855319	5.610435	0.919776
C	-2.933295	4.514459	-0.506888
H	-3.288564	4.977389	0.417516
H	-2.967011	5.275655	-1.289132
H	-3.632035	3.713176	-0.767795
H	-1.871424	2.243528	-1.562445
H	-1.595461	3.297906	0.591421

Vibrational frequencies

-1198.2494	17.4360	23.2867
28.3577	33.6539	34.5883
36.4138	44.7554	50.9515
54.7900	64.2164	75.5723
78.3101	84.2297	89.8972
102.4555	106.6456	115.4139
124.3297	131.3615	143.4881
148.1868	149.5596	158.6289
172.8992	177.7109	183.4209
185.6851	193.2718	200.0696
213.8651	216.2841	216.7587
228.3969	233.5210	243.5614
251.0727	254.6621	260.3318
265.5639	275.6316	281.8602

283.9305	290.1911	296.9485
299.8169	313.7638	320.9276
322.0969	331.6889	335.8002
349.4514	371.3263	378.1737
378.6208	381.3866	402.4988
415.3527	419.9291	426.2616
434.3338	447.6131	456.9453
465.9311	471.5543	489.9636
510.6546	520.5506	526.9331
538.9348	551.3723	564.2772
574.4365	579.7336	589.6431
605.8612	621.1716	638.0263
649.0036	662.3979	676.5786
681.2169	689.4202	713.0480
723.5211	728.9396	738.4179
745.4803	751.9359	753.3823
763.3933	783.2994	792.8740
803.3694	814.8513	824.9794
835.7287	841.2202	854.9252
860.0604	862.4935	878.8303
886.3571	898.1596	910.1636
910.2167	919.2966	925.0649
927.6212	935.8093	941.6569
953.1454	956.7334	966.9918
970.1366	978.8784	982.1380
985.4986	993.6082	1000.5784
1001.4669	1007.8247	1016.5799
1035.9142	1039.8039	1043.4445
1045.4289	1062.4226	1064.9638
1074.2399	1080.1706	1082.1167

1088.2452	1104.6007	1108.2089
1130.0940	1138.6490	1158.5265
1163.9280	1172.1163	1184.9856
1187.4211	1197.5959	1200.9037
1204.8532	1218.7336	1220.1394
1223.7183	1226.6809	1233.0788
1234.2405	1236.6414	1243.3862
1276.2781	1281.8522	1282.1832
1285.5477	1288.2974	1294.8551
1307.0684	1315.2446	1326.3255
1333.0331	1336.2946	1340.5935
1348.7306	1349.2259	1358.8820
1361.7169	1364.6420	1379.6089
1396.2641	1400.5631	1402.6453
1413.3417	1418.4781	1421.1006
1423.6174	1431.4142	1438.5327
1439.5916	1444.6868	1456.5880
1464.9810	1469.2940	1472.4477
1476.1020	1480.2301	1482.7545
1486.8361	1489.3660	1490.7117
1493.1469	1494.9127	1495.7951
1497.4121	1500.1091	1504.7323
1507.0567	1509.5299	1510.7805
1511.1586	1520.0986	1526.2220
1527.7104	1544.2203	1551.7460
1552.2968	1576.6950	1600.6690
1635.0279	1638.6326	1642.3133
1680.0466	1683.7267	1684.2103
1695.1124	1730.5346	1753.4226
1824.1400	2391.4650	2958.8601

3068.7158	3072.6575	3075.5110
3079.3006	3081.3726	3082.6613
3084.6183	3085.0426	3087.0500
3092.6817	3095.9588	3101.8713
3143.7061	3145.3439	3145.6343
3146.2449	3147.2041	3150.4657
3153.3680	3160.1288	3162.7191
3167.3942	3168.1478	3168.3919
3171.3647	3172.4832	3174.1396
3174.9012	3177.2367	3178.8554
3178.9165	3182.9381	3188.7922
3202.8339	3204.7543	3207.2249
3207.6713	3213.9742	3221.0263

R_p -INT2

Zero-point correction= 0.706790

Thermal correction to Energy= 0.745388

Thermal correction to Enthalpy= 0.746332

Thermal correction to Gibbs Free Energy= 0.639781

Sum of electronic and zero-point Energies= -1784.993256

Sum of electronic and thermal Energies= -1784.954658

Sum of electronic and thermal Enthalpies= -1784.953714

Sum of electronic and thermal Free Energies= -1785.060265

Cartesian coordinates

C	-4.373156	-1.061848	0.495988
C	-3.854292	0.168613	0.043891
C	-2.922743	0.791609	0.871609
H	-2.546165	1.770244	0.593790
C	-2.297593	0.097342	1.905950

H	-1.456269	0.562795	2.414985
C	-2.604815	-1.240628	2.159475
C	-3.754546	-1.741258	1.549881
H	-4.086060	-2.754848	1.775337
C	-5.423168	-1.807036	-0.223494
C	-4.015793	0.673451	-1.372067
H	-5.062910	0.731528	-1.671941
H	-3.589863	1.681203	-1.410560
C	-3.255534	-0.234786	-2.432369
H	-2.735008	0.435133	-3.124903
H	-4.001091	-0.791436	-3.005544
C	-2.295897	-1.211693	-1.789694
C	-1.144180	-0.755624	-1.149315
H	-0.820992	0.258131	-1.343044
C	-0.495804	-1.486836	-0.138774
C	-1.112903	-2.695894	0.292124
C	-2.079952	-3.253622	-0.545789
H	-2.505867	-4.216311	-0.269677
C	-2.659587	-2.544277	-1.595585
H	-3.506223	-2.963601	-2.132997
C	0.758388	-1.026091	0.452891
C	-1.048541	-3.220514	1.718548
H	-1.701310	-4.098281	1.765414
H	-0.053470	-3.540431	2.028001
C	-1.579525	-2.171978	2.769266
H	-0.742553	-1.566862	3.135631
H	-1.973464	-2.725391	3.628280
O	-5.937125	-1.486951	-1.277334
O	1.443543	-1.956742	1.249377
H	-5.732772	-2.746673	0.281062

C	3.395059	1.156376	-0.377811
C	1.552058	0.025817	0.075571
N	2.928861	0.052518	0.291941
N	1.284719	1.240916	-0.580631
N	2.508923	1.930069	-0.885134
C	0.248478	2.157724	-0.191566
C	-0.491434	2.769916	-1.212092
C	-1.437026	3.735294	-0.858246
C	-1.639651	4.114027	0.468506
C	-0.851119	3.517787	1.455187
C	0.105973	2.550333	1.149383
H	-2.018839	4.211515	-1.644210
H	-0.968407	3.829440	2.490661
C	-0.219371	2.463855	-2.661282
H	-0.077830	1.394367	-2.834334
H	0.704949	2.956784	-2.979479
H	-1.035772	2.823807	-3.290981
C	-2.700554	5.118754	0.834239
H	-3.641972	4.610762	1.069675
H	-2.893928	5.809128	0.010335
H	-2.410433	5.698420	1.713600
C	1.006252	2.012198	2.231680
H	2.057095	2.091397	1.934995
H	0.805659	0.956222	2.438715
H	0.867743	2.576899	3.155176
C	3.983144	-0.970684	0.278351
C	5.207555	0.007481	0.286036
O	4.718724	1.173639	-0.476158
C	5.481145	0.481240	1.710118
H	6.192439	1.309709	1.692371

H	5.908722	-0.335675	2.296826
H	4.559690	0.814214	2.195283
C	6.487005	-0.449850	-0.383271
H	6.882390	-1.328009	0.131989
H	7.226941	0.351117	-0.312240
H	6.337165	-0.690613	-1.435068
C	3.769520	-1.958743	-0.884302
C	4.782705	-3.107776	-0.883798
H	4.954323	-3.488482	0.128200
H	5.746306	-2.817829	-1.307072
H	4.396778	-3.932709	-1.488284
C	3.648505	-1.290374	-2.257057
H	3.469200	-2.053673	-3.018980
H	4.552359	-0.743439	-2.539882
H	2.806310	-0.591257	-2.294345
H	3.970839	-1.530396	1.216957
H	2.793952	-2.403869	-0.655987
H	1.458063	-1.630951	2.158855

Vibrational frequencies

22.9270	36.8962	41.7453
51.6745	62.1577	63.2681
66.5017	80.2179	88.0483
90.5537	97.4077	103.5392
117.7126	120.4416	124.3435
142.4820	153.7128	161.8968
165.1343	175.0834	190.8756
200.3974	204.1086	206.8642
215.2466	218.6508	240.9163
245.5296	253.4836	255.4725

262.5844	272.5915	275.0742
280.9345	283.0527	288.1850
298.6783	307.4416	315.1254
326.5625	330.8176	335.4921
348.8206	353.7982	367.2826
372.8788	385.0707	390.5452
412.2625	414.6183	432.3534
436.3936	446.3852	460.1286
465.6567	476.2114	487.3572
500.7052	512.8482	521.5899
531.0604	543.1765	550.1191
556.2390	575.5693	587.6219
592.2412	610.3523	623.9200
640.2247	666.6341	670.8581
682.6220	684.8536	694.7705
724.7820	735.1412	739.2748
747.6132	759.7454	763.4702
777.1888	783.4682	803.9262
806.7189	817.5894	843.7577
849.9855	863.9462	878.7861
884.2492	886.1774	898.4818
916.1476	916.3881	920.5109
929.5933	940.4656	942.9908
951.3803	956.7450	959.9094
961.4530	971.1919	977.4411
981.2938	983.0854	993.8338
1000.6630	1008.0211	1015.2156
1030.6066	1037.3846	1039.5461
1043.2719	1047.6083	1057.6888
1063.0708	1065.4342	1071.8754

1092.0287	1108.5868	1134.9823
1153.1634	1155.7076	1166.4136
1173.6657	1181.2626	1186.9666
1198.8963	1203.0233	1208.6831
1213.0325	1214.8423	1219.0023
1225.2787	1226.1513	1234.1312
1237.1309	1258.4693	1270.6130
1276.7131	1279.2412	1288.5363
1295.1450	1299.4015	1312.6439
1315.2671	1325.2774	1328.8817
1346.7007	1347.7529	1350.3985
1352.9854	1356.6501	1364.8310
1370.8869	1384.8531	1394.3323
1396.4575	1412.5988	1417.7564
1418.2592	1419.1139	1427.1070
1428.6740	1437.8655	1438.9911
1460.8006	1467.9550	1472.3360
1478.3305	1480.8640	1482.5888
1483.0899	1486.4417	1486.7090
1489.3095	1491.2304	1494.3408
1494.4200	1498.9845	1501.1779
1503.3893	1504.3609	1505.0197
1511.3522	1517.3649	1522.0315
1527.8813	1535.8591	1543.4156
1550.9573	1628.1328	1643.2639
1650.4931	1666.0120	1685.5284
1687.2416	1693.3689	1778.7529
1827.6667	2960.8425	3072.1508
3072.6383	3072.9331	3074.1010
3077.2694	3078.0599	3079.9677

3083.0773	3088.1403	3090.8525
3093.4351	3097.2474	3120.8471
3130.8457	3138.8840	3142.7228
3142.9138	3145.3036	3146.0512
3149.5733	3159.0292	3165.5994
3167.2680	3167.7152	3170.1924
3170.6382	3171.5981	3172.0674
3175.3143	3176.5594	3178.6524
3185.8049	3197.6282	3200.0142
3204.9736	3205.2061	3210.9086
3254.3087	3299.0790	3838.2271

DQ

Zero-point correction= 0.622671

Thermal correction to Energy= 0.655348

Thermal correction to Enthalpy= 0.656292

Thermal correction to Gibbs Free Energy= 0.559919

Sum of electronic and zero-point Energies= -1240.374768

Sum of electronic and thermal Energies= -1240.342090

Sum of electronic and thermal Enthalpies= -1240.341146

Sum of electronic and thermal Free Energies= -1240.437519

Cartesian coordinates

C	-1.458545	-1.234205	-0.058868
C	-0.693867	0.000001	0.000018
C	-1.458546	1.234206	0.058909
C	-2.808196	1.280938	0.067868
C	-3.572502	-0.000002	0.000041
C	-2.808195	-1.280940	-0.067811
H	-0.914853	-2.164299	-0.127266

H	-0.914856	2.164302	0.127296
O	-4.800136	-0.000002	0.000028
C	2.808196	-1.280938	0.067823
C	3.572502	0.000003	0.000008
C	2.808195	1.280941	-0.067826
C	1.458545	1.234207	-0.058874
C	0.693867	0.000002	0.000012
C	1.458546	-1.234204	0.058881
H	0.914854	2.164303	-0.127262
H	0.914856	-2.164300	0.127261
O	4.800136	-0.000002	-0.000092
C	-3.583763	-2.595743	-0.150623
C	-3.583766	2.595741	0.150678
C	3.583766	-2.595743	0.150596
C	3.583763	2.595745	-0.150651
C	-4.455735	-2.612054	-1.420897
H	-4.981494	-3.570234	-1.486429
H	-5.193362	-1.810215	-1.408271
H	-3.832438	-2.506249	-2.314657
C	-2.640384	-3.803158	-0.216400
H	-1.998901	-3.771757	-1.103149
H	-2.005364	-3.873365	0.672878
H	-3.238005	-4.717208	-0.271140
C	-4.469704	-2.761020	1.099427
H	-5.209856	-1.964672	1.171278
H	-4.992468	-3.721666	1.047294
H	-3.856585	-2.758271	2.006409
C	-4.455702	2.612073	1.420977
H	-4.981460	3.570255	1.486507
H	-5.193329	1.810234	1.408387

H	-3.832379	2.506285	2.314721
C	-4.469743	2.760992	-1.099349
H	-5.209894	1.964639	-1.171165
H	-4.992510	3.721636	-1.047219
H	-3.856650	2.758228	-2.006349
C	-2.640388	3.803159	0.216406
H	-1.998880	3.771777	1.103138
H	-2.005393	3.873350	-0.672891
H	-3.238010	4.717208	0.271145
C	2.640388	-3.803163	0.216296
H	1.998885	-3.771804	1.103032
H	2.005389	-3.873330	-0.673000
H	3.238011	-4.717213	0.271008
C	4.455707	-2.612109	1.420891
H	4.981465	-3.570293	1.486393
H	5.193334	-1.810270	1.408319
H	3.832388	-2.506344	2.314641
C	4.469738	-2.760959	-1.099439
H	5.209887	-1.964603	-1.171238
H	4.992507	-3.721604	-1.047336
H	3.856641	-2.758175	-2.006436
C	4.469583	2.761119	1.099472
H	5.209748	1.964794	1.171443
H	4.992329	3.721774	1.047328
H	3.856379	2.758412	2.006396
C	2.640381	3.803148	-0.216602
H	1.998994	3.771690	-1.103419
H	2.005265	3.873402	0.672603
H	3.238002	4.717199	-0.271332
C	4.455857	2.611969	-1.420843

H	4.981629	3.570141	-1.486386
H	5.193477	1.810125	-1.408094
H	3.832645	2.506111	-2.314656

Vibrational frequencies

8.6400	18.7784	21.7915
43.9682	60.7455	68.2413
69.6189	77.7636	112.9763
126.6174	147.9039	151.8216
161.1348	162.1740	162.3839
191.1589	208.7237	217.8002
220.9982	225.7426	250.7928
251.0484	251.5679	251.8386
268.7482	273.4435	275.3470
290.1250	293.6512	302.4861
309.2192	315.7642	321.3506
337.0157	359.0627	359.6960
363.6718	367.6505	369.1655
370.0582	382.4638	384.0705
384.6575	397.4871	399.3234
402.1422	407.0047	440.4432
442.4637	447.0554	451.4733
467.6141	515.7444	523.3007
527.3516	546.4425	569.6151
579.4528	586.9803	640.1168
671.6599	680.4038	686.0788
763.9986	765.3463	804.5991
817.9227	821.4705	822.8041
833.4614	860.8662	889.0936
902.6428	911.8591	913.5710

915.3145	933.9864	945.0284
953.2712	953.3711	953.4918
953.9402	957.5924	958.0444
958.0699	958.1305	965.9360
965.9415	966.0284	966.0398
1027.6883	1048.0375	1053.6346
1054.2343	1054.6321	1055.1409
1055.5975	1055.9997	1069.5120
1113.7238	1118.7696	1216.9721
1223.3331	1246.3908	1246.5112
1246.5852	1247.0594	1253.3426
1256.8007	1257.3040	1257.9130
1296.0957	1307.6851	1312.6707
1317.2427	1339.5561	1382.9242
1392.1049	1395.3263	1395.3517
1395.3994	1395.4732	1397.4938
1399.4013	1404.1990	1407.0923
1419.6145	1428.1579	1428.8207
1429.3734	1430.3664	1463.8352
1472.9803	1486.3257	1486.3576
1486.4468	1486.4870	1502.2966
1502.4408	1502.5234	1502.6908
1502.9262	1502.9630	1503.1063
1504.6553	1506.5430	1507.1005
1507.1414	1507.2913	1517.6133
1517.7322	1517.9265	1518.0655
1534.4319	1534.5965	1534.8559
1535.2639	1594.9417	1669.4595
1680.7985	1717.9186	1735.1368
1740.3005	1759.0350	3062.8215

3062.8688	3063.0914	3063.1348
3069.9551	3069.9595	3069.9916
3070.0236	3073.3239	3073.3255
3073.3504	3073.7766	3139.8596
3139.9134	3139.9936	3140.0587
3141.1099	3141.1114	3141.1726
3141.2170	3141.8099	3141.9707
3142.1055	3142.1713	3151.2744
3151.2827	3151.3332	3151.4855
3195.4499	3195.4575	3195.5968
3195.6040	3199.3949	3199.4094
3199.5616	3199.5728	3272.0405
3272.2565	3304.7509	3306.6315

R_p -INT03

Zero-point correction= 1.329901

Thermal correction to Energy= 1.403187

Thermal correction to Enthalpy= 1.404132

Thermal correction to Gibbs Free Energy= 1.223185

Sum of electronic and zero-point Energies= -3025.394799

Sum of electronic and thermal Energies= -3025.321513

Sum of electronic and thermal Enthalpies= -3025.320569

Sum of electronic and thermal Free Energies= -3025.501515

Cartesian coordinates

O	1.651930	-0.988090	-1.041778
H	1.521642	-1.487314	-0.220056
C	-3.778802	-1.689909	0.815625
C	-4.560494	-1.966668	-0.377701
C	-5.617536	-1.221825	-0.763964

C	-6.047288	-0.077972	0.100041
C	-5.244895	0.234427	1.320920
C	-4.205023	-0.566425	1.632581
C	-2.597922	-2.364463	1.080400
C	-2.078132	-3.382304	0.183050
C	-0.779242	-3.759259	0.169189
C	0.154192	-3.077790	1.104461
C	-0.412836	-2.269321	2.215948
C	-1.730355	-1.969790	2.176943
H	-4.253365	-2.790578	-1.004537
H	-3.627297	-0.335629	2.514306
H	-2.760283	-3.841697	-0.518345
H	-2.148349	-1.365796	2.969548
O	-7.039100	0.584205	-0.185162
O	1.378145	-3.169361	0.955348
C	0.527444	-1.738537	3.298088
C	-0.246244	-0.993896	4.392857
H	-0.743862	-0.096274	4.008212
H	-0.998629	-1.634143	4.864519
H	0.454898	-0.672781	5.167876
C	1.285027	-2.903402	3.960977
H	0.585528	-3.585250	4.455056
H	1.869145	-3.465556	3.231245
H	1.967600	-2.508509	4.720566
C	1.530979	-0.748545	2.669657
H	2.208162	-1.246031	1.973544
H	1.010633	0.052475	2.129915
H	2.131700	-0.289179	3.462789
C	-5.634350	1.440320	2.175698
C	-7.042256	1.226654	2.763463

H	-7.792041	1.145959	1.976383
H	-7.070146	0.318147	3.373650
H	-7.299177	2.075208	3.405976
C	-5.604238	2.727695	1.329716
H	-4.593719	2.911688	0.952401
H	-6.293625	2.673764	0.487398
H	-5.888981	3.576962	1.959550
C	-4.654660	1.638086	3.339262
H	-4.657694	0.788111	4.029561
H	-3.631895	1.794522	2.975778
H	-4.949098	2.526461	3.904790
C	-6.382665	-1.491780	-2.058613
C	-5.780604	-2.671847	-2.831351
H	-4.738674	-2.484805	-3.111968
H	-5.827346	-3.602449	-2.256499
H	-6.352049	-2.821259	-3.751484
C	-7.852514	-1.833282	-1.747692
H	-8.377203	-2.053664	-2.683071
H	-7.912375	-2.720401	-1.109057
H	-8.357572	-1.005798	-1.250715
C	-6.307296	-0.249431	-2.967813
H	-6.810501	-0.464040	-3.916102
H	-6.787587	0.613069	-2.506263
H	-5.263733	0.001627	-3.185395
C	-0.223758	-4.796240	-0.807575
C	-1.353461	-5.510285	-1.560160
H	-1.921524	-4.822391	-2.194649
H	-0.920060	-6.274071	-2.211641
H	-2.046574	-6.005868	-0.872622
C	0.675221	-4.105281	-1.851140

H	1.499473	-3.562060	-1.386723
H	1.090542	-4.859634	-2.528579
H	0.093160	-3.397454	-2.449877
C	0.581597	-5.864893	-0.044405
H	0.921109	-6.631105	-0.748372
H	1.455197	-5.434702	0.446236
H	-0.042931	-6.352793	0.710898
C	1.451176	1.479900	-1.041518
C	0.873285	1.691465	-2.315691
C	0.383125	2.965044	-2.603493
H	0.012774	3.168108	-3.606337
C	0.189715	3.915675	-1.603129
H	-0.323640	4.846522	-1.834905
C	0.456008	3.585608	-0.273789
C	1.195449	2.424706	-0.038687
H	1.477218	2.172997	0.982575
C	2.216045	0.258609	-0.720606
C	0.537955	0.550548	-3.247986
H	1.341043	-0.190100	-3.277825
H	0.408940	0.948484	-4.258729
C	-0.805898	-0.204305	-2.833730
H	-1.447729	-0.274367	-3.717273
H	-0.540500	-1.218347	-2.525204
C	-1.534690	0.473972	-1.697436
C	-2.290570	1.631493	-1.885483
H	-2.614959	1.906187	-2.888946
C	-2.471622	2.557232	-0.851993
C	-1.916748	2.320653	0.424480
C	-1.465294	1.024888	0.667194
H	-1.101909	0.769171	1.661092

C	-1.256610	0.125851	-0.375944
H	-0.726115	-0.801299	-0.180707
C	-3.071699	3.847075	-1.238961
H	-3.483951	3.862033	-2.269528
C	-1.515134	3.417698	1.386439
H	-1.215302	2.938513	2.324196
H	-2.338087	4.101165	1.603006
C	-0.290881	4.275980	0.845622
H	-0.680226	5.229533	0.479187
H	0.368331	4.487406	1.694283
O	-3.135273	4.843307	-0.544854
C	5.332845	-0.544605	0.738645
C	3.459029	0.231066	-0.170719
N	4.132158	-0.939310	0.211844
N	4.338969	1.237264	0.239953
N	5.517352	0.720620	0.834040
C	4.179056	2.637022	0.099864
C	3.968889	3.412013	1.247492
C	3.708229	4.772050	1.088569
C	3.632184	5.357893	-0.175765
C	3.882479	4.563948	-1.295677
C	4.172492	3.205778	-1.181794
H	3.527035	5.381263	1.971586
H	3.847217	5.012808	-2.285998
C	3.963439	2.765234	2.605704
H	3.648755	3.474525	3.373627
H	3.280337	1.907564	2.616685
H	4.952747	2.377886	2.864201
C	3.243588	6.805049	-0.333915
H	2.163590	6.890277	-0.498740

H	3.489817	7.384990	0.558454
H	3.743103	7.260435	-1.192562
C	4.476098	2.371103	-2.396379
H	5.469432	1.918838	-2.308538
H	3.754112	1.555658	-2.514418
H	4.455256	2.985153	-3.298963
C	4.274972	-2.296357	-0.328405
C	5.375489	-2.788789	0.672825
O	6.150742	-1.569783	0.973124
C	6.360598	-3.828746	0.180329
H	7.073405	-4.046212	0.979612
H	5.831823	-4.752032	-0.067430
H	6.914346	-3.489499	-0.694338
C	4.717773	-3.240703	1.973551
H	4.147843	-4.158240	1.802239
H	5.484215	-3.434201	2.727585
H	4.030952	-2.477437	2.348891
C	4.536823	-2.252354	-1.844845
C	5.733575	-1.386503	-2.245215
H	5.633056	-0.365109	-1.864642
H	6.682903	-1.789197	-1.880866
H	5.795636	-1.324975	-3.335427
C	4.586265	-3.644261	-2.482658
H	4.422435	-3.561069	-3.560483
H	5.551022	-4.134672	-2.336618
H	3.806645	-4.297790	-2.076568
H	3.366266	-2.876348	-0.143054
H	3.634812	-1.757433	-2.229786

Vibrational frequencies

12.7964	15.5531	17.8385
23.8768	27.8215	28.9371
31.7696	36.3711	39.5762
42.5408	47.9830	52.3661
53.2232	58.3978	58.8279
61.0723	63.2789	71.1262
74.7300	75.8049	80.0665
83.1686	86.9782	92.8010
99.3157	102.9666	120.1062
122.6241	127.1542	134.6539
140.7973	145.9018	150.5560
153.1381	155.5988	158.3404
158.7133	166.9469	168.6390
178.3865	179.3829	185.9208
193.5875	195.5517	198.7774
211.0175	211.5948	215.5026
220.7722	222.1371	229.0384
236.5811	238.5987	240.4818
243.3932	249.3414	251.5391
252.8932	254.0544	257.5423
267.8848	271.6184	273.7399
275.8443	279.6317	281.8341
283.5515	283.8572	293.6579
298.2832	301.7434	303.6245
306.8013	312.8730	315.8028
316.8311	318.9156	320.5853
322.5284	329.7543	339.7158
342.0679	342.8382	349.8599
354.0117	362.7292	363.4112
365.1842	366.5504	370.1687

379.0587	380.4487	381.2375
383.6040	385.9760	386.8381
389.6068	396.8547	398.3325
402.0430	404.4628	410.5821
418.1644	427.7719	431.8318
441.1855	442.0435	443.2658
444.2468	451.0247	456.8534
468.4587	468.8388	472.4727
486.8062	506.4696	511.0994
517.6851	521.7564	522.7321
526.0341	527.1165	541.2151
546.5387	553.5367	563.5641
575.0684	575.7462	577.2966
583.8497	585.5360	589.3982
603.9536	631.0942	635.7042
643.2290	651.6589	664.5921
676.5804	676.9077	682.0811
683.4973	685.7320	695.0489
719.2585	730.4159	739.5199
754.8303	756.9842	763.5359
765.2815	768.4938	775.7505
795.1531	805.2200	805.7308
809.4328	820.0873	822.3617
829.0371	831.2080	837.6026
845.5565	853.4030	860.9847
866.4768	879.0294	887.5166
893.9813	894.8796	907.2325
908.8434	911.1911	912.7266
915.3081	917.3915	919.1663
925.5078	929.3002	939.1393

939.8118	940.6084	945.1388
949.8368	952.3123	953.1371
953.7761	954.9961	955.3800
956.4600	957.4643	958.8150
959.9726	961.2421	963.3766
964.6629	965.8946	966.6604
966.9083	974.6832	981.2295
983.5307	993.2772	996.2950
1000.9006	1005.2065	1008.8760
1026.4045	1033.3269	1035.0886
1039.1109	1043.7022	1047.6899
1052.1983	1053.7719	1054.7657
1055.5308	1056.7099	1057.3511
1059.1673	1061.1138	1063.3192
1066.2247	1067.5001	1078.0642
1095.8573	1113.1173	1114.7633
1120.5295	1135.2853	1151.5081
1158.3794	1167.7560	1180.4946
1187.7539	1191.6037	1195.0238
1203.3619	1210.6468	1215.2575
1215.8603	1216.4817	1217.9896
1222.7725	1227.1442	1227.6721
1232.6422	1243.3897	1245.0921
1246.5762	1247.2832	1247.5340
1251.5773	1256.1013	1256.4760
1257.2712	1259.4089	1276.0353
1278.3240	1281.8083	1282.6622
1284.4383	1294.4299	1302.0882
1306.6275	1312.0913	1316.3114
1318.1760	1320.5863	1326.8810

1330.1272	1332.5620	1335.4195
1347.2746	1351.4250	1353.7596
1356.3700	1362.6091	1371.2869
1380.6172	1384.7843	1390.7023
1392.7916	1393.6852	1393.9837
1396.4256	1397.3025	1399.9068
1400.2984	1404.4457	1406.7834
1413.9865	1414.9940	1416.4016
1417.3898	1417.9393	1425.3633
1426.7272	1428.2783	1428.9049
1429.9080	1430.2371	1430.9658
1437.5138	1437.8368	1461.5894
1464.7292	1466.8541	1469.2101
1472.3758	1477.1600	1478.6977
1479.8500	1481.7937	1482.2335
1483.9236	1484.5770	1485.3572
1486.3770	1486.4816	1489.1392
1490.3605	1494.5131	1495.4204
1496.1107	1498.0186	1498.3482
1499.9001	1502.0846	1502.2011
1502.6867	1502.7476	1503.8686
1504.6251	1504.8791	1505.5544
1505.9196	1506.2943	1506.8652
1507.0202	1507.5917	1509.5958
1516.6492	1517.0189	1517.8207
1520.0327	1520.9349	1522.4358
1527.0295	1532.6000	1535.4493
1536.1709	1537.1639	1540.5215
1548.4060	1554.7745	1594.8903
1636.1337	1641.4295	1663.1298

1669.6424	1672.7316	1680.8361
1685.4336	1693.0614	1705.2530
1715.8689	1724.0871	1734.7873
1759.9992	1788.3444	1824.4609
2966.0291	3057.7757	3058.1463
3060.4810	3061.9563	3063.7622
3065.8390	3068.0444	3068.3049
3068.7915	3069.1998	3069.8165
3069.9652	3071.0326	3072.5097
3073.0152	3074.0490	3077.0562
3077.9550	3078.5283	3081.1432
3084.4218	3087.0540	3093.6782
3095.9730	3127.2030	3134.0791
3134.7784	3135.0435	3135.3007
3135.4377	3137.7671	3138.6672
3139.0044	3139.5048	3139.8842
3140.4637	3140.5046	3141.0207
3141.7714	3142.6998	3142.8726
3146.1570	3149.2035	3150.8750
3151.1207	3152.4834	3152.9744
3153.1278	3155.1435	3157.4161
3160.7242	3165.7069	3165.9087
3166.6534	3168.9075	3169.6614
3172.8675	3175.0924	3179.7043
3183.5302	3184.3019	3185.3427
3186.4070	3189.5640	3190.5420
3191.0148	3191.2140	3193.9960
3194.2599	3196.0021	3197.2691
3201.8766	3202.1961	3206.0064
3238.0466	3266.0377	3270.1776

3298.4627

3307.8156

3776.6801

R_p-TS3

Zero-point correction= 1.325817

Thermal correction to Energy= 1.397090

Thermal correction to Enthalpy= 1.398034

Thermal correction to Gibbs Free Energy= 1.225202

Sum of electronic and zero-point Energies= -3025.384685

Sum of electronic and thermal Energies= -3025.313412

Sum of electronic and thermal Enthalpies= -3025.312467

Sum of electronic and thermal Free Energies= -3025.485300

Cartesian coordinates

O	1.191409	0.875577	-1.082445
H	0.970929	1.673080	-0.328023
C	-4.730616	1.026886	0.751973
C	-5.216692	0.138908	1.762668
C	-6.299152	-0.674398	1.596021
C	-7.035762	-0.638499	0.313562
C	-6.572077	0.310715	-0.720369
C	-5.484139	1.093141	-0.463167
C	-3.474075	1.692909	0.870820
C	-3.032088	2.632030	-0.108288
C	-1.722637	3.020177	-0.235760
C	-0.754169	2.440566	0.668485
C	-1.210667	1.707752	1.828474
C	-2.541435	1.371177	1.900772
H	-4.694084	0.113821	2.710438
H	-5.133478	1.756008	-1.242735
H	-3.765500	3.040349	-0.789966

H	-2.878795	0.773930	2.736372
O	-8.010963	-1.382644	0.112532
O	0.514167	2.576072	0.443211
C	-0.215812	1.299638	2.922489
C	-0.919628	0.583849	4.083179
H	-1.366842	-0.365553	3.768123
H	-0.185556	0.361639	4.862697
H	-1.702712	1.205890	4.527679
C	0.861331	0.339232	2.376319
H	1.464102	-0.042913	3.208586
H	0.401341	-0.520068	1.874246
H	1.529920	0.835966	1.672507
C	0.462667	2.559274	3.492599
H	0.974909	3.124569	2.712377
H	-0.278104	3.211963	3.965136
H	1.195926	2.271408	4.254017
C	-7.296794	0.352161	-2.066364
C	-6.679509	1.384973	-3.017512
H	-5.633285	1.153634	-3.247919
H	-7.235777	1.380031	-3.959475
H	-6.727814	2.398487	-2.605666
C	-8.775632	0.730846	-1.860712
H	-9.285276	0.763286	-2.829864
H	-9.278709	0.006396	-1.221018
H	-8.854699	1.722589	-1.403278
C	-7.197175	-1.026278	-2.747246
H	-6.147043	-1.288812	-2.920678
H	-7.656466	-1.800475	-2.133006
H	-7.702956	-0.996522	-3.718550
C	-6.761786	-1.640378	2.687418

C	-8.212807	-1.324769	3.096245
H	-8.284517	-0.305850	3.490808
H	-8.887634	-1.422215	2.246302
H	-8.531790	-2.016305	3.883663
C	-6.665710	-3.087781	2.167730
H	-5.629123	-3.327998	1.905881
H	-6.986298	-3.783175	2.951154
H	-7.293802	-3.230818	1.288896
C	-5.889680	-1.542268	3.944998
H	-6.256620	-2.253759	4.690529
H	-4.843256	-1.790624	3.734540
H	-5.926678	-0.542707	4.390405
C	-1.284977	4.024045	-1.309897
C	-0.489089	5.171457	-0.660747
H	0.410808	4.802362	-0.167315
H	-0.195740	5.893822	-1.429703
H	-1.104996	5.694598	0.077990
C	-0.426207	3.333958	-2.385137
H	0.495025	2.925178	-1.973149
H	-0.984893	2.516915	-2.854610
H	-0.167298	4.059153	-3.164570
C	-2.494968	4.643256	-2.023113
H	-3.062634	3.896039	-2.588456
H	-3.172624	5.137465	-1.319747
H	-2.141219	5.394510	-2.734869
C	3.434640	0.025075	-0.659523
C	4.164442	0.806845	-1.595307
C	5.534992	0.566247	-1.668365
H	6.110328	1.065229	-2.444626
C	6.212027	-0.133365	-0.670366

H	7.297722	-0.191023	-0.696081
C	5.526860	-0.568056	0.465737
C	4.135011	-0.592467	0.388483
H	3.560143	-1.011475	1.213359
C	1.980593	-0.126564	-0.755658
C	3.606736	2.016372	-2.310083
H	2.618956	1.830699	-2.737665
H	4.286929	2.266624	-3.128910
C	3.493398	3.283211	-1.350516
H	3.831530	4.157989	-1.913963
H	2.438727	3.436672	-1.102223
C	4.264158	3.121981	-0.058679
C	5.657257	3.113850	-0.011522
H	6.230625	3.515951	-0.846556
C	6.342002	2.416583	0.991611
C	5.631304	1.730600	1.998909
C	4.276406	2.038286	2.116541
H	3.699830	1.600983	2.929245
C	3.600904	2.710740	1.100571
H	2.519075	2.794825	1.145483
C	7.795031	2.265285	0.786395
H	8.216491	2.956216	0.026638
C	6.165763	0.516424	2.723475
H	5.479469	0.288519	3.543832
H	7.155860	0.691457	3.145022
C	6.257171	-0.756567	1.774268
H	7.312158	-0.953131	1.566772
H	5.857650	-1.617246	2.320879
O	8.518139	1.464098	1.345757
C	-0.201166	-2.951717	-0.600967

C	1.352794	-1.394959	-0.660588
N	-0.008879	-1.605908	-0.629252
N	1.868851	-2.669426	-0.636823
N	0.888534	-3.647910	-0.583293
C	3.229603	-3.098900	-0.712967
C	3.803121	-3.672755	0.425573
C	5.150382	-4.022066	0.362046
C	5.908947	-3.802651	-0.788556
C	5.280371	-3.273850	-1.917133
C	3.932367	-2.922569	-1.909710
H	5.624341	-4.450858	1.241835
H	5.855081	-3.125980	-2.828267
C	3.002064	-3.857006	1.686203
H	2.251797	-4.643211	1.563702
H	3.654165	-4.123047	2.519746
H	2.459906	-2.940642	1.947485
C	7.386979	-4.089551	-0.801687
H	7.650815	-4.860178	-0.074309
H	7.721454	-4.412915	-1.790083
H	7.945774	-3.182672	-0.544333
C	3.255615	-2.383257	-3.141113
H	3.905117	-2.494260	-4.010891
H	2.322485	-2.920952	-3.336477
H	3.013217	-1.320588	-3.033889
C	-1.292647	-0.932489	-0.901293
C	-2.231498	-2.065854	-0.342020
O	-1.472661	-3.307275	-0.631372
C	-3.602108	-2.221762	-0.964414
H	-3.548538	-2.440480	-2.030573
H	-4.122236	-3.044294	-0.466782

H	-4.184050	-1.307887	-0.809754
C	-2.341336	-1.977460	1.174747
H	-2.970000	-1.127218	1.442997
H	-2.802975	-2.891214	1.556421
H	-1.361386	-1.853361	1.645164
C	-1.366538	-0.530611	-2.389644
C	-1.079359	-1.683839	-3.354835
H	-1.810127	-2.492930	-3.270158
H	-1.110321	-1.312750	-4.382427
H	-0.083449	-2.109562	-3.193909
C	-2.662897	0.205334	-2.748797
H	-2.938782	0.924810	-1.971920
H	-2.515665	0.757484	-3.681976
H	-3.505340	-0.472485	-2.902768
H	-1.387979	-0.037719	-0.274473
H	-0.550481	0.194841	-2.488734

Vibrational frequencies

-1489.8718	19.8198	20.5895
25.4807	30.3835	34.8969
42.3822	45.5933	48.9328
54.3254	57.4598	59.9980
61.7160	68.4144	69.8978
70.8835	73.1910	78.5623
82.3254	83.2294	84.2699
91.8356	93.0487	97.8362
100.5807	106.9606	116.6782
121.8408	135.2214	136.4062
137.3164	140.4812	145.9465
149.6235	158.5590	161.0704

163.8778	170.4376	171.6917
176.6144	183.0518	191.2716
197.4886	203.0421	205.6413
214.5909	218.8619	227.6131
228.6850	231.4138	233.2740
236.8358	241.2806	243.2274
249.1248	250.6164	251.8825
256.6025	260.0292	264.4374
272.4626	278.4146	279.1590
280.6504	283.2745	285.4210
288.3269	294.3431	299.1739
301.5366	309.2274	312.0318
316.9364	318.8714	320.8125
324.0364	324.8267	329.0189
330.3450	332.4736	346.2800
349.1866	358.3235	365.0957
366.1792	367.4541	367.8420
370.8125	373.2262	374.4594
376.7625	381.6606	383.4873
388.9906	393.0807	397.0749
400.3729	404.1395	407.0151
409.3290	412.3133	416.0668
424.0436	430.7847	435.3545
443.0643	443.7276	456.1397
459.2140	463.5138	466.8178
468.6219	484.3059	503.4325
505.5276	512.0379	522.5997
524.8956	526.5424	530.5227
534.9250	538.5174	547.6777
549.5670	562.0583	574.0780

577.8488	587.6187	592.2399
596.5324	607.8816	611.8882
620.2608	630.2043	649.8080
650.1487	664.4460	671.5783
674.2553	677.5604	681.2418
684.1698	686.8601	706.5601
731.4342	737.6590	742.6057
755.9957	758.0312	763.3242
768.9474	772.2968	773.6251
790.3096	800.9103	805.8504
809.4209	816.1771	817.1356
831.5254	833.9881	846.2246
847.3125	855.8865	864.7448
870.1460	880.4224	885.4285
895.3966	904.3853	910.8361
914.3032	914.9064	915.6540
919.2772	920.3812	924.6749
925.5083	931.9007	933.5088
936.4509	947.5756	948.9994
951.4856	951.8003	952.3614
953.1710	954.2513	955.6210
956.5950	957.3604	957.5624
960.2077	961.8241	962.4287
962.6730	964.0145	965.0065
975.4530	979.2992	980.7456
985.9207	990.4721	998.6579
1005.7599	1009.6945	1018.3554
1030.5319	1036.5456	1039.6596
1039.7244	1042.6444	1047.8072
1049.8865	1051.7236	1052.2372

1054.4767	1056.2409	1056.8015
1059.0881	1059.8566	1064.1710
1066.8511	1096.4655	1099.9796
1107.4098	1114.5952	1121.5681
1137.4778	1142.0159	1148.4084
1158.1544	1162.0979	1173.2690
1182.2995	1194.9252	1198.0308
1203.9878	1211.0570	1218.9158
1219.5969	1221.9424	1224.2549
1225.4462	1227.3228	1231.5117
1234.0411	1235.0537	1243.0464
1245.2801	1245.5748	1248.2257
1249.9117	1253.9628	1256.8536
1258.4045	1273.8321	1276.2177
1280.6760	1284.5649	1289.2435
1294.0242	1295.9204	1297.3592
1304.8673	1310.7245	1319.2971
1319.9562	1324.4543	1333.5413
1336.2802	1339.8618	1343.6844
1349.0864	1359.3666	1360.5198
1363.3660	1363.5108	1376.3536
1376.8770	1379.5088	1381.9103
1388.9351	1390.2506	1390.9532
1391.1574	1393.4169	1396.6028
1396.8836	1400.1574	1408.4710
1412.7735	1413.5627	1413.6687
1416.8701	1418.3013	1423.6286
1425.1399	1425.8618	1426.7051
1426.9099	1427.5472	1431.4833
1436.2601	1438.2896	1442.4314

1463.8016	1465.8138	1472.6273
1475.1104	1477.1438	1480.5682
1482.8558	1483.4009	1484.4026
1484.6132	1484.6985	1485.7541
1486.2418	1487.4122	1489.4003
1492.7975	1494.0622	1495.2016
1495.4647	1496.2997	1497.8078
1499.4509	1500.3780	1501.0338
1501.3405	1501.6165	1502.2684
1502.7339	1503.0338	1503.8255
1504.2814	1504.6603	1506.2643
1508.1472	1509.8565	1515.5653
1516.4164	1517.3732	1517.9414
1518.6235	1519.5927	1520.0900
1521.2076	1521.7796	1528.1191
1530.9695	1532.7854	1533.0288
1534.0593	1536.4209	1545.4202
1550.1631	1552.3619	1582.3526
1613.2760	1625.4084	1635.7378
1641.7062	1671.1866	1674.5165
1677.8087	1686.3214	1690.9836
1692.7839	1729.9648	1731.4113
1825.1091	2963.1361	3056.5160
3057.1714	3059.5240	3060.1181
3060.3129	3062.4461	3062.5264
3066.5692	3067.3622	3067.5833
3068.2721	3068.4352	3070.2102
3071.3257	3071.4905	3076.8316
3081.7245	3082.6844	3087.9960
3088.4997	3091.7758	3096.8493

3100.4007	3101.8101	3111.7737
3127.3357	3128.2440	3130.5090
3133.6814	3134.3805	3134.6722
3134.9810	3135.3600	3135.8619
3137.4413	3138.1047	3138.9670
3139.2595	3139.3217	3140.6154
3141.4522	3143.2034	3144.8005
3145.2018	3148.8269	3149.9736
3150.4809	3154.8503	3156.3839
3165.2673	3166.8223	3168.5334
3171.1978	3172.2546	3172.7835
3174.3387	3174.5056	3178.8305
3180.7157	3183.3642	3187.1494
3191.9927	3193.4240	3193.8091
3194.0223	3194.1097	3194.9923
3195.9744	3200.9964	3202.3474
3203.9747	3204.3683	3210.4622
3219.5506	3236.9177	3249.9210
3257.8393	3280.1974	3282.1820

DQH

Zero-point correction= 0.633242

Thermal correction to Energy= 0.665630

Thermal correction to Enthalpy= 0.666574

Thermal correction to Gibbs Free Energy= 0.573217

Sum of electronic and zero-point Energies= -1241.113589

Sum of electronic and thermal Energies= -1241.081201

Sum of electronic and thermal Enthalpies= -1241.080257

Sum of electronic and thermal Free Energies= -1241.173614

Cartesian coordinates

C	-1.450903	-1.154545	-0.333066
C	-0.720265	-0.005450	-0.005368
C	-1.450939	1.140482	0.323355
C	-2.847302	1.178569	0.324835
C	-3.530971	-0.010550	-0.000350
C	-2.844700	-1.197132	-0.330259
H	-0.895143	-2.038957	-0.619939
H	-0.896523	2.025935	0.608651
O	-4.905235	-0.076134	-0.012122
C	2.880264	-1.191616	0.326051
C	3.641741	0.000906	0.000230
C	2.877806	1.190904	-0.329098
C	1.490493	1.149568	-0.322856
C	0.757955	-0.003767	-0.005761
C	1.492822	-1.154929	0.313751
H	0.932459	2.038851	-0.603185
H	0.936490	-2.046031	0.591577
O	4.921099	0.003151	0.003062
C	-3.602136	-2.487712	-0.685530
C	-3.599477	2.474685	0.682482
C	3.636298	-2.475818	0.690958
C	3.631218	2.477731	-0.690147
C	-4.488093	-2.269490	-1.926224
H	-4.998073	-3.204488	-2.183993
H	-5.240278	-1.499800	-1.754118
H	-3.873641	-1.972617	-2.782469
C	-2.640357	-3.638458	-1.013322
H	-2.013932	-3.411601	-1.881482
H	-1.987038	-3.876533	-0.168060

H	-3.224998	-4.533345	-1.247450
C	-4.462969	-2.943710	0.507600
H	-5.208177	-2.195251	0.776484
H	-4.980315	-3.875889	0.254313
H	-3.829443	-3.134989	1.379977
C	-4.457315	2.281776	1.952445
H	-4.993204	3.207883	2.183450
H	-5.198437	1.480541	1.889390
H	-3.807989	2.041882	2.799337
C	-4.452476	2.954336	-0.512980
H	-5.185717	2.228541	-0.874832
H	-4.996606	3.864331	-0.240864
H	-3.798801	3.186288	-1.358796
C	-2.633571	3.626686	0.997630
H	-2.002801	3.400536	1.861835
H	-1.987134	3.855944	0.145656
H	-3.214222	4.524066	1.231134
C	2.696453	-3.643896	1.013696
H	2.054801	-3.425322	1.874016
H	2.053381	-3.895941	0.163407
H	3.291835	-4.530545	1.257604
C	4.516072	-2.232275	1.930344
H	5.094164	-3.132806	2.172942
H	5.197158	-1.402742	1.740275
H	3.890211	-1.988368	2.796371
C	4.523482	-2.909878	-0.490132
H	5.210532	-2.104759	-0.750670
H	5.095798	-3.808748	-0.228198
H	3.902993	-3.145789	-1.362256
C	4.511643	2.914226	0.495147

H	5.200367	2.111379	0.758272
H	5.081909	3.815283	0.236267
H	3.886489	3.147434	1.364691
C	2.688898	3.642836	-1.016489
H	2.052057	3.422614	-1.879961
H	2.041000	3.892037	-0.168997
H	3.282343	4.531706	-1.257000
C	4.517314	2.237920	-1.925725
H	5.093066	3.140710	-2.165503
H	5.200733	1.410917	-1.733048
H	3.896134	1.991911	-2.794506
H	-5.274255	0.781203	0.214849

Vibrational frequencies

24.3240	30.4363	43.2057
49.9504	63.8732	73.5990
82.4735	83.8090	112.6945
127.7932	142.3768	167.3896
171.8595	179.8267	183.9021
198.7828	206.4953	224.5533
225.6584	232.5138	234.2325
254.1931	258.8505	263.3288
275.5398	278.1159	288.4222
294.8807	306.2727	312.5897
321.5358	325.9958	328.1591
336.6529	352.1735	361.7223
366.3584	370.4609	370.8653
378.5866	379.7416	385.6335
393.7819	403.2391	404.3994
408.5154	414.8166	435.7266

446.7690	450.5966	456.1368
469.9771	480.9736	525.0046
529.8149	543.4674	550.7027
591.9314	615.3046	638.5106
640.3137	641.3746	666.3019
684.1008	776.1407	777.9005
782.2518	783.5199	804.8097
834.3932	842.6067	871.4484
908.3889	919.2404	925.3634
929.9228	938.6288	941.7063
946.0363	946.5744	946.9363
952.2975	953.6191	954.9582
957.2452	963.4831	966.4040
966.4244	967.1022	973.6794
976.1672	1044.1384	1047.7686
1048.6984	1051.0825	1059.4372
1059.8141	1060.1249	1060.8066
1140.2098	1143.3634	1151.9236
1175.8766	1215.5726	1231.9492
1242.1357	1244.5171	1245.4325
1248.8995	1250.9741	1251.5516
1252.0815	1280.7566	1287.8174
1294.6339	1301.9030	1308.1023
1323.7644	1331.7726	1347.8350
1360.0157	1381.7886	1382.2410
1384.8083	1389.4984	1398.8880
1402.3219	1409.3014	1413.6995
1416.3672	1420.6287	1426.5690
1429.4201	1445.2887	1453.3037
1481.6035	1481.6464	1486.3195

1486.7001	1487.9271	1493.0898
1498.5913	1500.7477	1501.5430
1501.7726	1502.3635	1503.5786
1504.7314	1505.6092	1507.3355
1509.1138	1511.1326	1517.7180
1517.8970	1519.1166	1519.8357
1530.3338	1535.3827	1535.9649
1536.8565	1538.1836	1571.8416
1594.2282	1663.6146	1670.5076
1683.3780	3045.8461	3045.9890
3048.6848	3049.0465	3054.5242
3055.1047	3062.1335	3063.1610
3068.4509	3068.5572	3070.8144
3075.4574	3113.3705	3113.5513
3115.6038	3115.7994	3129.2454
3129.5047	3132.2795	3133.0405
3133.1566	3133.2834	3143.8458
3145.8216	3146.6951	3148.0347
3151.0930	3151.9254	3152.8585
3155.7736	3190.7239	3191.0747
3191.2965	3192.6050	3199.5034
3199.7373	3205.2048	3207.1944
3249.7386	3252.0197	3944.8328

R_p -INT3

Zero-point correction= 1.332187

Thermal correction to Energy= 1.404119

Thermal correction to Enthalpy= 1.405063

Thermal correction to Gibbs Free Energy= 1.229120

Sum of electronic and zero-point Energies= -3025.408910

Sum of electronic and thermal Energies= -3025.336978

Sum of electronic and thermal Enthalpies= -3025.336034

Sum of electronic and thermal Free Energies= -3025.511977

Cartesian coordinates

O	1.951928	-0.863972	-1.062139
H	1.487516	-2.872928	-0.854409
C	-4.176445	-1.421829	0.114916
C	-4.573805	-0.578505	-0.932857
C	-5.743886	0.163613	-0.904963
C	-6.620114	0.092082	0.251269
C	-6.217177	-0.804810	1.322644
C	-5.024818	-1.507848	1.227717
C	-2.868254	-2.097593	0.063344
C	-2.342367	-2.567578	-1.147451
C	-1.048080	-3.078690	-1.260560
C	-0.246988	-3.065263	-0.100986
C	-0.749871	-2.676654	1.155262
C	-2.068572	-2.219044	1.205051
H	-3.894274	-0.475448	-1.774902
H	-4.733067	-2.177452	2.033036
H	-2.985344	-2.531608	-2.018327
H	-2.473905	-1.854004	2.141164
O	-7.689249	0.788105	0.325634
O	1.085389	-3.456796	-0.195962
C	0.135162	-2.651656	2.412386
C	-0.662310	-2.270814	3.667980
H	-1.061346	-1.253507	3.610241
H	-1.495706	-2.958451	3.839720
H	-0.000087	-2.318506	4.537575

C	0.762426	-4.031727	2.678114
H	-0.021581	-4.777201	2.844347
H	1.381869	-4.365954	1.844901
H	1.381696	-3.987684	3.581422
C	1.237658	-1.591391	2.236459
H	1.890894	-1.844727	1.401204
H	0.797106	-0.607629	2.035134
H	1.840396	-1.515493	3.148886
C	-7.123666	-0.942993	2.552449
C	-8.515303	-1.442008	2.123874
H	-8.943153	-0.757285	1.391646
H	-8.438763	-2.439796	1.677377
H	-9.181377	-1.509963	2.993117
C	-7.262359	0.420942	3.252516
H	-6.286916	0.757072	3.621746
H	-7.648450	1.156970	2.547465
H	-7.941794	0.343455	4.110659
C	-6.573822	-1.937274	3.582430
H	-6.472798	-2.944003	3.162818
H	-5.595685	-1.627409	3.966178
H	-7.262647	-1.995912	4.432174
C	-6.102822	1.112641	-2.055178
C	-5.093482	1.046410	-3.208327
H	-4.089197	1.341975	-2.885235
H	-5.031493	0.039133	-3.635117
H	-5.406818	1.731081	-4.004217
C	-7.483555	0.751082	-2.631490
H	-7.757612	1.449586	-3.432027
H	-7.463024	-0.258896	-3.056683
H	-8.234523	0.787501	-1.842634

C	-6.123829	2.561815	-1.536465
H	-6.416186	3.253766	-2.336547
H	-6.829801	2.645879	-0.709451
H	-5.125422	2.849003	-1.184246
C	-0.558639	-3.713657	-2.579120
C	-1.608713	-3.569087	-3.690416
H	-1.803308	-2.518325	-3.931737
H	-1.239110	-4.059778	-4.595267
H	-2.555748	-4.042334	-3.418648
C	0.748646	-3.091121	-3.118650
H	1.634825	-3.483798	-2.612143
H	0.866022	-3.348220	-4.175806
H	0.749874	-2.000320	-3.035520
C	-0.330103	-5.217310	-2.338078
H	0.030107	-5.693557	-3.256741
H	0.409715	-5.377030	-1.550184
H	-1.264887	-5.703471	-2.043367
C	1.828994	1.491458	-0.653351
C	1.292011	1.959168	-1.873944
C	1.016736	3.326629	-1.927158
H	0.702497	3.761506	-2.872041
C	0.934307	4.090850	-0.767982
H	0.573730	5.114975	-0.830146
C	1.128090	3.515559	0.492986
C	1.728211	2.259603	0.514548
H	2.006380	1.814674	1.469318
C	2.420368	0.148170	-0.574526
C	0.792454	1.076910	-2.993606
H	1.426303	0.199121	-3.138700
H	0.815879	1.656039	-3.919661

C	-0.708002	0.587009	-2.745596
H	-1.297365	0.844170	-3.630407
H	-0.708314	-0.503234	-2.651993
C	-1.323727	1.174627	-1.499112
C	-1.904811	2.441354	-1.469535
H	-2.187945	2.930791	-2.401408
C	-1.947664	3.186725	-0.283380
C	-1.452148	2.642276	0.918535
C	-1.197387	1.270601	0.921083
H	-0.913477	0.787549	1.853698
C	-1.097622	0.555288	-0.268477
H	-0.712251	-0.461300	-0.250228
C	-2.317642	4.606936	-0.432183
H	-2.866943	4.836056	-1.368828
C	-0.915435	3.470910	2.063285
H	-0.783358	2.808934	2.923293
H	-1.596093	4.272968	2.348867
C	0.490330	4.128489	1.716579
H	0.333818	5.194665	1.537624
H	1.142613	4.024060	2.589368
O	-2.045122	5.498391	0.348481
C	5.546036	-0.982227	0.906822
C	3.774281	-0.023323	0.099887
N	4.325780	-1.226565	0.363942
N	4.692693	0.873083	0.487969
N	5.813465	0.291611	1.005300
C	4.645008	2.315142	0.432972
C	4.519107	3.002076	1.642888
C	4.389979	4.386373	1.567505
C	4.387003	5.057961	0.343093

C	4.573224	4.324102	-0.829637
C	4.715399	2.937993	-0.814836
H	4.268626	4.951411	2.487902
H	4.606013	4.841254	-1.784841
C	4.483779	2.282504	2.964769
H	4.149196	2.957285	3.753512
H	3.805958	1.421482	2.943123
H	5.474576	1.903401	3.229958
C	4.147817	6.542316	0.285210
H	3.074726	6.740654	0.187300
H	4.495570	7.037576	1.193845
H	4.647910	6.992875	-0.574474
C	4.931499	2.161071	-2.086558
H	5.702072	1.394959	-1.962098
H	4.010787	1.669348	-2.419114
H	5.246854	2.833002	-2.885657
C	4.183163	-2.685665	0.112473
C	5.235896	-3.174565	1.171354
O	6.225703	-2.060345	1.214022
C	6.003517	-4.442083	0.872731
H	6.719621	-4.610135	1.679906
H	5.313943	-5.288172	0.847477
H	6.545785	-4.391751	-0.069349
C	4.589356	-3.234868	2.549257
H	3.862927	-4.051166	2.575493
H	5.353433	-3.416020	3.307050
H	4.066735	-2.304183	2.788164
C	4.373532	-2.971253	-1.388971
C	5.703346	-2.481618	-1.967241
H	5.848974	-1.407833	-1.810653

H	6.566586	-3.002671	-1.548046
H	5.706890	-2.651518	-3.046323
C	4.087344	-4.440504	-1.719101
H	3.931349	-4.540696	-2.796293
H	4.913455	-5.098836	-1.446071
H	3.180991	-4.791827	-1.213284
H	3.192394	-3.020708	0.427839
H	3.582822	-2.379732	-1.868423

Vibrational frequencies

9.7793	16.9818	22.8909
30.3338	33.4807	36.8337
43.3167	44.8381	48.1766
52.3590	54.5707	56.0092
60.3172	63.7576	66.7129
70.1806	70.8062	72.5130
78.8532	82.2314	88.7048
95.0714	99.1431	101.8781
109.6166	109.8770	120.8648
124.9245	131.1572	133.3556
140.4040	141.1170	156.9427
158.1792	161.2346	169.9450
172.5632	177.3941	177.7625
183.7827	187.5714	191.6612
202.8106	205.4956	206.2637
208.1680	215.3572	223.6741
226.9237	232.2004	238.1882
240.4669	243.0431	250.8614
251.4693	253.0517	255.6989
260.6682	269.0215	275.4337

276.8217	278.8778	279.5098
281.4056	286.4323	288.3583
292.1466	293.3141	302.0325
305.5643	308.0674	314.8010
316.7411	319.6002	320.5411
321.9788	324.7634	326.9254
330.5568	333.1018	339.7990
340.8692	346.6643	357.4119
362.5883	364.7527	369.7507
371.7018	372.6724	373.4347
382.1244	382.6151	384.8685
385.0645	398.0844	403.0858
404.2763	404.6537	409.7140
411.8436	415.0723	419.4291
424.1284	427.1607	434.9598
441.1229	444.1387	452.0056
454.7625	458.0345	467.6710
480.4629	483.5272	485.7433
498.4714	506.2691	515.8683
525.2714	525.9395	531.1568
532.1510	543.9008	544.9507
557.0872	559.0821	565.8517
575.8822	587.5697	593.8854
606.8884	615.5121	616.4981
635.6104	641.1875	650.2978
656.2846	660.9602	671.5574
672.8440	678.5855	689.0390
690.5348	702.4733	731.0660
742.5387	745.3932	753.0340
755.1041	763.5041	774.4449

775.3108	776.8308	783.3567
783.6961	791.8914	803.5126
806.0765	809.6743	815.8668
834.8738	836.5139	841.6338
846.1132	852.0403	860.1949
871.2661	883.7959	887.6145
896.7099	907.4533	909.4067
914.8426	920.6946	921.5159
925.5684	926.0348	926.8027
931.7071	935.7015	939.6997
940.5016	945.7570	945.9635
947.2376	949.3824	950.5532
950.9171	951.8237	953.9196
956.3693	957.2456	960.8602
961.3709	962.8345	964.4614
964.8664	967.5756	975.0687
977.6070	983.7136	984.8619
994.4361	997.2294	1002.1851
1003.9395	1011.3478	1013.0758
1037.9246	1039.4399	1041.5476
1041.6585	1044.2911	1048.6975
1051.2230	1052.7008	1055.6474
1057.7962	1058.0619	1058.1286
1060.4046	1060.9847	1065.5344
1068.1356	1093.5273	1111.8307
1123.5521	1139.3521	1139.8927
1144.7934	1149.5456	1159.4167
1167.4077	1177.9376	1184.1883
1195.0556	1198.7777	1206.1207
1211.4764	1216.4800	1218.7182

1222.3217	1224.7940	1225.8870
1230.1876	1233.5183	1237.7292
1242.9351	1244.6713	1246.2910
1246.5030	1247.1716	1249.6438
1250.5894	1251.5139	1252.6201
1267.3944	1274.0288	1280.0300
1284.3981	1287.2527	1288.3206
1291.8591	1296.0051	1297.5673
1303.6357	1305.1242	1312.8378
1318.9742	1321.0011	1322.3978
1333.2331	1333.5995	1338.3226
1340.3950	1341.2559	1350.7661
1360.0001	1360.4578	1362.7503
1366.4503	1372.2359	1377.2908
1378.2245	1383.3154	1383.8868
1388.0901	1390.2322	1400.6850
1403.3279	1404.2840	1406.3904
1412.4862	1414.9068	1417.7002
1420.3716	1420.7597	1425.0406
1428.1478	1429.5854	1429.9666
1430.8768	1432.8769	1436.9576
1443.2457	1452.4124	1457.5823
1461.1456	1463.6522	1471.5510
1474.5240	1477.3030	1479.2809
1479.8054	1480.0078	1482.0795
1483.9870	1484.9517	1486.8541
1487.7221	1491.7611	1492.4338
1494.2772	1495.2594	1495.9450
1496.0878	1496.3849	1497.7972
1498.7048	1500.0911	1500.2474

1500.5360	1501.2352	1501.6880
1502.4137	1504.2526	1506.0306
1507.1022	1509.4487	1510.1085
1513.9995	1515.0691	1516.5850
1518.4635	1518.7406	1521.2037
1523.0420	1523.4924	1523.7830
1525.8247	1529.7895	1534.2191
1534.6763	1540.6282	1542.4646
1543.7157	1545.3602	1550.4128
1554.8932	1573.4854	1593.7575
1629.1688	1640.8028	1650.1295
1663.4392	1678.1363	1679.4946
1683.8861	1684.2311	1687.0664
1721.0434	1796.9513	1823.0324
2968.4272	3043.5248	3046.1197
3048.3102	3049.8709	3054.0258
3055.3310	3061.9881	3063.6212
3064.0082	3066.9859	3069.4068
3070.4446	3074.3982	3074.9527
3078.2321	3079.3810	3085.3912
3087.8995	3088.3863	3088.9504
3090.5650	3103.0351	3103.9600
3105.5289	3109.8661	3114.4682
3114.8181	3118.5538	3128.4695
3129.0171	3129.3539	3133.0981
3133.9299	3135.4420	3138.8556
3140.9443	3141.6104	3143.1464
3145.1978	3145.2436	3146.9557
3147.5151	3150.7133	3151.6422
3151.7221	3156.1562	3156.8837

3159.1768	3160.3421	3166.5145
3167.9298	3172.2514	3174.9652
3176.4438	3176.8275	3177.8349
3180.0989	3180.4443	3182.4179
3184.8662	3185.2732	3186.7698
3188.1774	3189.0027	3190.1858
3195.1225	3198.6846	3201.0777
3201.3998	3204.8167	3205.2431
3205.2936	3211.4103	3213.1590
3218.5182	3219.7507	3228.6307
3249.2355	3251.7322	3840.2997

MeOH

Zero-point correction= 0.051948

Thermal correction to Energy= 0.055274

Thermal correction to Enthalpy= 0.056218

Thermal correction to Gibbs Free Energy= 0.029198

Sum of electronic and zero-point Energies= -115.615753

Sum of electronic and thermal Energies= -115.612427

Sum of electronic and thermal Enthalpies= -115.611483

Sum of electronic and thermal Free Energies= -115.638502

Cartesian coordinates

C	0.047202	0.659609	0.000000
H	1.090190	0.982490	0.000000
H	-0.440195	1.075458	0.890379
H	-0.440195	1.075458	-0.890379
O	0.047202	-0.755364	0.000000
H	-0.870628	-1.048153	0.000000

Vibrational frequencies

313.7346	1072.4718	1123.1361
1186.3239	1384.5019	1498.1484
1508.7548	1527.2484	3040.0580
3097.1575	3155.7043	3895.3218

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Zero-point correction= 1.385843

Thermal correction to Energy= 1.462032

Thermal correction to Enthalpy= 1.462976

Thermal correction to Gibbs Free Energy= 1.274310

Sum of electronic and zero-point Energies= -3141.056996

Sum of electronic and thermal Energies= -3140.980808

Sum of electronic and thermal Enthalpies= -3140.979863

Sum of electronic and thermal Free Energies= -3141.168529

Cartesian coordinates

C	-4.635246	-0.385912	-0.546004
C	-5.900645	-0.747339	-1.054128
C	-6.541240	-1.800878	-0.398525
H	-7.556925	-2.059586	-0.685939
C	-5.840521	-2.645490	0.459899
H	-6.324563	-3.546100	0.831233
C	-4.474302	-2.458680	0.692951
C	-3.929290	-1.236123	0.308869
H	-2.886521	-1.005022	0.519045
C	-3.986098	0.846232	-1.029578
C	-6.455975	-0.233022	-2.363134
H	-6.350058	0.851028	-2.455452
H	-7.524560	-0.460796	-2.387573

C	-5.765889	-0.900054	-3.636819
H	-6.559948	-1.254521	-4.299863
H	-5.207043	-0.124725	-4.164959
C	-4.831870	-2.026983	-3.264414
C	-5.320792	-3.268848	-2.859583
H	-6.347985	-3.545591	-3.096266
C	-4.594480	-4.088367	-1.988871
C	-3.332431	-3.676848	-1.511683
C	-2.741686	-2.599543	-2.173397
H	-1.748000	-2.280859	-1.875257
C	-3.475877	-1.784351	-3.032921
H	-3.028970	-0.862332	-3.396982
C	-5.317746	-5.259064	-1.455602
H	-6.257611	-5.493094	-1.997684
C	-2.746406	-4.133252	-0.192034
H	-1.732574	-3.728114	-0.123188
H	-2.685806	-5.220635	-0.122566
C	-3.576034	-3.616078	1.057981
H	-4.184683	-4.439524	1.437949
H	-2.862297	-3.331425	1.837947
O	-3.941630	1.208780	-2.190059
O	-4.980027	-5.936085	-0.504727
C	-2.337967	3.574416	0.675851
C	-3.398827	1.830418	-0.041407
N	-2.726774	2.921732	-0.448318
N	-3.412443	1.895052	1.290848
N	-2.732062	2.985882	1.771508
C	-4.117521	1.035012	2.209630
C	-3.372817	0.217146	3.059828
C	-4.085675	-0.677690	3.856375

C	-5.477000	-0.762873	3.805038
C	-6.174779	0.121005	2.979478
C	-5.516166	1.046973	2.174960
H	-3.532719	-1.340345	4.516997
H	-7.261035	0.091411	2.961074
C	-1.873322	0.267596	3.089692
H	-1.425318	0.042135	2.115305
H	-1.515765	1.260845	3.376475
H	-1.487306	-0.456431	3.809011
C	-6.213327	-1.807716	4.599274
H	-6.357504	-2.705282	3.987832
H	-5.653463	-2.098892	5.490210
H	-7.200228	-1.453549	4.904898
C	-6.290601	2.019039	1.323482
H	-5.939753	3.043493	1.480037
H	-6.211332	1.791646	0.254610
H	-7.349329	1.981858	1.583040
C	-2.579575	3.818022	-1.618062
C	-1.445825	4.728700	-1.025492
O	-1.710162	4.706003	0.442787
C	-1.411840	6.181598	-1.443952
H	-0.596129	6.674867	-0.911075
H	-1.208552	6.248182	-2.514837
H	-2.339756	6.705145	-1.221143
C	-0.097566	4.060104	-1.242884
H	0.142892	4.062024	-2.309199
H	0.677762	4.608460	-0.704287
H	-0.111171	3.026637	-0.887277
C	-3.959429	4.404101	-1.978209
C	-4.657807	5.125730	-0.823026

H	-4.787432	4.475728	0.048408
H	-4.123927	6.020690	-0.495788
H	-5.656106	5.433538	-1.143046
C	-3.908008	5.255352	-3.250678
H	-4.923421	5.390143	-3.630556
H	-3.491125	6.248026	-3.073359
H	-3.320126	4.768106	-4.034071
H	-2.187787	3.258030	-2.468909
H	-4.558202	3.517826	-2.219140
C	-0.650859	0.488953	-1.685593
H	-1.233250	1.276697	-2.181478
H	-0.677566	-0.394708	-2.340008
H	0.394623	0.823784	-1.623281
O	-1.194802	0.237392	-0.414455
H	-0.446517	-0.157369	0.175346
H	10.670214	-0.802296	-0.669967
C	4.693855	-0.471013	0.414161
C	4.018414	0.502918	1.156668
C	2.655956	0.433524	1.430438
C	1.880755	-0.658268	0.903429
C	2.586955	-1.708768	0.221673
C	3.951562	-1.573548	-0.018946
C	6.143845	-0.354862	0.132991
C	6.740855	0.890834	-0.085277
C	8.102938	1.043125	-0.341536
C	8.887806	-0.127375	-0.393181
C	8.334753	-1.408373	-0.188204
C	6.966055	-1.482185	0.079812
H	4.603231	1.322930	1.561394
H	4.471410	-2.342088	-0.581899

H	6.101628	1.765507	-0.070778
H	6.514699	-2.446522	0.278364
O	0.586642	-0.722746	1.086711
O	10.224223	0.048578	-0.654317
C	9.197371	-2.683520	-0.243374
C	8.362728	-3.947181	0.013550
H	7.907833	-3.936387	1.008000
H	7.570392	-4.066389	-0.731036
H	9.015735	-4.822710	-0.047069
C	9.813678	-2.862478	-1.648692
H	9.014728	-2.981317	-2.386208
H	10.432639	-2.028246	-1.989653
H	10.435545	-3.762887	-1.669351
C	10.282517	-2.661406	0.855637
H	9.806072	-2.638379	1.839883
H	10.893621	-3.567142	0.791994
H	10.960443	-1.804706	0.815825
C	1.842621	-2.978819	-0.216601
C	2.775524	-4.012297	-0.861862
H	3.229446	-3.634458	-1.784015
H	3.578958	-4.315155	-0.182281
H	2.197517	-4.906229	-1.117790
C	0.752940	-2.637505	-1.242570
H	0.012212	-1.977650	-0.788462
H	1.184620	-2.136139	-2.116612
H	0.254602	-3.552704	-1.588359
C	1.188358	-3.647026	1.006647
H	1.952632	-3.948592	1.731316
H	0.497460	-2.953303	1.488161
H	0.642255	-4.546975	0.697046

C	1.992993	1.467803	2.351937
C	1.407864	0.739106	3.573741
H	0.860075	1.440936	4.214930
H	0.735046	-0.054433	3.250852
H	2.216855	0.299130	4.167250
C	2.988658	2.509905	2.880412
H	2.461052	3.205424	3.541625
H	3.795240	2.046871	3.457668
H	3.437615	3.095106	2.070663
C	0.897918	2.244363	1.601853
H	0.146013	1.578643	1.173631
H	0.399147	2.954427	2.275606
H	1.360150	2.819967	0.793340
C	8.719831	2.432835	-0.571544
C	7.666382	3.544389	-0.465347
H	6.881951	3.436278	-1.220814
H	7.195653	3.566607	0.522593
H	8.153778	4.510727	-0.625879
C	9.793380	2.722956	0.494256
H	9.350802	2.693624	1.495272
H	10.608731	2.001006	0.452871
H	10.206747	3.725270	0.336403
C	9.333160	2.521875	-1.981383
H	9.744288	3.524785	-2.141339
H	10.131755	1.793534	-2.120595
H	8.563923	2.346711	-2.740597

Vibrational frequencies

5.2269	11.7004	16.5311
22.3850	23.9521	27.7579

33.8965	36.7694	37.1959
42.0437	44.6034	48.0278
55.1322	58.9958	60.3138
63.4124	65.9800	69.7350
70.8463	76.0511	77.8467
86.4196	90.7861	93.2746
95.7644	103.8962	107.2801
108.9590	115.6004	120.9329
122.6844	131.0841	136.0211
139.8998	144.0844	146.8571
150.8228	152.8617	158.6186
163.5504	170.0664	170.4477
174.4776	179.8597	186.2642
188.4320	190.7980	199.0243
206.4733	207.6857	211.5608
211.9500	222.3482	223.4327
227.7217	229.5418	238.9025
242.2288	243.3098	248.8263
253.0915	258.3904	264.8534
272.4967	275.0390	277.9302
278.1783	280.5758	281.7370
284.0814	286.9448	289.4436
293.5987	295.8069	305.0937
310.1877	312.9776	319.3785
321.2824	323.9065	325.0180
326.7073	327.9573	331.8284
336.7244	340.7151	342.7055
353.6632	361.1976	363.4681
366.2986	370.5530	371.6444
373.6148	375.0902	378.3446

379.0925	380.4789	383.5780
390.0722	398.4628	400.3190
408.4396	409.4355	412.0350
415.2196	416.8263	419.3490
420.4981	429.3074	440.3081
442.6797	450.1029	451.8193
457.2789	457.3826	462.0774
472.7478	482.9692	492.5728
502.8049	510.7804	516.5417
525.6258	531.3039	532.1233
535.4906	545.1556	545.7917
555.1474	558.2079	565.1198
576.1255	591.8749	596.8127
605.4587	614.3590	625.6971
638.8006	642.3314	643.4305
649.1615	659.0174	669.3482
673.8270	677.1137	682.5687
684.6041	697.4776	727.8066
739.6568	740.4230	750.0302
753.3367	763.8827	773.7078
776.5612	781.2021	784.5067
786.1654	787.4226	804.8672
808.6199	811.1265	816.4866
829.7006	835.7691	844.9430
847.0731	854.0532	859.6794
872.6186	881.1003	885.0214
898.1119	908.9904	910.7129
914.8490	916.3103	919.8774
926.9768	931.5021	932.0815
935.2228	939.3781	944.4647

944.6118	947.2439	950.1693
950.7861	951.1643	952.9893
953.8595	953.9577	958.0892
961.5786	962.8592	964.0133
965.5366	966.3881	966.7377
971.5839	976.8235	977.3199
979.8833	983.5584	985.4664
989.7226	993.1004	995.2183
999.9771	1007.1787	1012.8386
1024.6929	1035.6346	1037.7443
1039.7358	1043.2214	1045.8365
1049.4710	1051.5530	1051.7279
1053.7749	1059.1604	1059.8102
1061.1991	1061.2176	1062.4139
1065.0459	1072.6084	1095.2207
1105.0257	1120.9036	1134.9901
1141.0289	1147.5072	1151.3313
1156.0750	1158.0638	1164.1243
1171.8070	1176.3827	1180.9978
1186.5441	1189.1033	1192.9051
1201.0367	1205.8831	1212.0138
1217.0117	1219.1896	1225.6066
1227.0932	1228.2312	1230.6347
1232.2624	1237.6215	1242.3769
1246.2469	1247.4012	1247.9735
1249.1146	1251.2464	1252.7968
1255.0653	1274.6663	1281.0513
1282.6583	1282.7380	1288.7581
1289.1455	1290.7227	1296.9269
1297.4480	1304.8505	1308.9786

1310.4046	1316.9785	1322.9404
1325.4950	1329.9204	1335.4985
1339.9322	1341.0884	1345.3181
1349.1446	1349.4009	1352.1964
1361.3854	1363.4821	1370.1605
1377.9095	1380.5417	1386.6188
1388.1767	1393.5714	1394.9790
1399.2471	1400.9466	1403.8204
1410.6756	1413.5599	1416.0077
1418.9786	1420.2967	1421.0723
1421.5470	1422.6863	1426.4852
1430.5479	1431.2342	1436.8091
1442.9591	1445.8300	1454.2798
1459.4360	1461.4719	1466.5972
1468.2491	1472.4690	1473.3213
1476.8382	1478.7599	1480.0134
1480.9034	1482.5592	1483.7652
1484.7973	1487.3298	1488.2248
1488.7337	1490.0290	1492.9071
1493.1711	1494.2287	1494.8869
1497.4563	1498.3291	1499.2042
1500.2899	1501.1908	1501.9789
1502.2215	1503.8441	1504.3458
1504.6883	1505.8012	1506.5759
1507.8173	1508.4188	1509.2607
1511.4492	1514.3861	1517.3151
1517.8900	1518.3499	1518.5282
1521.3755	1521.9053	1523.2833
1524.5128	1526.4552	1533.4552
1536.1867	1536.8023	1537.7978

1540.8719	1543.9952	1544.8083
1550.9343	1553.1163	1578.0352
1604.9844	1612.1581	1635.6233
1640.7336	1666.6247	1675.9388
1680.8786	1683.1005	1683.6804
1686.3252	1688.4605	1719.0420
1804.6180	1828.2130	2551.4094
2966.2646	3019.2260	3045.6892
3046.9287	3050.5526	3052.6294
3058.1059	3058.8681	3062.8416
3064.6759	3069.3775	3069.5625
3070.6509	3072.9371	3073.0794
3073.5208	3077.3110	3082.6065
3083.1660	3085.8175	3086.7743
3088.0684	3089.8973	3093.0888
3097.2574	3101.3129	3102.0917
3104.1778	3115.2088	3120.2613
3121.4932	3124.0720	3133.0382
3133.4548	3134.4449	3135.6707
3137.6142	3138.5897	3139.4090
3143.2062	3145.0704	3145.3955
3146.1649	3148.4291	3150.5535
3150.6800	3152.6653	3152.9629
3153.6241	3153.9466	3154.9189
3156.1460	3159.2918	3161.8606
3161.9083	3165.2532	3172.4090
3174.6193	3175.1860	3175.9876
3177.9175	3178.2440	3178.6038
3179.6055	3183.2232	3185.0551
3189.5176	3191.0336	3195.9369

3197.4610	3200.9257	3206.5602
3208.3795	3209.6390	3209.9085
3211.1437	3212.4759	3215.7166
3219.9452	3222.3540	3246.5513
3247.7375	3252.5763	3941.3403

R_p -TS4

Zero-point correction= 1.382624

Thermal correction to Energy= 1.457976

Thermal correction to Enthalpy= 1.458920

Thermal correction to Gibbs Free Energy= 1.273685

Sum of electronic and zero-point Energies= -3141.053815

Sum of electronic and thermal Energies= -3140.978463

Sum of electronic and thermal Enthalpies= -3140.977518

Sum of electronic and thermal Free Energies= -3141.162754

Cartesian coordinates

C	-3.857454	-0.628382	-0.414306
C	-5.228447	-0.809681	-0.697060
C	-5.878154	-1.822275	0.009871
H	-6.953655	-1.937322	-0.102981
C	-5.156263	-2.797318	0.692120
H	-5.677780	-3.658758	1.102923
C	-3.760174	-2.785492	0.677105
C	-3.129929	-1.608196	0.260209
H	-2.051328	-1.498515	0.332799
C	-3.237754	0.613582	-0.971033
C	-5.944828	-0.150645	-1.859353
H	-5.662254	0.899646	-1.978037
H	-7.018393	-0.171777	-1.652192

C	-5.684419	-0.874014	-3.255757
H	-6.654327	-1.061235	-3.725106
H	-5.130944	-0.182801	-3.896057
C	-4.898737	-2.153509	-3.106973
C	-5.488121	-3.327855	-2.641392
H	-6.572130	-3.436183	-2.670593
C	-4.740660	-4.288830	-1.949787
C	-3.360113	-4.096891	-1.736336
C	-2.751313	-3.094379	-2.491873
H	-1.677707	-2.956661	-2.420015
C	-3.503412	-2.129180	-3.154999
H	-3.000706	-1.261816	-3.572461
C	-5.516868	-5.356587	-1.292581
H	-6.566562	-5.433596	-1.645488
C	-2.590438	-4.700286	-0.581800
H	-1.529506	-4.494862	-0.750572
H	-2.724176	-5.780993	-0.518267
C	-2.993586	-4.079050	0.823415
H	-3.613600	-4.805948	1.353426
H	-2.072189	-3.935038	1.396319
O	-3.128727	0.844457	-2.163115
O	-5.112227	-6.103884	-0.423422
C	-2.851787	3.879196	0.561320
C	-3.149342	1.823555	-0.064291
N	-2.718103	3.026691	-0.489444
N	-3.528090	2.010351	1.202169
N	-3.330623	3.310261	1.627513
C	-4.222385	1.121753	2.107288
C	-3.483423	0.382137	3.028216
C	-4.196209	-0.427381	3.911672

C	-5.589743	-0.487994	3.892671
C	-6.284557	0.307361	2.979592
C	-5.619510	1.130484	2.074717
H	-3.643952	-1.022646	4.634102
H	-7.371209	0.287641	2.968783
C	-1.987530	0.463797	3.064838
H	-1.535329	0.066439	2.150819
H	-1.651749	1.501939	3.159970
H	-1.596351	-0.100075	3.912813
C	-6.330545	-1.414165	4.820287
H	-7.316466	-1.018060	5.073095
H	-6.476886	-2.388530	4.342104
H	-5.772626	-1.579722	5.744289
C	-6.371873	1.996729	1.103504
H	-6.113064	3.052319	1.237057
H	-6.138419	1.722008	0.069294
H	-7.448103	1.886402	1.242716
C	-2.451116	3.797123	-1.726145
C	-1.837684	5.072397	-1.037895
O	-2.523981	5.123260	0.281712
C	-2.065327	6.412686	-1.701094
H	-1.613251	7.187276	-1.077836
H	-1.573398	6.428177	-2.675801
H	-3.121835	6.641898	-1.828476
C	-0.361580	4.846849	-0.747581
H	0.198345	4.805596	-1.685416
H	0.025015	5.667007	-0.139262
H	-0.209400	3.908200	-0.209962
C	-3.746141	3.904546	-2.555741
C	-4.942690	4.462573	-1.781228

H	-5.178141	3.853563	-0.901840
H	-4.791977	5.491649	-1.445534
H	-5.825684	4.449488	-2.425038
C	-3.526226	4.625490	-3.890274
H	-4.347391	4.377434	-4.567024
H	-3.508126	5.711264	-3.785180
H	-2.593904	4.309657	-4.368252
H	-1.680414	3.290771	-2.310537
H	-3.973249	2.861877	-2.799910
C	-0.312488	0.914262	-1.368961
H	-0.862168	0.825044	-2.320393
H	0.634936	0.365452	-1.488779
H	-0.045749	1.977796	-1.233812
O	-1.060106	0.412128	-0.304947
H	-0.233089	-0.150473	0.454591
H	10.565183	-0.785440	-0.619393
C	4.593711	-0.427982	0.460225
C	3.929754	0.539173	1.216556
C	2.563967	0.473115	1.490396
C	1.807556	-0.608196	0.950836
C	2.481330	-1.644595	0.244411
C	3.848904	-1.515566	0.002632
C	6.046290	-0.317403	0.179946
C	6.643821	0.925849	-0.043117
C	8.005815	1.071529	-0.302130
C	8.785562	-0.103254	-0.346561
C	8.229246	-1.381984	-0.134054
C	6.860191	-1.449450	0.132471
H	4.519887	1.349785	1.629034
H	4.363501	-2.272885	-0.577747

H	6.007273	1.802558	-0.031198
H	6.403760	-2.410887	0.333775
O	0.485153	-0.696841	1.165979
O	10.120441	0.066366	-0.608549
C	9.087656	-2.660035	-0.182161
C	8.248065	-3.918842	0.082270
H	7.792657	-3.900213	1.076406
H	7.456152	-4.040409	-0.662430
H	8.897968	-4.796957	0.027838
C	9.702914	-2.848894	-1.586642
H	8.903577	-2.967752	-2.323681
H	10.326406	-2.019848	-1.931979
H	10.320263	-3.752399	-1.602181
C	10.172910	-2.634970	0.916654
H	9.696962	-2.604473	1.900903
H	10.780477	-3.543299	0.857930
H	10.854310	-1.781297	0.871596
C	1.725938	-2.889809	-0.243799
C	2.667937	-3.922579	-0.881050
H	3.146782	-3.538352	-1.787409
H	3.450425	-4.242694	-0.185531
H	2.087501	-4.806662	-1.162803
C	0.690731	-2.507043	-1.312361
H	-0.098734	-1.867324	-0.908109
H	1.173094	-1.980738	-2.143854
H	0.240330	-3.420905	-1.717462
C	1.025416	-3.587646	0.936885
H	1.763407	-3.911894	1.678711
H	0.315127	-2.915851	1.419262
H	0.495517	-4.479728	0.580082

C	1.911728	1.517835	2.409762
C	1.295231	0.805815	3.625990
H	0.752473	1.524335	4.252054
H	0.610625	0.021986	3.306263
H	2.086969	0.356221	4.235074
C	2.928155	2.533839	2.951647
H	2.410611	3.229750	3.619554
H	3.723448	2.049069	3.526299
H	3.388881	3.121673	2.150817
C	0.850344	2.324467	1.643082
H	0.044891	1.699458	1.252368
H	0.414267	3.091614	2.296666
H	1.332370	2.835645	0.801572
C	8.627893	2.457290	-0.540723
C	7.577898	3.572631	-0.440230
H	6.792339	3.462527	-1.194266
H	7.108711	3.602943	0.548258
H	8.068156	4.536265	-0.607411
C	9.703146	2.749757	0.522742
H	9.261591	2.726838	1.524345
H	10.517030	2.026033	0.484318
H	10.118518	3.750183	0.359009
C	9.240176	2.535503	-1.951662
H	9.653793	3.536290	-2.117689
H	10.036969	1.804560	-2.087195
H	8.469970	2.357952	-2.709272

Vibrational frequencies

-568.4350	10.2139	11.9223
16.4995	21.6280	33.7312

35.1779	39.3664	40.1464
42.8757	43.3350	46.8349
47.8199	52.6011	54.3822
58.7604	64.6328	67.0942
67.2596	74.6029	76.2263
81.0154	83.7177	93.3315
94.7481	99.0200	106.5890
113.8332	118.5010	123.3177
128.9179	132.5747	135.8411
140.0094	142.7197	148.5545
154.9135	159.4590	165.6520
167.2079	171.2991	177.9297
179.3710	184.6405	185.8930
190.8560	196.5608	199.6979
204.1811	211.4797	214.3748
218.0258	219.7235	226.9561
229.1205	233.3872	238.3290
240.2581	242.7598	249.5237
252.8857	256.9266	261.4939
272.5038	275.3656	276.5108
277.8458	279.2805	280.2521
282.5675	285.7408	289.2964
293.6328	296.0651	304.0194
310.2446	311.3949	315.2517
321.2438	321.9139	324.2119
327.5504	329.7381	331.9883
333.9111	339.9971	340.8969
344.1135	348.7350	357.1726
357.7337	369.1905	370.9225
374.4444	375.0865	380.6003

381.4594	382.1951	384.3740
390.2021	394.5156	401.3847
408.7502	412.2127	413.8359
416.2953	417.3380	418.7725
423.2560	429.1655	437.5380
443.0614	443.8881	452.1950
457.7381	458.3187	465.5733
473.5627	483.6943	491.4973
503.3210	514.0938	517.2492
526.2280	529.3211	534.3921
535.4003	545.2626	546.3605
556.7537	564.6353	566.7172
576.7960	594.0184	594.8900
606.6240	622.4137	628.8933
634.1377	642.0973	644.8245
650.3839	658.2947	662.3548
674.4176	675.0420	681.3064
684.1844	707.2577	723.5773
728.6196	739.8112	744.0511
751.2542	754.0821	763.3604
769.9744	776.9349	778.4288
781.6327	787.9830	795.0378
798.5785	808.8764	813.9365
827.3092	830.7904	837.9091
847.3938	851.2992	856.1001
863.2171	881.5189	882.0922
885.7520	897.6862	909.1048
913.7110	914.6674	916.0283
920.3390	929.0398	932.1916
933.1795	934.3882	941.1648

945.6102	947.5494	947.9179
951.7688	953.0549	953.2250
953.7100	954.2467	956.0423
958.3519	960.6820	962.8287
964.1311	966.3196	966.5803
967.3311	970.5721	977.5727
978.1740	979.1180	983.2464
984.2768	988.8884	992.4861
994.5227	1000.8346	1004.9748
1011.1766	1034.7851	1038.5239
1041.6568	1043.5783	1046.3372
1049.9689	1051.7419	1054.5271
1055.6611	1061.2590	1061.6336
1061.8414	1062.3860	1062.6235
1064.0906	1078.2051	1093.8891
1106.8920	1112.5810	1139.3110
1151.7504	1153.1814	1153.5582
1155.0362	1159.8406	1160.7982
1164.5296	1175.6062	1181.9921
1187.6974	1189.8438	1193.1659
1197.3168	1199.5617	1201.3870
1210.1285	1218.3082	1219.7851
1222.2518	1230.2999	1230.8827
1232.1851	1234.8907	1240.8929
1242.5505	1242.5926	1248.3479
1249.2495	1249.6855	1250.7153
1251.7816	1255.5244	1272.9669
1280.9290	1283.3103	1284.1562
1286.3058	1290.0554	1290.4363
1294.6310	1299.2608	1305.8849

1306.9270	1308.7170	1311.4622
1316.0867	1323.6422	1326.9420
1329.3425	1334.6032	1335.7048
1338.8659	1348.6214	1350.9489
1352.2816	1361.6479	1365.1029
1368.8022	1386.5075	1388.4084
1391.2871	1395.6655	1399.8066
1399.9483	1401.9787	1403.8604
1404.2478	1411.0589	1413.8348
1417.3690	1420.9261	1421.3430
1421.8621	1425.0715	1426.3301
1429.8724	1431.1215	1432.7279
1437.3499	1440.6100	1446.2563
1453.5944	1463.1756	1465.6109
1469.5142	1473.4711	1475.9730
1477.9724	1479.8945	1480.7142
1481.8274	1482.1152	1485.0760
1486.4410	1487.4290	1488.2247
1488.4865	1489.3451	1490.8441
1492.5814	1494.4089	1494.6147
1496.0104	1496.8134	1498.3805
1500.0876	1501.1785	1502.0689
1502.2163	1503.7235	1504.5092
1505.1491	1506.0591	1506.8248
1507.5276	1508.3275	1509.9078
1510.0188	1511.7488	1514.5584
1515.7317	1518.5857	1518.7894
1520.4715	1523.0680	1524.6414
1527.1453	1527.8010	1529.8619
1530.2698	1535.2413	1537.5593

1538.9959	1539.3951	1541.3927
1546.4224	1551.9241	1554.0976
1579.6340	1630.7292	1636.4179
1642.9534	1669.1141	1675.4627
1680.1784	1684.4298	1685.7971
1687.0749	1688.3016	1691.4753
1730.5199	1785.1821	1825.8161
2964.5066	2983.6045	3032.1745
3045.0805	3051.5500	3053.7120
3054.9553	3057.0092	3061.6855
3062.5658	3063.2180	3065.4991
3069.6847	3070.2328	3073.0935
3073.7020	3075.0830	3077.8292
3079.6392	3080.7426	3084.2510
3086.6098	3089.9228	3090.0754
3096.4509	3103.2850	3104.8388
3114.2915	3116.2695	3121.7221
3123.9704	3124.7283	3133.5488
3134.3800	3135.3557	3137.4324
3139.2775	3139.9737	3142.2029
3143.0582	3145.0154	3146.0353
3147.0317	3149.1898	3149.3184
3150.3547	3151.4048	3153.1561
3153.4142	3153.7630	3154.2509
3155.6604	3156.2209	3156.8134
3159.6558	3165.7898	3168.9379
3169.7834	3172.5568	3176.4046
3177.9111	3178.8946	3179.6051
3182.5017	3183.6759	3184.1463
3185.1367	3188.8041	3191.4784

3194.5104	3201.4996	3208.4414
3210.0596	3210.5590	3214.5803
3216.5231	3224.6010	3228.1898
3235.2781	3237.8628	3247.2530
3248.6079	3253.2283	3938.6161

R_p -INT4

Zero-point correction= 1.387727

Thermal correction to Energy= 1.463069

Thermal correction to Enthalpy= 1.464014

Thermal correction to Gibbs Free Energy= 1.278896

Sum of electronic and zero-point Energies= -3141.063774

Sum of electronic and thermal Energies= -3140.988432

Sum of electronic and thermal Enthalpies= -3140.987488

Sum of electronic and thermal Free Energies= -3141.172605

Cartesian coordinates

C	-3.478073	-0.699572	-0.297537
C	-4.880818	-0.724832	-0.440698
C	-5.576154	-1.716505	0.250774
H	-6.664181	-1.700668	0.240053
C	-4.917820	-2.821756	0.786160
H	-5.496974	-3.654466	1.179846
C	-3.540109	-2.953843	0.628275
C	-2.828950	-1.816811	0.223581
H	-1.743577	-1.855520	0.209771
C	-2.715716	0.507021	-0.861932
C	-5.627840	0.089772	-1.477491
H	-5.256132	1.116030	-1.543715
H	-6.682075	0.130944	-1.184372

C	-5.533096	-0.528409	-2.941984
H	-6.545749	-0.582282	-3.353912
H	-4.946733	0.161340	-3.551577
C	-4.872984	-1.886583	-2.961535
C	-5.540104	-3.032839	-2.532935
H	-6.627697	-3.029074	-2.460689
C	-4.842562	-4.121991	-1.996022
C	-3.435449	-4.088897	-1.906561
C	-2.793619	-3.090639	-2.638786
H	-1.707930	-3.068255	-2.658543
C	-3.492684	-1.997571	-3.145160
H	-2.941468	-1.137732	-3.511077
C	-5.665993	-5.158471	-1.350449
H	-6.750774	-5.073841	-1.572754
C	-2.641603	-4.850202	-0.867540
H	-1.580268	-4.712450	-1.098949
H	-2.857442	-5.919651	-0.882819
C	-2.901192	-4.323849	0.607849
H	-3.560977	-5.034284	1.112063
H	-1.939169	-4.327225	1.130966
O	-2.879950	0.787150	-2.104596
O	-5.265441	-6.043477	-0.618651
C	-3.045179	3.925930	0.530591
C	-3.061243	1.803908	0.009929
N	-2.720115	3.030624	-0.441569
N	-3.584220	2.032575	1.223695
N	-3.572489	3.375806	1.578751
C	-4.307655	1.138989	2.099291
C	-3.610655	0.239722	2.904341
C	-4.361717	-0.620004	3.704698

C	-5.754801	-0.570684	3.732716
C	-6.404738	0.385754	2.952533
C	-5.701869	1.252804	2.119467
H	-3.838810	-1.342413	4.326353
H	-7.489708	0.449092	2.976837
C	-2.111103	0.211428	2.924878
H	-1.706455	-0.102296	1.959849
H	-1.702886	1.203134	3.146478
H	-1.752312	-0.485083	3.684567
C	-6.539393	-1.551670	4.562852
H	-6.693740	-2.479998	4.002340
H	-6.008535	-1.807751	5.482596
H	-7.522009	-1.154413	4.826127
C	-6.428069	2.255471	1.264397
H	-6.199259	3.279903	1.571421
H	-6.139747	2.153191	0.213726
H	-7.506476	2.104354	1.333276
C	-2.427164	3.762185	-1.694577
C	-1.967863	5.107187	-1.031214
O	-2.794818	5.180810	0.202318
C	-2.205608	6.387515	-1.800737
H	-1.868219	7.229300	-1.191817
H	-1.619892	6.375292	-2.722430
H	-3.255906	6.534327	-2.046206
C	-0.515720	5.002701	-0.580375
H	0.139594	4.947763	-1.453489
H	-0.247037	5.882916	0.007028
H	-0.353664	4.111681	0.032927
C	-3.667931	3.724715	-2.608492
C	-4.947331	4.268940	-1.968572

H	-5.176441	3.770540	-1.020299
H	-4.908682	5.344474	-1.777101
H	-5.790555	4.082627	-2.639212
C	-3.397930	4.348157	-3.981099
H	-4.173010	4.023002	-4.679803
H	-3.413932	5.439676	-3.962585
H	-2.432571	4.025473	-4.383157
H	-1.588905	3.294543	-2.211913
H	-3.802381	2.648543	-2.761766
C	-0.351986	0.962266	-1.323081
H	-0.664169	0.870713	-2.364489
H	0.622183	0.482188	-1.181474
H	-0.243874	2.023480	-1.060177
O	-1.275197	0.308871	-0.469876
H	-0.064065	-0.483180	0.632126
H	10.578487	-0.584998	-0.558770
C	4.595877	-0.464161	0.486224
C	3.904581	0.449888	1.281758
C	2.541357	0.321552	1.554040
C	1.858225	-0.773054	0.977773
C	2.529178	-1.738691	0.196753
C	3.892722	-1.548311	-0.038048
C	6.045866	-0.294672	0.217868
C	6.595823	0.974122	0.023360
C	7.952478	1.172701	-0.226477
C	8.774062	0.026560	-0.282601
C	8.263976	-1.275859	-0.096941
C	6.896168	-1.397659	0.154209
H	4.466229	1.264804	1.722148
H	4.433127	-2.248570	-0.663191

H	5.927600	1.826732	0.048057
H	6.471380	-2.378270	0.331404
O	0.518026	-0.957703	1.256991
O	10.101987	0.249194	-0.528166
C	9.169005	-2.520453	-0.158401
C	8.373390	-3.812807	0.078455
H	7.908826	-3.826478	1.068467
H	7.593630	-3.951978	-0.675965
H	9.055486	-4.665522	0.016945
C	9.802230	-2.663294	-1.560281
H	9.014221	-2.798214	-2.306627
H	10.399053	-1.807280	-1.886349
H	10.451618	-3.543718	-1.584640
C	10.243201	-2.473086	0.950435
H	9.758410	-2.474728	1.930814
H	10.883088	-3.358227	0.883281
H	10.894017	-1.595213	0.923811
C	1.799378	-2.951964	-0.404613
C	2.772290	-3.900081	-1.122649
H	3.254230	-3.422542	-1.981191
H	3.550469	-4.270212	-0.447760
H	2.213316	-4.763332	-1.495422
C	0.776502	-2.484722	-1.453497
H	-0.026671	-1.880752	-1.023943
H	1.268518	-1.896145	-2.235530
H	0.325016	-3.362424	-1.929885
C	1.098908	-3.776535	0.691465
H	1.830563	-4.139068	1.421119
H	0.345197	-3.191157	1.217257
H	0.616249	-4.650373	0.237783

C	1.835705	1.327164	2.480220
C	1.245603	0.593131	3.697277
H	0.708565	1.303730	4.336006
H	0.558942	-0.195181	3.392922
H	2.050507	0.146732	4.290372
C	2.806853	2.386963	3.021382
H	2.257574	3.061824	3.684486
H	3.618142	1.937193	3.601498
H	3.244832	2.990338	2.219825
C	0.740433	2.087347	1.710481
H	-0.052859	1.434848	1.341739
H	0.280052	2.838855	2.363724
H	1.186887	2.608693	0.856096
C	8.525450	2.583024	-0.441970
C	7.433500	3.657095	-0.339311
H	6.658874	3.525499	-1.101242
H	6.955898	3.660633	0.645628
H	7.888801	4.639803	-0.493025
C	9.578291	2.901795	0.636173
H	9.128065	2.850537	1.632801
H	10.419230	2.209841	0.597867
H	9.957550	3.918764	0.488266
C	9.148175	2.700630	-1.845742
H	9.524696	3.718339	-1.995426
H	9.973804	2.002484	-1.981767
H	8.392865	2.503235	-2.613326

Vibrational frequencies

10.4302	11.2703	17.0722
22.1524	29.0630	32.6599

34.9726	39.0069	41.1162
43.9205	44.9515	47.2972
52.3651	57.0526	58.5380
62.9294	66.0467	69.6739
75.5212	79.7459	83.7991
87.4033	93.8393	95.0070
103.0088	107.0867	114.2303
117.8891	121.4938	129.0186
133.5302	138.0131	142.3458
145.8560	152.6967	154.4386
162.5164	164.0048	166.7738
171.4228	178.4529	185.8506
187.0824	193.3346	197.5875
205.2563	207.5994	212.9102
215.8891	222.4208	223.8833
225.1877	228.5509	232.5047
236.0384	239.7428	242.5307
250.9544	255.8007	259.2176
259.6916	266.4637	269.0636
275.2452	277.2313	277.3516
280.0917	282.4659	284.9272
288.4393	290.7886	297.1586
300.5024	302.9297	308.7434
311.6016	316.0470	318.3250
319.6775	322.2622	325.6916
330.3681	330.9190	335.6824
341.7252	343.1476	346.2174
354.3323	357.3098	369.0424
372.1510	375.5657	375.7909
376.5418	381.1158	382.5644

384.7081	388.0525	392.5270
400.8331	402.3920	404.2379
414.0834	414.6210	417.2422
418.6825	424.6757	426.6758
432.0354	442.9812	443.7501
445.2787	452.0340	456.0856
459.9026	472.6393	475.2022
478.5268	482.6630	488.1047
504.7958	516.9087	519.7523
526.1390	532.6947	535.0189
535.7021	544.5799	547.1739
558.7020	560.5384	566.5599
591.8968	594.3078	597.0105
601.4654	619.5333	629.2125
634.5604	640.1796	642.1274
649.6392	652.0365	660.4509
673.0095	678.0930	683.6977
688.8567	697.3536	726.1040
729.3363	738.4311	749.4391
752.7805	761.4136	768.4002
773.8391	778.2196	780.9647
782.8556	789.2742	790.2227
795.4837	807.7343	814.8651
829.4128	834.2488	841.1663
842.7660	848.1562	852.1446
856.3067	868.2559	877.4687
882.2414	893.0662	909.9608
910.1193	910.5375	914.6467
920.2911	927.6934	929.3882
933.1002	934.9198	940.5156

943.7509	945.2483	945.8786
948.2978	951.6337	951.8521
953.7158	954.6476	956.2064
956.9519	957.9697	961.7074
962.5095	964.3023	964.9451
966.0580	966.5835	972.8614
977.2568	978.4944	979.5655
981.0194	984.0660	990.1096
990.5658	999.3876	1006.2355
1010.2903	1033.6666	1036.5276
1041.6563	1041.7935	1046.6000
1050.5389	1051.9181	1053.8943
1057.8583	1059.4618	1060.1600
1060.4106	1060.5146	1062.2037
1063.4284	1066.7021	1074.6122
1096.3876	1103.5648	1110.1923
1130.0383	1152.0031	1152.8498
1153.4832	1155.8571	1160.4949
1172.0582	1173.0671	1181.6530
1182.0039	1186.5733	1197.9194
1201.5367	1206.6319	1211.2617
1213.8186	1218.0653	1221.2941
1223.5330	1230.5947	1231.2482
1233.7778	1236.8054	1237.6141
1242.7664	1245.2240	1249.3898
1249.4507	1250.8552	1251.5440
1258.6507	1260.5604	1262.4564
1276.4397	1278.6433	1281.4540
1282.2016	1289.3503	1289.8672
1290.3493	1299.0280	1300.0362

1304.2865	1306.6164	1308.1640
1312.1738	1315.3695	1323.6838
1324.7845	1328.3005	1334.6200
1335.9772	1348.6149	1349.8753
1352.6800	1359.2310	1360.4009
1362.3514	1388.2829	1390.0396
1398.1558	1399.1835	1399.4231
1399.5760	1403.6286	1403.7508
1403.9041	1411.3555	1412.2014
1414.0048	1417.4763	1421.1771
1421.6519	1422.3939	1425.9228
1430.6457	1430.6872	1431.0539
1432.8873	1438.4670	1439.8599
1446.4816	1452.0539	1455.4386
1463.0912	1464.5278	1471.0218
1472.6689	1475.3435	1477.8941
1479.2879	1481.8511	1482.8524
1483.3947	1485.1801	1486.6078
1487.5002	1487.7298	1487.9392
1489.2376	1492.0385	1492.4873
1493.4696	1494.3558	1494.7045
1496.2108	1499.2413	1500.2442
1500.8946	1501.6604	1502.3322
1503.4794	1504.0440	1504.9272
1506.0569	1506.5181	1508.2180
1508.9855	1510.4588	1511.3870
1511.5605	1514.6137	1518.0445
1518.7569	1518.8946	1520.0265
1521.2910	1522.8393	1523.6167
1525.7329	1530.1877	1531.2809

1534.0003	1536.7472	1538.3588
1539.0853	1539.7990	1544.6095
1553.2935	1554.0524	1640.1932
1646.1623	1647.3528	1671.0127
1680.7207	1682.8260	1684.8978
1686.3948	1686.4549	1693.2159
1738.7816	1823.3460	2956.4913
3047.8590	3056.2615	3060.3545
3061.7595	3063.2276	3063.3924
3066.7563	3067.3966	3067.7740
3069.8898	3071.1834	3072.7903
3074.1928	3075.4916	3077.2887
3078.2721	3080.4791	3082.1347
3083.2745	3083.4339	3084.5267
3089.1730	3090.4235	3099.5268
3101.6990	3118.3699	3124.0730
3129.5634	3131.5387	3132.6295
3134.1094	3136.1041	3137.0225
3143.4060	3143.7644	3144.0347
3144.7758	3145.3448	3146.6299
3147.5236	3147.6724	3148.7606
3150.1014	3152.0464	3152.6953
3152.7849	3153.1201	3154.7069
3155.9575	3156.7826	3160.0774
3160.4870	3161.4872	3162.2519
3167.7921	3170.2716	3171.7776
3172.3091	3175.3019	3175.7934
3175.8255	3175.9214	3177.3513
3181.4764	3185.4961	3187.2599
3189.4972	3193.6084	3197.1143

3197.4839	3202.3744	3203.1651
3206.9625	3212.4639	3215.6866
3221.0407	3230.0822	3242.6389
3244.2001	3247.3291	3251.7620
3254.7536	3619.8192	3939.0529

DQH₂

Zero-point correction= 0.646751

Thermal correction to Energy= 0.679845

Thermal correction to Enthalpy= 0.680789

Thermal correction to Gibbs Free Energy= 0.585386

Sum of electronic and zero-point Energies= -1241.597835

Sum of electronic and thermal Energies= -1241.564741

Sum of electronic and thermal Enthalpies= -1241.563797

Sum of electronic and thermal Free Energies= -1241.659200

Cartesian coordinates

C	-1.458420	-1.139745	-0.387027
C	-0.742032	-0.001683	-0.009901
C	-1.460531	1.131349	0.369560
C	-2.856288	1.165255	0.381338
C	-3.535240	-0.010585	-0.002040
C	-2.851497	-1.182185	-0.391091
H	-0.898104	-2.009923	-0.707730
H	-0.903137	2.004286	0.687119
O	-4.902556	-0.078008	-0.016701
C	2.856334	-1.165340	0.381148
C	3.535216	0.010530	-0.002214
C	2.851436	1.182162	-0.391122
C	1.458363	1.139668	-0.387001

C	0.742034	0.001545	-0.009956
C	1.460575	-1.131491	0.369406
H	0.897982	2.009844	-0.707601
H	0.903220	-2.004445	0.686982
O	4.902532	0.077969	-0.016736
C	-3.609025	-2.452466	-0.811165
C	-3.611590	2.437680	0.808572
C	3.611735	-2.437656	0.808590
C	3.608886	2.452503	-0.811168
C	-4.489527	-2.171063	-2.043076
H	-4.998184	-3.092100	-2.347916
H	-5.243083	-1.411435	-1.836696
H	-3.871806	-1.832742	-2.881270
C	-2.644650	-3.584309	-1.192635
H	-2.014576	-3.313564	-2.045581
H	-1.996567	-3.867057	-0.357022
H	-3.227952	-4.465428	-1.475521
C	-4.473551	-2.966973	0.355223
H	-5.222952	-2.235627	0.656888
H	-4.986503	-3.886579	0.053251
H	-3.843771	-3.199575	1.220078
C	-4.461340	2.172786	2.070955
H	-4.999342	3.083199	2.352376
H	-5.200336	1.373615	1.969351
H	-3.807041	1.891342	2.900933
C	-4.472470	2.976504	-0.355567
H	-5.210873	2.272219	-0.747941
H	-5.012666	3.871601	-0.032379
H	-3.825458	3.250956	-1.193577
C	-2.646126	3.573313	1.179292

H	-2.009090	3.302726	2.026091
H	-2.007626	3.852735	0.336236
H	-3.227723	4.454109	1.465926
C	2.646311	-3.573317	1.179345
H	2.008870	-3.302503	2.025765
H	2.008218	-3.853178	0.336122
H	3.227944	-4.453892	1.466573
C	4.461375	-2.172455	2.070958
H	4.999986	-3.082565	2.352207
H	5.199766	-1.372750	1.969269
H	3.806936	-1.891572	2.901012
C	4.472814	-2.976634	-0.355333
H	5.212447	-2.273059	-0.746707
H	5.011888	-3.872450	-0.032259
H	3.826146	-3.249968	-1.193970
C	4.473338	2.967121	0.355228
H	5.222805	2.235859	0.656924
H	4.986203	3.886771	0.053243
H	3.843525	3.199685	1.220069
C	2.644414	3.584256	-1.192668
H	2.014470	3.313486	-2.045700
H	1.996205	3.866854	-0.357102
H	3.227633	4.465470	-1.475427
C	4.489449	2.171192	-2.043059
H	4.998033	3.092276	-2.347880
H	5.243065	1.411636	-1.836637
H	3.871794	1.832817	-2.881280
H	-5.279145	0.762633	0.257601
H	5.279015	-0.763184	0.256124

Vibrational frequencies

17.3449	33.5986	39.1810
48.3441	51.9712	73.2257
75.3240	82.8423	105.9511
126.4091	142.3320	155.1841
162.4027	172.1418	176.8450
178.7949	187.0184	198.5843
214.6757	215.0237	227.8905
230.2498	249.5332	250.3031
265.2104	276.2898	276.7342
283.4695	285.9321	310.9440
320.8014	326.4860	327.0988
332.8148	348.6454	357.8738
359.4311	371.5884	372.7449
375.4470	380.1761	380.2815
394.9799	401.0054	408.9231
413.9992	417.7105	437.5501
439.6621	450.2639	451.0207
455.6316	471.0344	476.0991
530.9904	532.7552	544.3601
555.2407	594.8094	627.3489
639.1598	641.5395	641.8476
671.2143	684.7139	772.7379
776.3666	778.2922	788.6462
789.8965	833.2753	839.0172
866.5262	909.7307	917.7216
923.6363	935.4528	943.3314
944.4923	946.7191	946.8329
952.8520	952.9462	958.1308
958.2380	963.1140	963.1961

966.6543	966.6626	975.4577
975.4764	977.5211	1045.0840
1047.6428	1050.6333	1051.3123
1059.3398	1059.3735	1060.7551
1060.7966	1150.8292	1152.8270
1154.7741	1179.3050	1179.8407
1230.8690	1233.2720	1242.2076
1242.2330	1248.8989	1248.9040
1250.0455	1251.9942	1279.6266
1289.0959	1290.5306	1297.5711
1300.5855	1308.6951	1310.5917
1325.0210	1348.4250	1355.4390
1388.7639	1400.6579	1400.6753
1403.5645	1403.5740	1409.8899
1410.0741	1420.8425	1420.8731
1430.9519	1431.0936	1445.8444
1445.9950	1453.2594	1484.3058
1486.7868	1486.9420	1488.4420
1488.4640	1491.3445	1494.2275
1499.6829	1501.8937	1501.9100
1503.0326	1504.7640	1506.4295
1506.4648	1508.4774	1510.8857
1512.3235	1517.9690	1517.9829
1518.5110	1518.5199	1527.1107
1533.7293	1535.1496	1536.0547
1536.6072	1545.7347	1661.9318
1675.5841	1684.4251	1687.9015
3063.0692	3063.0725	3066.6266
3066.6366	3069.4590	3069.4619
3071.0971	3071.1760	3073.5788

3073.5913	3077.6664	3077.7407
3135.2103	3135.2256	3136.2048
3136.2160	3144.1233	3144.1494
3147.5652	3147.6494	3149.7527
3149.7606	3151.3457	3151.3904
3152.4002	3152.4976	3153.6664
3153.7552	3155.2550	3155.2914
3156.0855	3156.1632	3195.5886
3195.5921	3201.7067	3201.7106
3246.5921	3247.2666	3252.5127
3253.1002	3935.6165	3936.0451

R_p -INT05

Zero-point correction= 0.739179

Thermal correction to Energy= 0.780317

Thermal correction to Enthalpy= 0.781261

Thermal correction to Gibbs Free Energy= 0.668405

Sum of electronic and zero-point Energies= -1899.453139

Sum of electronic and thermal Energies= -1899.412002

Sum of electronic and thermal Enthalpies= -1899.411057

Sum of electronic and thermal Free Energies= -1899.523914

Cartesian coordinates

C	0.814141	-0.220562	-0.133906
C	1.044511	-0.765875	1.145515
C	2.183244	-0.335352	1.833691
H	2.336721	-0.678333	2.855116
C	3.209184	0.347542	1.187807
H	4.148446	0.529001	1.706388
C	3.109119	0.614138	-0.177043

C	1.852178	0.461493	-0.770144
H	1.714684	0.754384	-1.806098
C	-0.515835	-0.507984	-0.870851
C	0.302788	-1.964038	1.702750
H	-0.778018	-1.870142	1.587264
H	0.522690	-2.024514	2.773900
C	0.738824	-3.333602	1.021376
H	0.919675	-4.066597	1.814487
H	-0.096702	-3.675843	0.409581
C	1.961988	-3.180161	0.146254
C	3.233443	-3.019544	0.694909
H	3.411260	-3.297944	1.733737
C	4.236749	-2.318916	0.015061
C	3.987379	-1.785145	-1.266821
C	2.839004	-2.241519	-1.913150
H	2.637579	-1.904029	-2.927085
C	1.832368	-2.911420	-1.218843
H	0.862299	-3.045937	-1.686683
C	5.440361	-1.999396	0.801393
H	5.506691	-2.550315	1.763466
C	4.703071	-0.571467	-1.819183
H	4.386303	-0.446747	-2.858830
H	5.787360	-0.691690	-1.806575
C	4.353723	0.758927	-1.023347
H	5.201060	1.001105	-0.376741
H	4.249373	1.565703	-1.756375
O	-0.963112	-1.720929	-0.856808
O	6.312205	-1.207850	0.496902
C	-3.624379	1.154706	0.322176
C	-1.640219	0.447389	-0.248612

N	-2.938498	0.093287	-0.182327
N	-1.621997	1.702549	0.207597
N	-2.869583	2.178425	0.580397
C	-0.468772	2.547335	0.349054
C	-0.038906	3.286596	-0.751287
C	1.140581	4.017667	-0.601848
C	1.858807	4.011330	0.592862
C	1.349679	3.303166	1.684701
C	0.174951	2.565011	1.590366
H	1.511769	4.592568	-1.446693
H	1.889911	3.313683	2.628219
C	-0.794636	3.266254	-2.052252
H	-0.611869	2.319993	-2.569847
H	-1.872364	3.353875	-1.884742
H	-0.475322	4.090283	-2.692553
C	3.179716	4.725240	0.706413
H	4.000409	4.002013	0.643359
H	3.311462	5.453598	-0.096243
H	3.271968	5.241975	1.664957
C	-0.396826	1.826421	2.769767
H	-1.345076	2.274312	3.083813
H	-0.586463	0.777124	2.523572
H	0.297830	1.853716	3.611030
C	-3.831611	-1.071652	-0.323039
C	-5.189793	-0.280835	-0.370391
O	-4.922256	0.933819	0.444384
C	-6.413913	-0.942264	0.223222
H	-7.256330	-0.251169	0.145341
H	-6.657087	-1.844137	-0.342334
H	-6.273777	-1.204096	1.270897

C	-5.462181	0.196853	-1.791954
H	-5.692721	-0.660027	-2.429606
H	-6.313869	0.879922	-1.796110
H	-4.594595	0.715447	-2.210975
C	-3.546003	-2.084073	0.800420
C	-3.593673	-1.486365	2.208361
H	-2.899302	-0.645860	2.318627
H	-4.590855	-1.135467	2.488573
H	-3.294211	-2.247157	2.934552
C	-4.389777	-3.356769	0.680152
H	-3.914892	-4.155351	1.255920
H	-5.402225	-3.233888	1.069500
H	-4.459704	-3.693935	-0.358850
H	-3.644663	-1.547411	-1.288008
H	-2.509486	-2.363144	0.584335
C	-1.371185	-0.288487	-3.103473
H	-1.532961	-1.369016	-3.101387
H	-1.055487	0.042637	-4.095081
H	-2.324219	0.211712	-2.863574
O	-0.349755	0.072713	-2.203548

Vibrational frequencies

24.4307	32.3187	34.1286
38.8259	44.2461	56.5335
64.3687	68.4334	75.9076
82.1200	88.4835	92.4772
108.9861	110.6558	113.5762
120.8531	135.1981	142.8856
151.3519	164.8949	169.5831
179.8017	182.9070	186.3532

202.0283	203.4317	206.8007
219.5572	228.8637	230.2844
238.1027	243.0235	257.0775
259.1317	276.0184	279.8103
280.4889	284.9124	285.8525
306.4693	308.6092	316.4528
320.0013	321.9602	327.4257
338.7254	352.4954	370.4044
373.8383	374.9604	386.5040
397.4480	417.0997	423.2807
425.7473	433.0437	447.7321
460.4311	473.4410	484.7307
490.2104	510.7406	517.0162
522.6039	535.7200	547.3646
560.6563	567.9227	586.0449
588.4257	604.5043	618.8936
640.6083	654.1758	660.4230
669.9530	680.5551	709.1941
728.0860	735.7012	737.9031
750.9141	752.7868	759.7972
776.9406	781.5676	789.9974
804.0456	814.1533	825.0379
844.6884	848.9089	852.4044
875.9926	876.7703	892.3688
897.3713	909.0251	910.8528
913.4668	930.7132	934.7945
940.0514	945.3988	952.4337
956.0565	962.9503	966.8398
975.6219	978.6896	981.5229
989.8190	991.4340	1000.8837

1005.2345	1009.9340	1034.9247
1037.9471	1040.0815	1042.3032
1058.4011	1059.8950	1065.7736
1067.7592	1070.6873	1102.4621
1109.0842	1127.9327	1140.4511
1150.3265	1164.2041	1171.4076
1174.3111	1183.2842	1185.3277
1195.8063	1201.1247	1203.3150
1207.8736	1214.5462	1218.5774
1221.8004	1226.4523	1229.5241
1233.3520	1246.4641	1259.4947
1276.4635	1278.6052	1279.8672
1288.5235	1289.8528	1301.3034
1307.4864	1324.9164	1331.0568
1334.6220	1336.4710	1347.5635
1357.9413	1359.8249	1360.4875
1366.0004	1380.1424	1396.3565
1403.3269	1408.8971	1413.5965
1421.2831	1422.6810	1424.1080
1432.1639	1437.6129	1439.4661
1454.7758	1464.8398	1465.3460
1469.5697	1472.5529	1475.5833
1480.8684	1481.5202	1482.2165
1486.0535	1488.0550	1489.8471
1491.4168	1492.4440	1495.1328
1498.1583	1499.9914	1501.5205
1502.0469	1506.0923	1509.6471
1520.3973	1521.9653	1523.3941
1524.5305	1527.0283	1534.5606
1540.4740	1551.8354	1564.2841

1638.9895	1644.7488	1681.8083
1684.9398	1685.2657	1691.9288
1733.1638	1822.6642	2958.0307
3006.4565	3069.0970	3070.1449
3075.0163	3078.6000	3078.8472
3079.7121	3081.3883	3081.5434
3090.1993	3095.3900	3100.6330
3116.5941	3117.4184	3139.8077
3140.2709	3141.6606	3143.2978
3150.9108	3151.9678	3153.5987
3158.7032	3159.9696	3163.2322
3164.2387	3166.7027	3170.4016
3170.7891	3173.5308	3174.3477
3174.9551	3175.8205	3178.6191
3182.6752	3183.2857	3199.9196
3200.8768	3203.2216	3204.9208
3210.7851	3230.3829	3237.3495

R_p -TS5

Zero-point correction= 0.738077

Thermal correction to Energy= 0.779055

Thermal correction to Enthalpy= 0.780000

Thermal correction to Gibbs Free Energy= 0.666294

Sum of electronic and zero-point Energies= -1899.449846

Sum of electronic and thermal Energies= -1899.408868

Sum of electronic and thermal Enthalpies= -1899.407923

Sum of electronic and thermal Free Energies= -1899.521629

Cartesian coordinates

C -0.666284 -0.731783 -0.024584

C	-0.861093	-1.790399	-0.938142
C	-1.774829	-1.564826	-1.974572
H	-1.899087	-2.332340	-2.735538
C	-2.669780	-0.496012	-1.948447
H	-3.463027	-0.441145	-2.690817
C	-2.677930	0.373660	-0.858396
C	-1.583532	0.317655	0.006940
H	-1.510919	1.040990	0.815203
C	0.446626	-0.779016	1.016402
C	-0.435214	-3.228513	-0.686414
H	0.640831	-3.344762	-0.560471
H	-0.741114	-3.811818	-1.561222
C	-1.116517	-3.857337	0.596812
H	-1.319378	-4.913039	0.388050
H	-0.396704	-3.798406	1.415084
C	-2.370977	-3.118252	1.001875
C	-3.487150	-3.078720	0.165621
H	-3.589548	-3.816646	-0.630094
C	-4.373712	-1.999250	0.187730
C	-4.170579	-0.928124	1.084638
C	-3.252643	-1.144827	2.110775
H	-3.098977	-0.367886	2.855323
C	-2.356065	-2.213444	2.064398
H	-1.528835	-2.235495	2.769494
C	-5.365123	-1.963773	-0.903709
H	-5.421588	-2.906546	-1.487579
C	-4.646778	0.480577	0.802899
H	-4.421697	1.088315	1.684095
H	-5.722813	0.522824	0.628005
C	-3.925256	1.127118	-0.456520

H	-4.628876	1.132258	-1.292480
H	-3.689399	2.167618	-0.207336
O	1.127353	-1.817058	1.190137
O	-6.076893	-1.024275	-1.200594
C	3.672153	1.178192	-0.302834
C	1.667950	0.480125	0.292047
N	2.964352	0.117472	0.171150
N	1.690452	1.761516	-0.094773
N	2.945682	2.237673	-0.478788
C	0.562347	2.641328	-0.193145
C	0.193749	3.393313	0.922602
C	-0.935492	4.204134	0.807779
C	-1.667638	4.274466	-0.378985
C	-1.252208	3.512038	-1.473054
C	-0.134218	2.684012	-1.403453
H	-1.250025	4.792754	1.666032
H	-1.824558	3.546945	-2.397036
C	0.962398	3.287663	2.210861
H	0.751562	2.325382	2.686185
H	2.040473	3.343561	2.035785
H	0.677212	4.085251	2.898740
C	-2.874256	5.171205	-0.486877
H	-3.335318	5.332721	0.490004
H	-2.593430	6.150391	-0.887972
H	-3.623365	4.743144	-1.157608
C	0.271862	1.805632	-2.554342
H	1.335451	1.922017	-2.784178
H	0.092236	0.752167	-2.304218
H	-0.306793	2.047470	-3.447318
C	3.784020	-1.098741	0.120245

C	5.189815	-0.403049	0.148405
O	4.952333	0.906224	-0.513554
C	6.322847	-1.077407	-0.593703
H	7.218658	-0.457655	-0.509718
H	6.533565	-2.047308	-0.137613
H	6.096941	-1.222488	-1.649150
C	5.583373	-0.100119	1.589926
H	5.816098	-1.031720	2.111337
H	6.465725	0.542910	1.605308
H	4.770867	0.400973	2.124255
C	3.334105	-1.938471	-1.089591
C	3.365500	-1.191617	-2.425584
H	2.746260	-0.288733	-2.397459
H	4.374297	-0.899890	-2.729571
H	2.957524	-1.836570	-3.208478
C	4.034550	-3.296739	-1.161402
H	3.472711	-3.959260	-1.825474
H	5.050772	-3.225643	-1.555525
H	4.080192	-3.771890	-0.176454
H	3.635786	-1.678007	1.033082
H	2.282073	-2.129851	-0.849511
C	0.929700	-0.199898	3.244020
H	1.042117	-1.247287	3.532141
H	0.511566	0.376661	4.070896
H	1.923582	0.199002	2.990909
O	0.035107	-0.058692	2.158816

Vibrational frequencies

-176.2450	16.7028	26.3328
35.1480	35.9266	41.7582

50.3125	56.6461	62.9280
68.9812	79.6811	84.0738
94.6776	97.8549	102.3268
107.8050	121.2648	130.9031
146.1615	153.3640	164.5351
166.8489	173.1675	180.2647
194.1895	198.0307	202.7977
210.5096	219.5428	231.4876
239.8323	243.3884	248.2381
250.3064	257.7944	271.0315
279.3929	284.4178	288.2871
291.2708	299.4288	312.2579
318.6622	319.6986	326.3188
329.8294	352.1386	365.6852
371.6979	379.2109	383.9891
396.2830	412.3139	416.6284
420.4472	435.6489	448.3363
458.3477	467.6814	484.5367
495.1581	505.4441	510.6067
524.1543	534.6349	549.0070
552.5655	562.9313	573.7592
588.5241	599.2291	608.1213
632.2130	646.3783	659.1442
667.0852	681.1684	691.9957
704.9208	729.8349	736.2314
747.1164	751.7482	756.8497
768.9249	780.2169	783.6762
787.2417	804.6210	821.4886
827.1489	847.4917	858.3950
877.0968	878.3566	886.5979

897.1173	911.6162	914.1548
919.8032	938.2547	941.8811
944.4920	949.5999	949.9444
963.6491	964.4675	972.1272
978.7465	980.3201	980.9365
989.9148	998.1472	1001.0717
1011.5332	1012.2531	1021.8312
1034.4524	1037.6334	1038.7693
1041.9148	1059.4007	1062.1613
1064.6955	1070.0284	1088.1223
1104.7470	1131.1223	1144.5771
1161.1103	1162.0356	1172.7705
1180.9404	1184.1204	1191.7804
1195.3087	1199.9815	1201.8443
1210.9832	1214.1319	1217.3499
1220.9229	1224.8041	1225.5674
1233.2312	1246.8647	1268.3839
1272.6599	1275.7798	1278.9223
1287.1284	1293.0600	1299.6944
1311.2743	1324.9723	1330.3421
1334.7271	1342.7613	1347.7480
1351.5614	1356.5455	1361.6596
1364.1370	1388.5780	1390.4293
1408.3146	1414.7735	1419.0362
1419.5637	1425.0458	1427.9992
1434.6746	1440.2126	1440.9879
1447.8936	1463.4538	1467.7061
1471.2800	1472.2138	1477.3546
1480.8942	1482.2433	1484.9093
1488.2656	1488.4036	1491.0950

1493.3078	1493.8635	1493.9752
1496.9445	1498.5480	1498.9245
1503.6855	1506.5179	1507.9165
1510.8242	1517.3395	1519.8083
1521.5987	1523.7693	1543.1880
1551.9194	1562.8104	1598.8928
1641.2980	1644.5023	1681.3714
1685.2394	1688.4685	1691.2685
1729.1333	1827.1217	2961.4120
3029.2312	3061.3488	3074.8577
3075.0387	3077.6877	3081.4411
3082.3042	3082.5271	3083.8643
3090.2774	3096.7945	3098.4555
3100.6066	3126.5635	3131.9036
3144.9722	3145.8862	3146.4085
3149.5799	3158.3932	3159.5617
3160.5222	3162.4547	3163.5608
3165.3279	3167.6119	3167.6830
3172.3001	3173.2674	3174.9316
3175.9203	3177.1317	3178.6084
3180.8244	3186.5815	3201.3213
3201.8325	3204.0857	3205.9399
3208.3409	3214.4412	3217.1325

R_p -P

Zero-point correction= 0.330641

Thermal correction to Energy= 0.348730

Thermal correction to Enthalpy= 0.349675

Thermal correction to Gibbs Free Energy= 0.285602

Sum of electronic and zero-point Energies= -959.817175

Sum of electronic and thermal Energies= -959.799085

Sum of electronic and thermal Enthalpies= -959.798141

Sum of electronic and thermal Free Energies= -959.862214

Cartesian coordinates

C	1.284527	-0.267537	0.887853
C	0.766002	0.940353	1.395650
C	-0.442416	0.849148	2.092982
H	-0.836115	1.738597	2.578128
C	-1.247549	-0.283551	2.003871
H	-2.252972	-0.256321	2.417566
C	-0.854829	-1.373935	1.223857
C	0.477025	-1.407069	0.813868
H	0.854221	-2.274877	0.280787
C	2.615676	-0.306854	0.222115
C	4.360164	-1.672377	-0.533419
H	4.604829	-2.732131	-0.519624
H	5.124198	-1.095211	-0.010028
H	4.279815	-1.309850	-1.559942
C	1.279013	2.313362	1.012904
H	2.356180	2.403665	1.155955
H	0.788798	3.040708	1.665820
C	0.960569	2.699746	-0.497258
H	0.594134	3.730449	-0.507300
H	1.893497	2.665198	-1.062184
C	-0.040693	1.761997	-1.130233
C	-1.376728	1.762157	-0.730655
H	-1.778659	2.624299	-0.198879
C	-2.160891	0.608135	-0.814672
C	-1.617386	-0.586307	-1.331464

C	-0.407711	-0.468503	-2.017850
H	0.011572	-1.346676	-2.502545
C	0.374620	0.682296	-1.913783
H	1.383980	0.676980	-2.317850
C	-3.477034	0.676445	-0.149654
H	-3.784021	1.704540	0.133952
C	-2.117963	-1.960250	-0.940551
H	-1.574601	-2.694031	-1.542561
H	-3.183809	-2.079890	-1.140921
C	-1.878988	-2.291062	0.594506
H	-2.829120	-2.181786	1.121500
H	-1.574451	-3.339606	0.663434
O	3.216121	0.653599	-0.214732
O	3.102905	-1.554065	0.136221
O	-4.200268	-0.265936	0.105549

Vibrational frequencies

32.4035	60.1219	88.3609
101.7354	108.6191	136.8593
160.1184	167.9081	180.2960
202.5722	225.7769	244.5598
271.7326	291.3363	308.3216
320.3947	330.9966	363.9512
380.2319	391.2887	416.2174
429.6088	437.3114	463.1758
486.3731	523.7353	539.4425
553.8107	614.9506	660.1495
669.7175	690.2610	726.4086
735.6595	742.3602	758.6730
795.1315	801.4829	802.3878

819.8661	839.0435	859.0115
892.1891	904.5231	919.8388
935.0324	942.8633	951.0596
967.9659	988.4831	998.7258
1007.1282	1013.8163	1037.5952
1042.6685	1126.2397	1145.9022
1171.6376	1181.7131	1185.8779
1195.0841	1201.3962	1218.1572
1219.8255	1223.3960	1225.1562
1234.3516	1250.1190	1275.6665
1287.5822	1289.3650	1308.8068
1328.4592	1334.7208	1342.6425
1349.7987	1362.1859	1366.2426
1437.7562	1459.1810	1471.9442
1481.0630	1484.6844	1489.1881
1496.0250	1500.3691	1503.0353
1506.4471	1549.5617	1551.5917
1640.4047	1645.6241	1682.8658
1686.2148	1827.6717	1829.5107
2968.1203	3092.4642	3094.6541
3095.1640	3100.6900	3104.1684
3154.3678	3160.4613	3167.4566
3173.9426	3176.9257	3179.3417
3198.1161	3199.2318	3213.1046
3214.9175	3215.0895	3224.8569

R_p -TS1-1

Zero-point correction= 0.704910

Thermal correction to Energy= 0.743541

Thermal correction to Enthalpy= 0.744485

Thermal correction to Gibbs Free Energy= 0.634706
Sum of electronic and zero-point Energies= -1784.974919
Sum of electronic and thermal Energies= -1784.936288
Sum of electronic and thermal Enthalpies= -1784.935344
Sum of electronic and thermal Free Energies= -1785.045123

Cartesian coordinates

C	0.959114	-0.432874	-0.131986
C	1.448864	-0.322601	1.184612
C	2.583243	0.471713	1.374741
H	2.941130	0.642678	2.388050
C	3.374083	0.884228	0.299810
H	4.335196	1.355848	0.491326
C	3.040108	0.501119	-1.000183
C	1.755484	-0.018188	-1.196036
H	1.428024	-0.257421	-2.208546
C	-0.353079	-1.124572	-0.472346
C	0.975515	-1.206977	2.318167
H	-0.112125	-1.205860	2.400373
H	1.390368	-0.808742	3.249664
C	1.443651	-2.718424	2.161212
H	1.825029	-3.057724	3.129473
H	0.566335	-3.312899	1.903826
C	2.488458	-2.882628	1.081563
C	3.781571	-2.389149	1.252711
H	4.143110	-2.165264	2.256345
C	4.554519	-1.979750	0.161864
C	4.047799	-2.087294	-1.150316
C	2.909975	-2.879192	-1.309720
H	2.524235	-3.050829	-2.311846

C	2.132042	-3.260312	-0.215454
H	1.152044	-3.697096	-0.385809
C	5.799068	-1.259958	0.490773
H	6.085313	-1.324895	1.561428
C	4.492894	-1.189437	-2.285351
H	4.002075	-1.541734	-3.197167
H	5.571801	-1.233813	-2.442386
C	4.104754	0.335088	-2.060706
H	5.002495	0.877586	-1.756266
H	3.778502	0.738412	-3.024523
O	-0.804242	-2.061343	0.226134
O	6.488469	-0.625286	-0.283547
H	-0.502865	-1.140299	-1.572535
C	-2.170687	2.325135	0.826742
C	-1.482000	0.476758	-0.172068
N	-1.099951	1.703541	0.261505
N	-2.767491	0.439732	0.194543
N	-3.239840	1.592418	0.829464
C	-3.690086	-0.625127	-0.072346
C	-3.960385	-1.556630	0.932207
C	-4.886834	-2.557690	0.646983
C	-5.522240	-2.638525	-0.594197
C	-5.222743	-1.683246	-1.566368
C	-4.306405	-0.659781	-1.324889
H	-5.116617	-3.294447	1.412990
H	-5.718043	-1.729947	-2.532990
C	-3.239524	-1.493361	2.249061
H	-2.193529	-1.769775	2.079838
H	-3.264002	-0.483452	2.668252
H	-3.683173	-2.183507	2.968827

C	-6.495564	-3.752403	-0.882731
H	-5.963635	-4.658372	-1.190589
H	-7.082755	-4.002449	0.004084
H	-7.181688	-3.480332	-1.687600
C	-3.995387	0.382907	-2.366358
H	-4.193747	1.388122	-1.980210
H	-2.940597	0.347089	-2.657806
H	-4.603888	0.230234	-3.258932
C	-0.002083	2.658152	0.074588
C	-0.426109	3.677097	1.188608
O	-1.906046	3.559580	1.235446
C	-0.101970	5.139583	0.976278
H	-0.502975	5.713818	1.814844
H	0.981615	5.275473	0.956649
H	-0.526583	5.530106	0.052553
C	0.101180	3.189462	2.534854
H	1.187799	3.305050	2.565204
H	-0.341416	3.776834	3.341950
H	-0.132211	2.131610	2.690816
C	0.060541	3.064911	-1.409197
C	-1.241503	3.652661	-1.958241
H	-2.081060	2.962480	-1.824880
H	-1.508884	4.601885	-1.487481
H	-1.135775	3.833113	-3.031132
C	1.283262	3.929131	-1.721126
H	1.428710	3.979543	-2.803406
H	1.175243	4.953075	-1.357001
H	2.186603	3.495289	-1.279570
H	0.950618	2.204428	0.358942
H	0.217694	2.103765	-1.918528

Vibrational frequencies

-190.0418	13.7603	25.2670
31.5674	34.3293	37.1380
42.4332	52.1928	60.4081
73.7597	80.8321	86.8213
101.7089	103.7461	116.2226
123.9471	131.9450	152.7522
154.2725	165.9717	169.4789
180.6350	191.4340	201.0960
205.9042	217.6204	220.0794
223.6227	236.0186	241.2208
245.4086	254.3518	267.7427
275.2444	279.9385	287.2862
289.7261	292.7369	303.6597
311.2821	317.2316	328.9194
334.9687	348.2379	366.9452
371.2882	374.5110	389.9520
406.7886	418.1953	422.4681
430.2806	441.4185	459.2689
463.8757	480.9458	502.3808
505.2857	520.7183	525.1727
540.2409	543.1042	560.1744
570.7921	587.5450	589.8955
603.3672	634.4199	640.8847
654.2365	660.9407	673.2514
682.7255	713.5201	733.7088
738.3816	747.3872	750.1052
757.9606	765.6726	777.7892
782.0737	805.7542	809.4405

819.9194	831.2667	849.4988
852.0473	879.5711	885.9634
886.7441	904.8349	915.4661
917.0469	920.7310	931.5205
937.4295	938.3889	950.5346
952.2902	963.6655	965.2087
978.6431	979.6756	981.1209
988.2925	990.1581	997.4442
1002.7934	1005.1018	1008.8559
1035.3671	1036.9375	1041.9339
1043.4679	1063.1052	1063.9172
1069.4895	1071.0680	1084.2254
1108.7374	1128.3234	1132.4649
1149.3770	1164.4301	1169.6506
1177.2355	1181.7509	1194.9652
1199.5780	1201.1039	1218.1391
1218.5290	1222.6842	1227.0113
1231.8723	1233.9719	1254.4294
1263.4017	1276.4909	1278.5394
1279.5302	1286.9198	1288.6240
1304.2440	1307.3476	1323.6760
1327.0856	1333.8619	1339.0140
1345.5685	1346.8074	1355.8240
1360.3354	1362.5514	1375.3887
1395.4427	1399.6125	1404.5348
1415.6732	1416.5653	1418.3216
1422.2062	1425.2356	1431.4437
1438.1837	1438.7011	1450.5005
1464.4574	1468.5174	1471.9203
1474.6959	1480.3292	1481.6802

1486.0489	1487.7251	1488.7991
1491.0798	1491.9477	1494.3105
1495.2613	1497.6306	1499.9052
1502.6247	1506.7059	1510.0236
1510.8730	1520.1453	1522.6398
1524.9685	1541.4208	1551.2624
1563.1458	1604.6124	1638.8769
1644.5182	1682.2522	1682.8038
1685.3965	1691.8101	1726.6017
1826.1860	2916.0612	2964.2375
3056.2103	3069.7387	3070.7869
3075.5791	3076.2942	3077.9609
3078.4429	3083.7610	3086.7939
3094.4278	3097.0247	3099.0777
3134.0520	3145.8535	3146.9621
3148.6182	3149.2759	3150.7883
3156.7856	3160.3696	3161.3847
3163.1825	3165.3146	3165.9419
3169.8765	3170.3883	3172.2247
3173.4296	3175.1754	3175.2484
3176.2294	3179.4223	3189.5706
3198.8881	3201.8673	3206.4045
3207.5928	3209.2434	3222.6366

R_p-TS1-2

Zero-point correction= 0.705119

Thermal correction to Energy= 0.743459

Thermal correction to Enthalpy= 0.744403

Thermal correction to Gibbs Free Energy= 0.636845

Sum of electronic and zero-point Energies= -1784.975370

Sum of electronic and thermal Energies= -1784.937030

Sum of electronic and thermal Enthalpies= -1784.936086

Sum of electronic and thermal Free Energies= -1785.043644

Cartesian coordinates

C	0.933246	-0.296643	0.026209
C	1.765301	0.510744	0.821232
C	2.860699	1.103036	0.182309
H	3.480138	1.797664	0.746561
C	3.292765	0.681004	-1.072863
H	4.242013	1.041949	-1.462892
C	2.623535	-0.352901	-1.733162
C	1.372233	-0.709730	-1.231373
H	0.783282	-1.464743	-1.755143
C	-0.324225	-0.960893	0.545024
C	1.717490	0.531251	2.337201
H	0.730444	0.797703	2.714032
H	2.426745	1.294003	2.675478
C	2.116632	-0.857806	2.993643
H	2.739241	-0.652233	3.870341
H	1.200872	-1.346968	3.329906
C	2.827347	-1.765716	2.016610
C	4.084584	-1.431979	1.514143
H	4.695389	-0.698068	2.039701
C	4.498754	-1.855392	0.248698
C	3.653283	-2.656731	-0.546733
C	2.563575	-3.238251	0.102729
H	1.923713	-3.922079	-0.450041
C	2.149001	-2.795346	1.359984
H	1.195820	-3.137584	1.756335
C	5.745443	-1.247668	-0.255211

H	6.306551	-0.674729	0.512513
C	3.712630	-2.666085	-2.059406
H	2.991378	-3.408832	-2.412907
H	4.699437	-2.951810	-2.427547
C	3.348303	-1.259949	-2.702994
H	4.275344	-0.777056	-3.020357
H	2.749369	-1.455206	-3.598227
O	-0.680861	-0.915970	1.739257
O	6.172761	-1.319886	-1.390502
H	-0.575595	-1.856460	-0.063527
C	-3.854636	0.814855	-0.567193
C	-1.746420	0.141284	-0.444901
N	-3.034007	-0.271761	-0.580535
N	-1.895489	1.470746	-0.393569
N	-3.213312	1.935138	-0.470075
C	-0.835973	2.414355	-0.196910
C	-0.058602	2.798246	-1.291362
C	0.986860	3.687526	-1.055173
C	1.258493	4.175557	0.224974
C	0.450400	3.768416	1.286869
C	-0.609586	2.881267	1.098502
H	1.613218	3.997378	-1.888645
H	0.653755	4.140411	2.288344
C	-0.329977	2.239697	-2.662003
H	-0.061114	1.178490	-2.696666
H	-1.389785	2.322363	-2.920348
H	0.256800	2.767135	-3.416069
C	2.428478	5.098084	0.450425
H	3.370369	4.542524	0.389814
H	2.464873	5.883317	-0.309247

H	2.379683	5.570585	1.433569
C	-1.464858	2.400385	2.240308
H	-2.512687	2.679488	2.091719
H	-1.414883	1.306566	2.305497
H	-1.121220	2.825824	3.185354
C	-3.818575	-1.503617	-0.467685
C	-5.187518	-0.932251	-0.993477
O	-5.143493	0.503804	-0.630411
C	-6.464040	-1.493985	-0.405497
H	-7.313337	-0.966259	-0.845914
H	-6.552416	-2.553334	-0.655627
H	-6.505811	-1.377659	0.676715
C	-5.212682	-0.998076	-2.516900
H	-5.299423	-2.038081	-2.841060
H	-6.070128	-0.438294	-2.895763
H	-4.298239	-0.576636	-2.944083
C	-3.681017	-2.067909	0.959417
C	-4.013250	-1.051405	2.053677
H	-3.339646	-0.190589	2.003382
H	-5.045048	-0.692463	2.000504
H	-3.869998	-1.515059	3.033253
C	-4.413712	-3.399587	1.145325
H	-4.019112	-3.909033	2.028029
H	-5.486732	-3.269044	1.297926
H	-4.268958	-4.061608	0.285326
H	-3.458798	-2.247401	-1.184930
H	-2.606989	-2.269321	1.060587

Vibrational frequencies

-160.7347

25.1471

26.6457

34.0884	39.7554	49.6999
58.5580	63.1070	68.4410
77.0900	87.1784	89.3143
92.9205	111.1599	113.3131
123.5446	134.9380	149.8526
161.0691	165.2853	170.9371
191.1001	197.3452	201.6231
210.6230	219.7018	226.5277
241.0973	242.8494	247.3437
254.5914	262.9832	270.3367
277.3136	281.5033	285.2039
291.9012	299.2476	311.1408
316.5688	318.8753	329.2023
334.2809	345.5952	367.7545
373.0722	373.9316	393.8094
415.2141	419.9124	421.8965
433.7222	441.4989	460.2441
463.3355	475.5476	496.7147
507.8416	517.0398	525.3236
536.4133	547.8568	559.9159
564.7389	581.9807	588.4613
601.0821	622.9008	635.4489
653.4959	662.5092	667.6132
681.2647	704.3860	732.9682
736.4846	744.0087	746.1180
755.7131	759.5808	773.6311
779.0267	802.1549	805.5742
818.4402	828.0922	852.9971
855.0316	877.3058	879.7714
887.0087	903.4428	909.8368

915.8165	920.5538	929.3916
938.2810	941.7068	951.8925
953.7803	964.0692	965.8246
977.0101	979.3562	982.6878
988.5306	989.0344	996.3942
1002.2035	1007.6993	1011.4255
1035.5032	1036.2483	1041.8397
1043.5446	1060.6811	1062.7909
1071.4830	1073.1426	1077.9712
1110.0677	1112.8285	1129.5880
1147.7686	1163.2269	1170.6539
1171.4174	1180.1432	1193.5604
1199.7005	1200.2954	1215.9807
1218.6972	1220.6202	1224.6029
1232.0044	1232.2032	1254.6366
1263.5679	1274.3757	1275.9576
1279.6698	1286.2218	1290.4003
1300.4933	1309.7570	1321.7809
1329.6467	1337.9323	1339.3656
1340.5954	1346.3762	1356.5559
1360.5752	1363.1335	1378.8416
1397.5698	1410.8733	1413.6652
1414.6424	1416.4543	1417.9456
1419.9908	1426.7781	1431.1219
1437.6246	1441.3907	1453.1473
1464.6328	1468.9724	1472.1231
1477.2877	1482.0234	1483.3205
1488.1604	1488.5080	1488.9060
1491.1740	1491.7737	1494.7985
1495.4743	1499.8552	1500.8936

1503.0021	1505.2091	1510.1573
1512.0788	1521.8879	1526.4447
1527.1259	1548.2288	1551.8041
1564.6655	1633.8630	1641.1592
1651.0059	1683.4479	1685.0406
1690.5427	1693.3100	1731.9887
1828.4535	2907.0689	2966.5138
3059.8593	3071.4860	3072.1011
3075.9698	3078.0904	3082.6312
3082.7620	3082.9524	3086.4233
3092.4441	3095.9043	3098.6970
3118.7472	3132.6051	3140.2096
3140.3115	3148.1515	3150.0545
3155.0928	3156.9671	3159.2681
3159.7578	3162.6118	3165.6852
3166.5111	3168.7664	3171.1948
3172.1071	3176.3836	3178.0370
3180.5190	3183.5500	3184.7559
3195.6006	3198.7479	3201.0252
3202.2520	3207.1670	3210.8318

R_p-TS1-3

Zero-point correction= 0.705077

Thermal correction to Energy= 0.743554

Thermal correction to Enthalpy= 0.744498

Thermal correction to Gibbs Free Energy= 0.634828

Sum of electronic and zero-point Energies= -1784.972672

Sum of electronic and thermal Energies= -1784.934195

Sum of electronic and thermal Enthalpies= -1784.933251

Sum of electronic and thermal Free Energies= -1785.042921

Cartesian coordinates

C	-0.862295	-0.211502	0.372450
C	-0.900433	-1.099674	-0.720315
C	-1.754747	-0.765812	-1.773865
H	-1.750672	-1.384493	-2.669099
C	-2.746369	0.207324	-1.628402
H	-3.496702	0.326777	-2.406666
C	-2.906310	0.868552	-0.410337
C	-1.862546	0.747382	0.514470
H	-1.915576	1.301220	1.453690
C	0.152955	-0.343438	1.500172
C	-0.283940	-2.481782	-0.664213
H	0.739947	-2.447996	-0.289874
H	-0.269353	-2.889963	-1.680550
C	-1.088448	-3.480849	0.276878
H	-1.221961	-4.423455	-0.263234
H	-0.472930	-3.669098	1.157421
C	-2.420119	-2.921070	0.716719
C	-3.481634	-2.799101	-0.179103
H	-3.470608	-3.371145	-1.106780
C	-4.459909	-1.813274	-0.018037
C	-4.407465	-0.933013	1.082920
C	-3.541865	-1.286931	2.118118
H	-3.519682	-0.675976	3.017393
C	-2.552582	-2.253908	1.936882
H	-1.770910	-2.362948	2.683283
C	-5.382801	-1.632577	-1.153909
H	-5.332161	-2.446781	-1.906939
C	-4.989480	0.463387	1.052809
H	-4.875638	0.891288	2.053069

H	-6.051791	0.461146	0.803993
C	-4.254325	1.410062	0.010869
H	-4.890830	1.508970	-0.871278
H	-4.163762	2.399090	0.471408
O	0.569083	-1.454938	1.892306
O	-6.144082	-0.699562	-1.320688
H	0.009786	0.483242	2.232986
C	2.251796	2.146378	-0.999686
C	1.519438	0.674830	0.480858
N	1.337796	1.920795	-0.016271
N	2.541814	0.226972	-0.260373
N	3.031547	1.135336	-1.205546
C	3.125408	-1.079157	-0.204137
C	3.089838	-1.871679	-1.358158
C	3.677522	-3.133399	-1.293327
C	4.273822	-3.607294	-0.123363
C	4.273452	-2.787465	1.004503
C	3.703019	-1.514042	0.992068
H	3.657413	-3.766514	-2.177222
H	4.731642	-3.144788	1.923437
C	2.404995	-1.404179	-2.616196
H	1.451799	-0.916673	-2.383090
H	3.016656	-0.677101	-3.156229
H	2.208584	-2.253290	-3.273897
C	4.871731	-4.989715	-0.072156
H	4.107431	-5.731306	0.181889
H	5.296622	-5.272460	-1.038045
H	5.657315	-5.052644	0.684031
C	3.687350	-0.665646	2.234623
H	3.966052	0.369884	2.019482

H	2.677400	-0.672137	2.657407
H	4.382727	-1.066043	2.974778
C	0.569540	3.134806	0.260863
C	0.819743	3.854116	-1.112408
O	2.150122	3.354232	-1.540062
C	0.889906	5.364821	-1.125396
H	1.097693	5.697596	-2.145095
H	-0.071805	5.781778	-0.819013
H	1.670888	5.747505	-0.469313
C	-0.197004	3.336055	-2.126176
H	-1.187788	3.731506	-1.887222
H	0.081650	3.662070	-3.130279
H	-0.256301	2.242334	-2.105765
C	1.033403	3.744005	1.596009
C	2.536964	4.020579	1.662204
H	3.122268	3.114835	1.476651
H	2.851839	4.779604	0.941441
H	2.798490	4.381753	2.660026
C	0.198711	4.957845	2.010816
H	0.359288	5.165179	3.071640
H	0.474713	5.857265	1.456815
H	-0.870664	4.777373	1.862053
H	-0.494562	2.890538	0.326563
H	0.820487	2.946467	2.322743

Vibrational frequencies

-180.9565	14.1077	21.3716
30.0933	30.4344	33.8775
45.3594	50.4424	60.8975
72.7362	77.8971	88.1142

98.1456	105.5970	109.1320
113.8336	133.5712	156.1836
163.8083	181.7842	189.3179
194.1440	199.3678	206.5802
215.4654	221.6071	224.1514
226.9915	239.5845	242.2008
245.0145	260.3234	272.3973
281.6304	283.2226	287.1546
289.7810	305.5870	310.0925
313.3074	322.2772	332.7895
338.2149	353.5539	363.9688
371.0881	375.6435	390.7930
407.2134	413.4917	417.7604
431.5526	444.4942	456.6333
461.0439	477.6035	499.3988
509.5549	516.6667	525.1021
539.2798	553.6772	556.1961
564.7168	582.9532	589.0719
602.9825	629.0872	644.6611
654.4605	664.3471	673.6377
686.5916	694.6109	733.1135
739.3815	745.0112	752.1985
754.5610	767.1525	775.2076
781.6840	804.1360	810.7083
819.6734	831.2022	850.3168
851.8900	883.1378	885.4038
886.0488	907.2384	913.0999
916.9123	920.0091	933.9269
939.0567	940.4711	949.7835
953.7879	965.2608	965.6020

979.4904	980.9506	982.2124
986.3190	989.3862	994.9968
1001.9679	1005.7898	1010.4308
1037.7515	1039.6888	1042.0736
1043.1069	1062.0239	1063.0371
1068.1537	1069.6521	1082.0114
1112.4860	1128.8908	1142.6371
1149.1657	1161.8239	1168.8255
1174.1941	1183.0746	1195.4424
1202.5581	1203.6415	1216.1845
1219.3974	1222.4184	1229.7158
1235.1080	1236.6328	1256.9174
1263.5285	1275.0241	1277.2659
1282.4056	1287.6751	1290.8297
1302.8014	1308.4515	1321.7661
1326.8612	1333.7783	1339.1039
1346.8904	1348.4208	1357.5084
1361.3160	1363.2014	1374.3120
1398.5083	1401.0365	1405.5643
1416.6047	1418.6916	1419.0725
1425.0081	1425.5106	1433.5424
1439.3308	1440.6258	1451.2988
1463.2973	1466.0665	1471.2700
1476.2165	1480.3233	1481.6973
1486.3743	1487.6415	1490.7314
1492.5962	1493.0244	1494.9685
1495.7250	1497.8860	1499.1694
1502.3574	1506.2362	1508.2807
1510.1445	1520.6240	1521.1421
1523.7391	1542.8775	1552.4693

1559.4040	1611.0317	1640.6104
1647.0239	1680.5949	1683.2934
1686.1721	1692.2927	1739.0080
1826.0081	2875.2453	2962.6014
3042.0854	3071.2456	3071.3952
3073.2899	3075.6039	3078.2522
3080.8029	3081.2265	3084.9733
3093.1210	3096.8923	3098.7498
3129.7669	3145.2785	3146.1458
3147.5226	3148.4829	3152.8990
3152.9209	3153.4915	3154.1956
3165.0398	3165.0657	3165.7126
3168.2418	3169.1255	3169.6074
3172.0445	3176.1090	3176.5195
3177.3928	3180.3791	3188.5335
3200.1674	3201.6206	3204.3632
3205.7237	3205.9069	3224.4278

R_p -TS1-4

Zero-point correction= 0.704807

Thermal correction to Energy= 0.743324

Thermal correction to Enthalpy= 0.744268

Thermal correction to Gibbs Free Energy= 0.635484

Sum of electronic and zero-point Energies= -1784.971492

Sum of electronic and thermal Energies= -1784.932975

Sum of electronic and thermal Enthalpies= -1784.932030

Sum of electronic and thermal Free Energies= -1785.040815

Cartesian coordinates

C	4.534847	-1.816129	0.434059
C	3.948865	-2.442428	-0.685269

C	2.803813	-3.200174	-0.438625
H	2.360280	-3.763292	-1.256433
C	2.093082	-3.075719	0.754184
H	1.105579	-3.517827	0.833011
C	2.523064	-2.198381	1.753751
C	3.824718	-1.713823	1.636202
H	4.246069	-1.102937	2.434547
C	5.793732	-1.054278	0.364396
C	4.310483	-2.106792	-2.115416
H	5.379818	-2.211411	-2.304964
H	3.779578	-2.810008	-2.763854
C	3.890571	-0.629932	-2.523945
H	3.511566	-0.667440	-3.550241
H	4.789694	-0.008984	-2.522243
C	2.876860	-0.031761	-1.574395
C	1.568829	-0.527009	-1.498854
H	1.176945	-1.127572	-2.320921
C	0.821680	-0.439580	-0.326212
C	1.394404	0.148902	0.816227
C	2.556105	0.897656	0.636079
H	2.968879	1.443439	1.482560
C	3.293275	0.810995	-0.544586
H	4.276393	1.274725	-0.597434
C	-0.492215	-1.195729	-0.268653
H	-0.812968	-1.468972	-1.303379
C	0.940036	-0.202040	2.212801
H	1.256785	0.594617	2.894790
H	-0.147571	-0.286275	2.257422
C	1.539591	-1.588142	2.726188
H	0.703608	-2.274544	2.870793

H	2.018153	-1.416326	3.695505
O	6.432949	-0.808649	-0.640710
O	-0.725439	-1.998675	0.671385
H	6.145980	-0.679108	1.348471
C	-3.822957	1.143130	-0.550149
C	-1.818699	0.253268	-0.262601
N	-3.140055	-0.026746	-0.426214
N	-1.820028	1.592932	-0.260780
N	-3.068623	2.189196	-0.437292
C	-0.690168	2.450610	-0.052019
C	-0.447261	2.923023	1.237824
C	0.672698	3.733644	1.424015
C	1.515946	4.067292	0.364351
C	1.208729	3.600425	-0.915747
C	0.102912	2.788192	-1.150745
H	0.893530	4.105361	2.421804
H	1.854926	3.864349	-1.749630
C	-1.374597	2.582129	2.373805
H	-1.590833	1.510243	2.402276
H	-2.331064	3.102276	2.260276
H	-0.935838	2.871834	3.330145
C	2.763090	4.879742	0.594592
H	3.639103	4.222504	0.630922
H	2.715428	5.426565	1.538600
H	2.925858	5.595967	-0.214596
C	-0.242744	2.292609	-2.528879
H	-1.243827	2.624876	-2.821335
H	-0.232198	1.199100	-2.561616
H	0.475655	2.663418	-3.261913
C	-4.037040	-1.162908	-0.675597

C	-5.426826	-0.437248	-0.537580
O	-5.113656	0.989677	-0.799701
C	-6.405344	-0.868793	-1.611085
H	-7.322223	-0.279668	-1.539684
H	-6.659533	-1.923253	-1.479078
H	-5.971184	-0.732752	-2.603919
C	-6.046613	-0.454979	0.850726
H	-6.373726	-1.459680	1.123628
H	-6.918392	0.203058	0.845522
H	-5.341493	-0.094254	1.603051
C	-3.719074	-2.412777	0.158625
C	-4.690466	-3.546879	-0.175438
H	-4.760833	-3.715414	-1.254841
H	-5.698145	-3.351829	0.205775
H	-4.342966	-4.474268	0.286650
C	-3.578121	-2.203981	1.668093
H	-3.017191	-3.046080	2.080006
H	-4.541021	-2.159089	2.181058
H	-3.002968	-1.302117	1.894872
H	-3.919281	-1.439951	-1.731266
H	-2.721686	-2.708596	-0.182843

Vibrational frequencies

-183.5668	17.4111	21.6676
31.1316	43.0219	49.5802
56.4223	60.6660	69.6202
72.1582	74.8020	83.8097
97.5249	105.2055	115.5994
121.3980	125.1610	135.0855
146.5562	161.9115	166.2799

183.9704	198.8574	207.6847
214.5026	222.4359	227.9601
233.8023	237.8513	242.9775
245.3895	262.6045	266.7383
277.5265	279.7476	281.2790
291.1332	302.2795	310.6771
316.2767	325.6216	331.1726
334.7164	353.6826	359.0239
373.1217	375.5758	381.1319
404.4699	418.4709	420.2876
429.8218	439.2905	460.4425
470.5846	480.6508	502.9662
508.8347	519.9817	524.6561
540.4518	545.1853	563.7524
565.6047	584.4486	588.6587
597.5516	630.2638	641.7998
660.5187	663.0727	675.9987
686.8150	704.0066	734.6465
738.5522	739.0124	752.9379
754.2154	768.0944	770.2696
775.9204	799.8069	806.0748
812.3559	827.5740	847.6547
860.2563	876.5978	880.4529
884.4402	902.1629	909.3491
915.6299	919.0774	925.1190
933.5218	941.6843	953.1358
955.9786	961.1474	962.7129
976.0489	980.3202	983.8190
984.3683	995.0503	1002.0639
1005.7330	1008.2009	1021.8277

1024.3202	1034.7761	1039.4412
1043.5810	1058.9225	1059.6492
1062.2207	1068.9779	1089.3250
1115.2013	1130.8056	1151.2005
1156.5146	1166.9119	1169.0858
1173.7227	1184.4827	1195.2158
1198.4152	1201.8459	1219.3912
1223.4196	1226.9471	1231.6377
1236.4193	1238.2234	1262.0589
1267.6839	1275.3835	1280.0641
1281.7775	1283.0303	1289.3225
1308.6471	1314.9744	1323.4704
1332.8066	1335.9940	1338.1102
1347.8809	1352.9763	1355.9846
1359.8647	1362.5723	1380.8924
1385.9502	1401.8143	1412.6771
1413.8936	1415.3132	1416.1429
1422.9375	1425.9948	1433.8520
1440.1316	1443.3528	1451.9115
1464.3043	1465.3345	1468.6660
1474.6879	1481.3348	1481.5961
1485.0264	1485.9652	1487.4754
1488.1653	1489.9003	1491.8768
1496.8768	1497.7343	1499.6759
1502.7315	1505.2713	1509.2202
1514.1043	1518.5532	1521.1629
1525.5500	1545.8193	1553.8636
1563.9755	1582.7881	1639.5374
1650.8492	1683.8455	1684.8030
1687.7803	1693.6629	1734.7302

1823.4519	2835.2460	2960.8272
3067.8174	3069.8337	3070.0927
3075.4464	3076.1067	3077.0044
3085.2559	3087.1565	3089.3300
3090.6726	3093.3477	3095.4764
3105.2932	3140.0140	3142.3636
3143.9988	3144.4676	3146.1693
3147.7420	3155.9940	3161.8651
3162.8607	3163.6863	3164.2170
3169.0279	3171.9356	3173.9769
3174.1916	3174.9916	3177.7287
3178.2554	3179.9206	3183.7809
3189.4424	3198.4997	3200.4795
3200.5736	3202.3083	3241.5620

S_p-TS1-1

Zero-point correction= 0.705042

Thermal correction to Energy= 0.743448

Thermal correction to Enthalpy= 0.744392

Thermal correction to Gibbs Free Energy= 0.635243

Sum of electronic and zero-point Energies= -1784.974092

Sum of electronic and thermal Energies= -1784.935686

Sum of electronic and thermal Enthalpies= -1784.934742

Sum of electronic and thermal Free Energies= -1785.043891

Cartesian coordinates

C	-4.526282	-1.541947	0.387754
C	-3.598688	-2.545308	0.737697
C	-2.865379	-2.328116	1.904977
H	-2.189869	-3.105279	2.254941

C	-2.807364	-1.067170	2.500699
H	-2.083173	-0.884453	3.290521
C	-3.503913	0.014709	1.956537
C	-4.476346	-0.288754	1.004377
H	-5.110174	0.506542	0.612258
C	-5.447188	-1.656816	-0.758884
C	-3.177931	-3.646086	-0.212687
H	-4.028887	-4.234988	-0.559010
H	-2.504195	-4.313163	0.333239
C	-2.417938	-3.099152	-1.496110
H	-1.603754	-3.796891	-1.717906
H	-3.111368	-3.116690	-2.339934
C	-1.905631	-1.689082	-1.303562
C	-0.944110	-1.414596	-0.331599
H	-0.366635	-2.242714	0.080704
C	-0.855635	-0.173721	0.302655
C	-1.768646	0.838117	-0.042581
C	-2.509961	0.648230	-1.215686
H	-3.159613	1.452109	-1.556583
C	-2.585242	-0.593058	-1.842357
H	-3.297002	-0.745041	-2.650820
C	0.091554	-0.074171	1.489822
H	0.465609	-1.088805	1.762249
C	-2.177078	1.950931	0.900180
H	-2.790923	2.658138	0.331740
H	-1.309359	2.483697	1.287264
C	-3.017089	1.432585	2.145048
H	-2.370651	1.472903	3.022818
H	-3.856312	2.118337	2.300031
O	-5.495268	-2.574881	-1.553948

O	-0.046383	0.788455	2.381931
H	-6.137025	-0.793694	-0.867583
C	3.803554	0.311647	-0.446553
C	1.773869	0.283782	0.435200
N	2.942000	-0.401136	0.331591
N	2.044597	1.393096	-0.259422
N	3.318834	1.448719	-0.830211
C	1.168368	2.513030	-0.435538
C	1.125516	3.488389	0.562626
C	0.278054	4.576958	0.358351
C	-0.509709	4.684736	-0.789578
C	-0.428699	3.684843	-1.761361
C	0.414140	2.585310	-1.607882
H	0.225097	5.352986	1.118186
H	-1.036586	3.760804	-2.659875
C	1.938752	3.332863	1.818281
H	1.544113	2.491177	2.398703
H	2.988183	3.126812	1.585911
H	1.888125	4.238729	2.425022
C	-1.459506	5.842399	-0.959394
H	-1.084985	6.738761	-0.459951
H	-1.618890	6.073386	-2.014998
H	-2.434797	5.603961	-0.521722
C	0.497693	1.491922	-2.637420
H	1.529067	1.348583	-2.973921
H	0.148220	0.543238	-2.212196
H	-0.124704	1.727557	-3.502417
C	3.475484	-1.739031	0.599382
C	4.989820	-1.442634	0.278773
O	4.949771	-0.313090	-0.677202

C	5.803026	-2.536086	-0.379578
H	6.806549	-2.151691	-0.576691
H	5.890206	-3.392002	0.292489
H	5.365072	-2.862354	-1.322487
C	5.676969	-0.926305	1.537759
H	5.776099	-1.737219	2.263546
H	6.671641	-0.551754	1.288372
H	5.098887	-0.118923	1.996826
C	2.666353	-2.784338	-0.189432
C	2.511945	-2.456453	-1.675595
H	2.003268	-1.498159	-1.823779
H	3.473970	-2.416628	-2.194822
H	1.903768	-3.226249	-2.158415
C	3.139799	-4.220469	0.051101
H	2.340346	-4.914538	-0.219517
H	4.011297	-4.476201	-0.553890
H	3.389479	-4.390760	1.103178
H	3.394042	-1.965563	1.666602
H	1.667524	-2.705532	0.259436

Vibrational frequencies

-156.1934	10.8026	20.3874
31.8851	35.2637	46.4178
51.1168	57.4561	66.7557
72.0667	81.6520	86.0589
93.4003	104.8078	111.8456
116.3173	135.5466	156.7633
164.2709	165.1416	186.3429
191.0570	199.1904	206.2366
215.1798	220.8874	223.3186

233.4508	240.1519	248.5563
253.2332	263.6506	270.6526
275.5557	280.5471	284.1676
289.7640	307.5412	315.9900
319.2927	323.3875	328.8994
338.0569	359.7053	366.2880
370.9561	373.8259	392.7434
409.3583	417.8729	423.7885
431.4986	445.0629	456.2829
460.4101	478.6349	498.4102
506.9575	513.9509	528.7658
536.5939	549.4465	567.0058
569.2053	577.5529	588.5987
602.7119	625.7962	640.1848
654.5125	663.5468	671.6551
683.8945	700.8421	732.3421
737.4005	742.5054	746.7483
755.5275	761.1689	774.1683
778.4759	801.7188	804.2969
817.6200	827.0233	853.1485
855.9452	879.1990	881.8744
886.6428	904.4903	910.8350
915.9486	920.7807	927.1707
937.3845	943.4799	953.1609
953.9435	963.1513	965.3750
976.8757	979.4802	983.4233
985.4981	991.4880	998.9231
1004.5306	1006.0357	1009.4305
1036.9948	1037.8156	1041.0257
1041.8372	1060.7353	1064.1936

1070.1280	1073.0854	1082.6295
1115.0664	1129.5730	1143.9676
1147.8048	1163.8443	1169.0091
1174.4336	1180.4987	1192.0175
1198.0533	1199.2935	1217.3719
1218.0639	1220.3012	1226.5471
1235.1651	1235.8752	1258.4815
1263.7289	1273.6886	1278.0067
1280.3764	1284.2121	1288.6598
1300.9157	1307.7239	1321.8200
1326.1127	1334.1017	1338.5060
1345.4428	1347.4338	1356.8303
1361.3028	1363.6904	1371.4559
1397.5805	1409.5392	1410.2905
1414.2393	1415.0800	1419.9479
1420.7124	1425.0864	1433.2724
1437.7942	1438.8647	1450.2991
1464.0907	1468.9006	1471.8720
1473.7702	1480.4580	1483.1766
1484.4709	1489.7906	1491.6102
1491.7176	1493.3287	1494.7906
1496.3143	1498.7783	1499.6144
1502.0606	1505.9321	1508.8654
1512.8024	1521.8050	1522.4911
1530.0816	1544.3885	1550.9992
1564.3088	1621.3928	1639.4909
1646.7356	1681.3975	1684.0248
1687.5253	1691.3069	1734.7972
1826.9359	2860.1601	2961.4863
3064.0169	3065.4761	3068.5328

3073.5218	3073.7563	3079.0793
3081.9642	3082.1140	3083.8894
3090.6879	3095.2891	3099.2852
3119.3131	3134.2368	3137.9903
3143.2677	3147.2537	3147.7168
3154.8382	3159.5513	3161.9847
3163.3921	3165.0769	3169.5260
3170.4128	3170.7945	3171.4106
3175.6802	3177.0842	3180.5176
3182.9688	3185.2439	3187.8643
3197.4122	3200.9727	3202.7569
3203.4048	3204.4370	3216.2622

S_p-TS1-2

Zero-point correction= 0.705014

Thermal correction to Energy= 0.743435

Thermal correction to Enthalpy= 0.744380

Thermal correction to Gibbs Free Energy= 0.635560

Sum of electronic and zero-point Energies= -1784.974128

Sum of electronic and thermal Energies= -1784.935707

Sum of electronic and thermal Enthalpies= -1784.934762

Sum of electronic and thermal Free Energies= -1785.043582

Cartesian coordinates

C	-4.566115	-1.500852	0.416043
C	-3.653212	-2.518108	0.764517
C	-2.906506	-2.306669	1.924308
H	-2.241797	-3.093405	2.273512
C	-2.821640	-1.043354	2.511745
H	-2.088224	-0.869120	3.294958
C	-3.503855	0.047184	1.966771

C	-4.489083	-0.245039	1.024331
H	-5.112059	0.558879	0.632393
C	-5.498618	-1.606577	-0.722122
C	-3.259481	-3.631370	-0.182864
H	-4.123216	-4.207971	-0.518105
H	-2.591989	-4.306399	0.360949
C	-2.502337	-3.104634	-1.476266
H	-1.702674	-3.817665	-1.701711
H	-3.204070	-3.115005	-2.313343
C	-1.964276	-1.702328	-1.296889
C	-0.990301	-1.437200	-0.334779
H	-0.422492	-2.270943	0.080130
C	-0.876167	-0.193021	0.288337
C	-1.775767	0.831103	-0.055074
C	-2.529198	0.645682	-1.221066
H	-3.168710	1.457481	-1.562392
C	-2.629117	-0.598547	-1.838574
H	-3.349248	-0.744228	-2.640759
C	0.086984	-0.099060	1.461164
H	0.458325	-1.115276	1.731209
C	-2.157530	1.955554	0.885049
H	-2.766256	2.668859	0.318711
H	-1.277918	2.477397	1.260110
C	-2.991959	1.457937	2.141974
H	-2.335746	1.493462	3.012841
H	-3.818290	2.158089	2.301793
O	-5.570463	-2.529194	-1.510062
O	-0.024340	0.770044	2.349947
H	-6.173308	-0.731606	-0.831189
C	3.838553	0.313770	-0.388333

C	1.768290	0.248632	0.392998
N	2.944823	-0.425796	0.325785
N	2.064639	1.379282	-0.255278
N	3.364759	1.458668	-0.762710
C	1.188877	2.497989	-0.441469
C	0.431154	2.559628	-1.611827
C	-0.411330	3.658714	-1.773110
C	-0.486975	4.668790	-0.811830
C	0.305204	4.571948	0.334350
C	1.150789	3.483835	0.546709
H	-1.022034	3.726549	-2.670358
H	0.255838	5.355621	1.086547
C	0.512803	1.458870	-2.633760
H	0.148769	0.516134	-2.207846
H	-0.097393	1.696604	-3.506837
H	1.546250	1.303228	-2.958970
C	-1.435886	5.825956	-0.989773
H	-1.606967	6.039984	-2.047106
H	-2.406529	5.597202	-0.536845
H	-1.053539	6.729464	-0.509459
C	1.966409	3.335581	1.801547
H	1.581921	2.487464	2.379300
H	3.017883	3.141801	1.568132
H	1.905408	4.238922	2.411030
C	3.468573	-1.771809	0.567244
C	4.995561	-1.456950	0.343401
O	4.998295	-0.299787	-0.580832
C	5.852829	-2.527294	-0.296637
H	6.864744	-2.134904	-0.421622
H	5.902925	-3.401917	0.355084

H	5.474363	-2.828676	-1.272828
C	5.606966	-0.972521	1.653317
H	5.674157	-1.803670	2.359615
H	6.610279	-0.583041	1.469990
H	4.997343	-0.183431	2.103150
C	2.711033	-2.780867	-0.314849
C	2.664811	-2.397800	-1.795422
H	2.177323	-1.428773	-1.943780
H	3.660561	-2.350668	-2.245323
H	2.084975	-3.142603	-2.346917
C	3.160272	-4.227985	-0.095740
H	2.382177	-4.906439	-0.454120
H	4.075164	-4.464631	-0.641755
H	3.328279	-4.441060	0.964692
H	3.327484	-2.045278	1.617174
H	1.682280	-2.709150	0.062415

Vibrational frequencies

-156.3987	17.0903	19.4657
33.0844	36.4935	47.9071
50.3269	56.3655	66.4300
69.8115	80.6834	84.9621
93.1434	105.1056	111.2697
114.6635	134.9468	155.3126
164.1771	170.0874	186.5806
191.4453	197.8296	204.4545
216.2026	218.6670	221.4604
232.7251	240.0439	249.5226
253.3084	263.4845	271.2069
274.6028	280.0997	283.3459

287.8646	306.5574	311.7492
317.8681	322.1904	328.3133
337.0508	359.8049	366.8743
370.2934	373.2117	391.6971
409.8657	418.0001	423.3892
431.8609	444.9623	456.8928
461.0067	479.0600	498.8901
507.1511	514.0270	529.3027
536.6209	549.3685	566.8746
567.9692	578.4155	588.8748
602.3655	625.9038	639.8217
654.5838	663.2318	671.8340
683.8137	701.0785	732.6955
737.5902	743.2427	747.0368
756.2649	761.2232	774.0214
778.8325	801.9793	804.3561
817.9321	827.1203	853.3638
854.3163	878.8593	881.7758
886.6772	905.3082	910.5404
915.2762	921.4421	928.8556
937.8024	940.6394	953.0881
953.2399	963.2497	965.5292
977.4161	979.4534	982.5988
985.4248	990.7628	998.0901
1003.6485	1006.1741	1009.3024
1036.9117	1038.1092	1041.0389
1042.0798	1060.5752	1064.7402
1070.8879	1073.2717	1082.0350
1113.7787	1130.5844	1140.1029
1147.9362	1163.1719	1169.6170

1174.2000	1180.9147	1192.9667
1199.3629	1199.5267	1217.3223
1218.3311	1220.6678	1227.3553
1234.1030	1237.5305	1257.6770
1264.7436	1274.1280	1278.2762
1279.0511	1286.0326	1289.2437
1301.5903	1308.2766	1321.6269
1326.8482	1334.2094	1339.0563
1344.8162	1345.8316	1356.7734
1361.6078	1365.5808	1372.3203
1396.9792	1407.2624	1410.9285
1414.4809	1415.3997	1418.7603
1421.6462	1425.3713	1432.7523
1438.0811	1438.2574	1450.7537
1464.1138	1469.0531	1472.0522
1474.4809	1480.3150	1483.6572
1484.2870	1489.7400	1490.8753
1491.2905	1493.6703	1495.0130
1496.0634	1497.9330	1499.9721
1502.4566	1506.3677	1509.5012
1512.9427	1522.0656	1522.2111
1528.9191	1544.9678	1551.0695
1564.9315	1624.3884	1639.6239
1647.4659	1681.4563	1684.1989
1687.9588	1691.5170	1733.6315
1827.3478	2860.4353	2962.0289
3064.1919	3066.7582	3067.1327
3073.6102	3074.6785	3079.4424
3080.3848	3081.8998	3084.3821
3091.0552	3095.5384	3099.6162

3116.8746	3134.5858	3137.9810
3143.3091	3148.1926	3148.4681
3153.4593	3160.0823	3162.4766
3162.7640	3165.1451	3166.8221
3169.4618	3171.2783	3171.4981
3174.3507	3176.6279	3178.6984
3181.8496	3184.8848	3187.4826
3197.1274	3201.2453	3202.9702
3204.2711	3205.1939	3215.8448

S_p-TS1-3

Zero-point correction= 0.704966

Thermal correction to Energy= 0.743509

Thermal correction to Enthalpy= 0.744453

Thermal correction to Gibbs Free Energy= 0.635281

Sum of electronic and zero-point Energies= -1784.973849

Sum of electronic and thermal Energies= -1784.935306

Sum of electronic and thermal Enthalpies= -1784.934361

Sum of electronic and thermal Free Energies= -1785.043534

Cartesian coordinates

C	4.595553	-1.681322	-0.183975
C	4.469345	-1.191103	1.132514
C	3.516150	-1.817224	1.936163
H	3.433300	-1.523147	2.979769
C	2.527687	-2.634296	1.387282
H	1.688106	-2.940683	2.003565
C	2.479778	-2.871660	0.011198
C	3.613694	-2.520564	-0.720469
H	3.667732	-2.768334	-1.780528
C	5.613147	-1.194030	-1.132823

C	5.081020	0.114554	1.592789
H	6.159824	0.142020	1.431593
H	4.895122	0.206178	2.666848
C	4.454780	1.378834	0.862446
H	4.347408	2.171771	1.609408
H	5.163883	1.723975	0.106593
C	3.136113	1.060477	0.194952
C	2.009434	0.716026	0.954319
H	1.976060	0.974284	2.013394
C	1.014652	-0.108954	0.439927
C	1.132631	-0.620498	-0.866242
C	2.078541	-0.021332	-1.697635
H	2.138591	-0.328727	-2.739715
C	3.072185	0.813349	-1.176406
H	3.891602	1.132940	-1.816391
C	-0.106758	-0.535014	1.364754
H	-0.158220	0.143253	2.248108
C	0.455778	-1.908842	-1.274040
H	0.459841	-1.976585	-2.366789
H	-0.580527	-1.933610	-0.926737
C	1.176223	-3.199471	-0.678890
H	0.492685	-3.653240	0.040042
H	1.340321	-3.906175	-1.498321
O	6.403901	-0.291034	-0.938958
O	-0.452878	-1.728238	1.480626
H	5.609688	-1.726605	-2.107033
C	-2.893386	2.248219	-0.032837
C	-1.554445	0.561180	0.478852
N	-1.640594	1.912893	0.384121
N	-2.786431	0.181644	0.124183

N	-3.663209	1.221526	-0.204888
C	-3.254497	-1.167971	0.006356
C	-3.341906	-1.717902	-1.276151
C	-3.802165	-3.028447	-1.386842
C	-4.169973	-3.770192	-0.261724
C	-4.064284	-3.178370	0.997311
C	-3.608341	-1.869874	1.158705
H	-3.871798	-3.481247	-2.372865
H	-4.341868	-3.749292	1.880073
C	-2.931219	-0.917549	-2.483647
H	-1.905114	-0.548849	-2.372009
H	-2.981254	-1.528074	-3.386645
H	-3.577503	-0.044576	-2.614481
C	-4.695958	-5.174938	-0.408840
H	-4.253838	-5.673293	-1.274569
H	-4.482947	-5.771664	0.480780
H	-5.781571	-5.167896	-0.550811
C	-3.461328	-1.250830	2.520823
H	-2.401652	-1.258106	2.795641
H	-3.815780	-0.216299	2.530503
H	-4.022898	-1.819077	3.264665
C	-0.767266	3.092149	0.341637
C	-1.889443	4.183878	0.463473
O	-3.062750	3.554612	-0.192157
C	-1.658352	5.512894	-0.221962
H	-2.542061	6.139316	-0.079520
H	-0.804017	6.018235	0.233652
H	-1.478840	5.402373	-1.290221
C	-2.256595	4.383774	1.930092
H	-1.440795	4.894317	2.447737

H	-3.157680	4.995813	2.004105
H	-2.437183	3.426623	2.427400
C	0.129388	3.020765	-0.909238
C	-0.635227	2.866359	-2.225716
H	-1.289856	1.988309	-2.208569
H	-1.246405	3.737829	-2.474384
H	0.081302	2.718139	-3.038319
C	1.174140	4.137453	-0.957345
H	1.953356	3.863774	-1.673914
H	0.757860	5.097471	-1.269843
H	1.655370	4.269509	0.017392
H	-0.137092	3.126466	1.235730
H	0.687749	2.090546	-0.768219

Vibrational frequencies

-163.0455	15.9281	20.1858
31.2171	39.5659	44.0622
52.0746	55.0474	60.5236
75.3406	79.9540	86.2711
101.0247	106.6587	115.4813
122.6260	128.8427	152.0062
159.8629	164.2214	168.4738
185.9986	196.7982	206.3111
213.3812	221.5524	225.1626
231.4289	237.9607	238.4824
246.5257	250.8059	260.5613
277.3067	280.0289	285.6907
290.0155	300.1900	310.5553
317.7819	323.2340	328.1754
337.5935	345.0974	364.2741

373.9797	378.2759	389.0420
399.6275	419.6246	420.4035
430.3565	446.8410	454.1417
461.4672	478.6109	498.4471
505.3925	513.8261	522.6514
538.5663	554.7725	557.2927
564.4206	575.0904	587.7865
607.6419	630.0253	638.3722
654.7962	662.1835	674.4115
688.9107	689.9045	734.3653
738.9459	747.3043	753.8900
754.2078	770.0201	775.5752
778.9288	803.1000	812.5845
820.9154	828.7397	848.9949
851.0968	878.1223	882.9077
885.0065	905.0165	914.7105
915.5352	921.1368	927.5478
935.1152	938.8119	952.3295
953.3926	963.0526	963.3907
977.0823	978.8813	982.4325
983.0475	989.7037	996.8474
1002.2471	1004.7340	1010.4402
1034.3333	1037.6768	1040.3115
1043.4243	1060.3564	1063.8491
1066.2138	1070.2509	1082.3950
1106.1560	1129.9790	1133.3881
1150.1702	1164.3129	1167.9539
1173.9135	1183.6484	1194.5511
1199.2569	1200.1628	1218.0125
1219.1909	1222.5050	1231.0005

1233.6134	1236.7723	1249.8158
1267.5302	1275.4924	1278.6968
1279.6075	1286.3459	1288.0327
1300.5902	1307.5390	1322.0200
1325.4893	1333.1142	1339.2654
1346.0165	1346.6763	1356.4080
1359.5374	1363.1444	1375.8462
1391.8513	1395.9340	1401.7946
1413.9877	1416.7817	1418.3203
1420.7641	1425.4474	1431.6493
1438.9903	1439.3859	1454.3650
1464.7467	1469.7528	1472.5067
1477.7462	1481.5467	1482.8882
1483.5235	1488.1599	1490.1685
1490.6544	1493.7060	1494.4412
1496.3253	1499.5793	1501.0160
1503.5167	1507.2460	1509.6529
1511.4550	1520.3449	1522.0024
1525.7435	1545.6033	1552.2777
1564.0969	1622.1630	1639.3498
1648.8167	1682.2818	1684.4244
1686.8676	1692.9872	1732.1366
1824.6674	2872.0104	2960.6562
3068.8165	3072.8191	3075.4317
3075.9566	3076.1862	3078.2785
3083.6794	3086.6072	3092.5777
3097.5274	3100.1465	3119.7426
3135.7406	3140.7759	3143.6001
3145.4880	3145.5159	3147.2741
3148.3289	3152.5023	3163.7307

3164.3430	3166.7014	3167.6482
3168.0254	3169.8858	3170.9394
3172.7737	3175.0087	3177.0585
3177.9581	3181.2784	3187.2834
3197.9137	3202.8831	3204.5253
3204.9221	3211.9287	3232.2036

S_p-TS1-4

Zero-point correction= 0.704997

Thermal correction to Energy= 0.743638

Thermal correction to Enthalpy= 0.744582

Thermal correction to Gibbs Free Energy= 0.634818

Sum of electronic and zero-point Energies= -1784.974895

Sum of electronic and thermal Energies= -1784.936254

Sum of electronic and thermal Enthalpies= -1784.935310

Sum of electronic and thermal Free Energies= -1785.045074

Cartesian coordinates

C	-4.528620	-1.762407	0.007470
C	-3.520865	-2.538471	-0.602830
C	-2.545173	-3.062430	0.245840
H	-1.788717	-3.726801	-0.164897
C	-2.385028	-2.581726	1.546964
H	-1.510825	-2.883876	2.119465
C	-3.210918	-1.571539	2.045178
C	-4.368848	-1.301144	1.316132
H	-5.093868	-0.586199	1.704955
C	-5.687222	-1.217864	-0.727636
C	-3.307115	-2.573376	-2.100926
H	-4.201471	-2.902667	-2.632157
H	-2.507906	-3.291812	-2.304419

C	-2.885421	-1.163178	-2.700629
H	-2.107322	-1.344105	-3.448703
H	-3.748870	-0.734207	-3.213657
C	-2.413219	-0.202369	-1.632413
C	-1.270140	-0.481421	-0.886095
H	-0.547233	-1.208615	-1.261596
C	-1.100029	-0.013243	0.416171
C	-2.110006	0.764053	1.010575
C	-3.087602	1.285943	0.150822
H	-3.841376	1.954862	0.561359
C	-3.241649	0.817778	-1.152382
H	-4.105649	1.128317	-1.735289
C	0.096478	-0.542180	1.191823
H	0.415953	-1.538148	0.820698
C	-2.366398	0.807135	2.507895
H	-3.214736	1.479414	2.673567
H	-1.513461	1.190666	3.068904
C	-2.723841	-0.613692	3.109210
H	-1.820753	-1.024004	3.565507
H	-3.470060	-0.469410	3.897069
O	-5.893125	-1.319258	-1.920775
O	0.293356	-0.226444	2.382071
H	-6.404963	-0.664943	-0.086242
C	2.540158	2.129678	-0.886876
C	1.494899	0.398901	0.015657
N	1.361182	1.689881	-0.370664
N	2.763103	0.142778	-0.330112
N	3.455674	1.212707	-0.909275
C	3.422408	-1.121030	-0.193597
C	3.599785	-1.905018	-1.336891

C	4.237037	-3.135076	-1.183946
C	4.684353	-3.576095	0.063425
C	4.480928	-2.760622	1.177920
C	3.853091	-1.519031	1.074726
H	4.381932	-3.765644	-2.057734
H	4.822394	-3.096085	2.154122
C	3.106684	-1.428893	-2.677083
H	2.053942	-1.132366	-2.622340
H	3.669603	-0.552467	-3.010513
H	3.208028	-2.214699	-3.427108
C	5.397856	-4.896679	0.199138
H	5.060614	-5.607701	-0.558347
H	6.477417	-4.765891	0.072343
H	5.232400	-5.335687	1.185482
C	3.639628	-0.636415	2.275817
H	4.041187	0.365569	2.092004
H	2.572530	-0.528624	2.503153
H	4.145199	-1.053890	3.148495
C	0.429098	2.802892	-0.190066
C	1.077241	3.789631	-1.225567
O	2.513539	3.410364	-1.235822
C	1.006990	5.272059	-0.930894
H	1.549408	5.812202	-1.710556
H	-0.034786	5.599536	-0.951218
H	1.440168	5.525813	0.035354
C	0.533424	3.482661	-2.617251
H	-0.513177	3.791269	-2.678976
H	1.108048	4.027593	-3.368990
H	0.588742	2.411573	-2.833724
C	0.344191	3.134370	1.310870

C	1.690046	3.474980	1.955955
H	2.412458	2.663349	1.820734
H	2.135034	4.393197	1.564968
H	1.550692	3.606654	3.032150
C	-0.746247	4.160078	1.619288
H	-0.935502	4.179465	2.696146
H	-0.469458	5.172487	1.315494
H	-1.683277	3.891662	1.119168
H	-0.565605	2.520344	-0.549077
H	0.027668	2.181445	1.756217

Vibrational frequencies

-145.6176	14.4509	24.7143
30.2261	35.1345	41.7940
47.9250	50.8211	67.6271
69.8097	82.1248	86.9850
91.0298	99.9712	112.5485
116.9783	122.5766	133.7422
160.1320	165.7349	171.1036
187.2544	190.9789	196.8373
201.6807	215.6189	220.3443
231.1760	237.8850	242.9070
244.6028	259.2764	266.7445
276.0794	283.7738	287.0001
293.6862	302.7359	306.5136
312.5563	320.7340	329.2848
330.8866	348.6158	368.7668
371.9478	375.2267	396.6451
414.8090	418.0056	424.7680
433.2589	442.3931	461.5095

467.8131	476.8297	494.9999
510.2662	524.9644	527.9627
539.3552	548.9772	558.3085
561.6594	583.1788	588.4378
605.2566	622.7082	636.5805
653.4565	658.8514	668.8384
680.7709	701.4683	732.5948
734.6930	742.9970	748.4797
757.9570	758.8075	775.3432
782.4898	803.5255	807.6610
817.2955	829.7460	849.5562
858.7640	879.4443	886.7502
890.2765	903.0629	917.0832
919.2915	920.8620	931.8789
940.2329	941.5747	952.7704
954.3492	963.5136	968.7107
979.4735	981.1486	982.2584
988.9321	989.3776	996.1831
1002.3940	1008.0669	1012.5524
1036.6402	1037.8294	1040.4103
1042.7815	1061.6668	1063.3561
1070.3360	1075.2104	1081.6509
1109.7081	1117.2833	1127.5541
1146.6641	1167.6548	1169.7470
1175.3165	1178.2068	1193.5010
1200.5064	1201.8451	1217.1608
1220.0074	1220.9793	1225.4590
1232.1782	1238.2384	1257.4679
1262.9887	1272.5970	1278.0185
1281.0569	1286.2677	1293.0610

1303.6457	1310.0811	1325.8115
1332.0689	1334.4421	1343.4769
1346.8452	1353.5708	1358.1473
1362.5782	1364.6247	1388.2919
1396.3160	1407.7301	1416.7531
1417.6882	1421.2088	1421.6410
1424.6938	1432.2270	1433.0187
1436.8652	1438.4868	1451.9104
1463.9760	1467.5641	1469.5975
1476.8946	1482.2524	1482.5100
1485.5982	1488.4157	1490.0530
1492.4713	1495.4752	1495.7854
1496.7856	1498.9367	1500.5322
1502.5379	1507.6052	1510.0408
1511.2341	1520.5289	1521.8003
1523.3438	1542.5147	1549.9354
1563.6035	1626.8771	1640.2635
1644.6201	1681.5425	1683.9903
1687.7317	1692.3349	1727.2954
1829.0086	2928.3657	2962.5059
3057.6045	3071.7721	3074.4788
3075.7316	3076.5891	3080.1676
3080.5947	3083.2711	3088.1325
3091.9072	3099.1588	3099.4043
3120.1205	3129.0207	3141.3591
3145.4034	3145.7110	3148.3669
3150.3434	3153.6742	3155.4206
3162.9081	3164.3403	3166.1253
3166.2346	3167.4005	3168.9646
3169.8946	3174.6480	3176.7319

3176.8492	3179.5209	3189.2592
3196.5544	3203.5610	3205.3201
3208.0775	3211.2127	3211.2152

R'_p -TS1-1

Zero-point correction= 0.704521

Thermal correction to Energy= 0.743209

Thermal correction to Enthalpy= 0.744153

Thermal correction to Gibbs Free Energy= 0.634749

Sum of electronic and zero-point Energies= -1784.968231

Sum of electronic and thermal Energies= -1784.929542

Sum of electronic and thermal Enthalpies= -1784.928598

Sum of electronic and thermal Free Energies= -1785.038003

Cartesian coordinates

C	-1.022312	-0.327100	1.372786
C	-2.106497	-0.777415	2.155182
C	-3.365328	-0.236879	1.887637
H	-4.201885	-0.507816	2.528166
C	-3.609806	0.481111	0.717061
H	-4.627940	0.769203	0.465017
C	-2.592498	0.641484	-0.222767
C	-1.288423	0.346339	0.185779
H	-0.470205	0.517682	-0.506423
C	0.364633	-0.726902	1.848133
C	-1.987997	-2.000673	3.039035
H	-1.093659	-1.964885	3.667010
H	-2.854688	-2.033759	3.705224
C	-1.932685	-3.362437	2.210803
H	-2.633743	-4.064321	2.672902

H	-0.926221	-3.773976	2.308701
C	-2.242625	-3.178081	0.742713
C	-3.528961	-2.867149	0.305891
H	-4.379368	-3.043887	0.964223
C	-3.742784	-2.150639	-0.876032
C	-2.648192	-1.734611	-1.662190
C	-1.423289	-2.342242	-1.384382
H	-0.565004	-2.112755	-2.013579
C	-1.218333	-3.048258	-0.199064
H	-0.212767	-3.350410	0.075733
C	-5.124615	-1.693098	-1.110066
H	-5.868771	-2.142869	-0.419538
C	-2.684711	-0.497522	-2.533479
H	-1.724528	-0.431546	-3.054898
H	-3.475075	-0.544978	-3.284449
C	-2.898345	0.831488	-1.691719
H	-3.938089	1.147077	-1.804597
H	-2.262106	1.609530	-2.128996
O	0.799973	-1.881191	1.738758
O	-5.485558	-0.896484	-1.954451
H	0.716170	-0.099509	2.691604
C	3.625636	0.788851	-0.343380
C	1.623989	0.518009	0.578053
N	2.806271	-0.086397	0.301067
N	1.846287	1.756700	0.103563
N	3.101791	1.965455	-0.481929
C	0.885815	2.818540	0.090469
C	0.506235	3.412713	1.294006
C	-0.474326	4.406745	1.246223
C	-1.063681	4.800396	0.047436

C	-0.658815	4.172968	-1.134778
C	0.313975	3.177863	-1.138340
H	-0.783628	4.880928	2.174359
H	-1.120617	4.460101	-2.076741
C	1.096167	2.979064	2.609068
H	2.159751	2.746086	2.517501
H	0.971839	3.761603	3.359781
H	0.590367	2.079410	2.975765
C	-2.103974	5.889863	0.013726
H	-1.671137	6.826968	-0.350533
H	-2.925560	5.626722	-0.657259
H	-2.515497	6.074971	1.007910
C	0.703508	2.475979	-2.412073
H	1.768615	2.595261	-2.625550
H	0.509289	1.398599	-2.337013
H	0.128298	2.864138	-3.254550
C	3.322176	-1.450315	0.163531
C	4.828098	-1.082356	-0.073286
O	4.770442	0.244941	-0.738517
C	5.643180	-1.994669	-0.964087
H	6.651510	-1.585575	-1.062182
H	5.718697	-2.982691	-0.504202
H	5.211183	-2.098230	-1.958332
C	5.520113	-0.870074	1.268923
H	5.633563	-1.828468	1.781420
H	6.509507	-0.436403	1.109648
H	4.938969	-0.201643	1.910288
C	2.490582	-2.169067	-0.917230
C	2.470700	-1.458448	-2.273480
H	2.094881	-0.433186	-2.185758

H	3.454169	-1.414963	-2.748423
H	1.801874	-1.992633	-2.954641
C	2.829381	-3.655067	-1.039509
H	2.040034	-4.162789	-1.601565
H	3.770245	-3.829703	-1.566614
H	2.893943	-4.126689	-0.053842
H	3.216196	-1.988498	1.107561
H	1.476133	-2.104989	-0.501883

Vibrational frequencies

-76.2763	16.5347	23.7171
31.2786	35.2288	39.2472
42.9621	58.2119	65.6350
71.9236	83.0097	92.0198
97.5195	104.7957	115.6063
132.9021	141.6680	148.9439
157.3883	158.9035	166.7779
182.3461	191.5461	196.7537
206.3156	211.0273	226.6438
230.2855	233.3646	240.0406
247.4013	250.0275	259.2571
265.3238	279.4180	283.2128
286.2645	301.7733	306.0802
312.0256	314.2524	327.6542
330.7740	358.1205	362.2507
373.1595	377.0595	385.3474
399.3917	415.5861	424.4060
433.1983	445.5589	459.9982
462.0144	472.4696	493.3588
508.9684	524.9153	529.8127

533.6355	546.9018	552.6690
563.5215	574.2708	587.2801
601.6626	605.8981	631.9082
653.9318	654.2287	669.9628
685.8340	700.6209	716.0018
737.2691	744.3012	748.6399
755.1563	760.8563	780.2996
790.1090	803.7569	806.5322
818.4178	823.7433	847.7147
848.6128	878.2553	879.5869
887.4824	907.0505	915.2605
918.7563	922.7605	929.8711
935.0758	940.2217	949.7038
954.7804	962.4856	970.4531
976.3318	978.2384	980.6171
983.1473	986.4205	994.4228
999.8580	1004.2624	1012.0977
1034.3941	1036.3077	1038.7000
1042.8311	1045.4206	1056.6841
1063.2858	1064.3389	1066.8128
1082.8359	1108.5894	1119.9608
1149.4190	1163.8866	1171.0364
1173.5792	1182.6311	1195.1037
1199.8175	1202.7339	1216.4214
1218.3628	1220.8104	1229.6381
1230.9913	1233.6316	1248.4552
1259.5731	1271.0490	1279.1646
1281.2004	1288.6997	1290.1500
1298.4503	1306.8868	1324.3902
1326.5181	1327.9745	1337.2123

1346.6696	1352.7407	1359.4257
1360.6254	1364.2957	1388.9034
1398.0792	1400.9208	1411.6514
1415.6049	1417.1320	1419.0657
1420.6716	1426.6646	1429.4012
1436.5074	1439.7012	1456.0485
1464.1879	1465.6541	1472.3363
1476.1956	1480.8202	1481.3624
1482.8959	1487.5306	1489.0749
1491.6375	1492.3414	1492.6906
1496.0163	1497.6011	1499.7674
1501.8831	1504.2499	1507.1055
1511.5242	1518.6972	1520.3224
1523.4430	1529.2347	1550.8371
1559.6932	1637.8180	1642.3283
1669.9602	1680.8943	1684.0873
1687.3127	1693.3566	1729.6064
1825.7364	2946.0477	2962.2082
3062.2193	3071.8773	3074.8041
3075.0595	3076.0436	3076.7458
3083.2548	3085.7974	3088.5918
3090.7970	3095.2121	3098.2311
3137.1962	3138.7323	3141.1195
3145.3249	3145.4280	3145.5721
3146.6345	3153.6801	3160.4037
3161.0940	3162.0509	3165.7692
3167.6022	3169.5444	3173.1560
3173.9359	3175.4725	3177.1921
3179.3816	3186.2883	3188.6885
3199.8469	3204.3592	3204.9324

3209.2174

3229.9805

3236.4871

R_p'-TS1-2

Zero-point correction= 0.705080

Thermal correction to Energy= 0.743524

Thermal correction to Enthalpy= 0.744468

Thermal correction to Gibbs Free Energy= 0.636548

Sum of electronic and zero-point Energies= -1784.967370

Sum of electronic and thermal Energies= -1784.928926

Sum of electronic and thermal Enthalpies= -1784.927982

Sum of electronic and thermal Free Energies= -1785.035901

Cartesian coordinates

C	4.504913	-1.428724	0.356452
C	3.912245	-0.228666	0.800374
C	2.868238	-0.355223	1.716208
H	2.429108	0.544838	2.140640
C	2.227185	-1.576211	1.916822
H	1.300026	-1.601597	2.479606
C	2.631645	-2.719499	1.221900
C	3.868414	-2.654440	0.582955
H	4.277394	-3.545524	0.106627
C	5.670590	-1.468314	-0.544269
C	4.139491	1.108995	0.134549
H	5.199524	1.351838	0.050162
H	3.658341	1.871684	0.754390
C	3.506472	1.179393	-1.322959
H	2.991942	2.143524	-1.408517
H	4.321803	1.163864	-2.050490
C	2.560723	0.034314	-1.611204
C	1.307211	-0.035277	-0.989430

H	0.902229	0.857887	-0.527751
C	0.653601	-1.246858	-0.799525
C	1.289043	-2.438460	-1.206935
C	2.375158	-2.326826	-2.075146
H	2.830492	-3.232715	-2.469892
C	3.001732	-1.100078	-2.291155
H	3.929519	-1.061700	-2.857204
C	-0.656454	-1.428125	-0.051544
H	-1.414482	-1.893490	-0.720502
C	1.016549	-3.757989	-0.516575
H	1.439536	-4.561815	-1.125915
H	-0.054958	-3.956634	-0.416779
C	1.653158	-3.837697	0.941853
H	0.839203	-3.778785	1.667095
H	2.131551	-4.816627	1.044987
O	6.202854	-0.513221	-1.076494
O	-0.691577	-1.703239	1.164742
H	6.053972	-2.492685	-0.736631
C	-3.745170	1.239864	-0.078646
C	-1.725696	0.331963	-0.269059
N	-3.064170	0.100222	-0.380053
N	-1.716096	1.627861	0.092606
N	-2.969706	2.232419	0.214023
C	-0.562360	2.444987	0.320207
C	0.128280	2.308142	1.524651
C	1.283414	3.075845	1.691756
C	1.739427	3.942119	0.697904
C	1.004190	4.055689	-0.486550
C	-0.153913	3.312734	-0.698401
H	1.844381	2.986690	2.619568

H	1.351403	4.727124	-1.268439
C	-0.335458	1.330904	2.570416
H	-0.276463	0.300723	2.195097
H	0.276464	1.414281	3.471249
H	-1.378962	1.519983	2.843011
C	3.016615	4.721969	0.873019
H	3.781491	4.365583	0.174290
H	2.860178	5.784904	0.670577
H	3.410255	4.616839	1.885973
C	-0.915962	3.380571	-1.993655
H	-0.936216	2.395853	-2.473486
H	-1.953423	3.681563	-1.824972
H	-0.450257	4.089398	-2.679661
C	-4.004995	-1.024128	-0.504573
C	-5.295873	-0.183955	-0.824643
O	-5.063185	1.103511	-0.130347
C	-6.628203	-0.708851	-0.335046
H	-7.405297	0.009990	-0.605526
H	-6.855608	-1.658467	-0.823642
H	-6.645149	-0.848453	0.744922
C	-5.346728	0.121846	-2.317975
H	-5.571541	-0.791679	-2.873991
H	-6.129253	0.856726	-2.517065
H	-4.390834	0.517203	-2.673236
C	-3.932256	-1.908670	0.755648
C	-4.118612	-1.129881	2.059897
H	-3.335127	-0.374985	2.180492
H	-5.089358	-0.630623	2.124778
H	-4.038801	-1.816963	2.906294
C	-4.837377	-3.141419	0.667986

H	-4.501783	-3.885745	1.394480
H	-5.881135	-2.915600	0.893121
H	-4.793642	-3.601981	-0.324345
H	-3.759464	-1.624975	-1.385190
H	-2.897393	-2.269636	0.774814

Vibrational frequencies

-118.3858	20.1127	29.9566
35.8305	40.2470	48.1655
57.0183	64.9885	69.8383
74.6748	81.6980	89.4738
98.6863	106.7916	115.3146
127.2796	134.9965	145.1783
154.0777	159.6871	167.7021
188.8535	193.7865	201.7854
210.2401	215.5867	224.0910
227.3436	238.5184	245.7918
249.2813	256.9868	267.5349
275.0631	280.2363	284.0323
285.6979	306.2464	314.2646
318.5653	322.2174	326.3723
333.8618	344.6311	359.9030
370.9440	375.8751	387.5723
409.1425	418.0006	422.5216
432.3583	445.9600	460.5896
465.0073	476.8184	495.8611
505.5792	526.9384	531.1175
531.7354	551.6702	558.7221
570.9864	586.5492	592.2253
603.3453	606.0278	635.5091

652.8335	656.3041	671.2358
696.6620	708.2874	718.2252
737.6627	748.3421	750.6895
757.8602	762.2082	778.5443
790.1349	799.6374	807.3408
817.8510	826.5835	846.4652
854.1688	877.0164	879.5362
887.3794	907.4692	913.6499
916.9456	919.9056	922.9624
933.1526	941.6568	952.3256
954.0428	963.0250	970.0142
978.2238	978.7615	981.2602
982.2937	989.3053	996.4758
1001.5855	1005.2816	1009.5206
1034.6421	1035.9941	1040.6928
1043.9811	1061.9629	1063.1528
1068.4636	1073.6559	1077.4690
1106.6609	1111.5199	1144.6958
1151.6352	1163.6149	1170.3429
1171.6594	1182.9989	1193.4574
1199.7752	1201.8400	1216.6628
1218.0875	1226.0010	1227.0883
1232.8158	1234.9529	1251.0946
1258.2900	1274.2367	1278.2473
1280.2046	1288.4759	1291.8881
1299.0892	1310.3883	1322.0711
1325.1109	1331.4904	1336.8697
1343.3600	1347.9009	1358.0688
1360.1435	1363.3559	1377.7677
1390.1147	1401.8297	1414.3173

1416.0888	1417.7174	1419.8744
1421.0582	1431.0602	1431.4618
1437.5012	1439.1598	1457.8404
1463.8784	1469.8610	1472.3709
1476.5843	1481.4265	1483.4077
1485.1441	1488.1022	1488.3089
1491.0726	1493.0664	1494.9767
1495.6577	1499.0577	1500.4346
1501.9029	1505.2642	1506.8520
1509.4219	1521.9629	1522.2826
1529.3565	1529.7260	1551.3154
1560.7916	1625.0232	1640.2793
1643.5150	1679.5191	1684.7470
1687.6353	1692.0194	1739.4045
1823.3582	2890.8135	2959.5133
3054.4351	3070.5799	3073.3800
3076.5558	3076.7357	3078.9815
3082.0418	3082.2017	3092.8882
3098.5398	3099.3367	3100.1360
3122.4031	3126.1393	3131.9706
3139.4355	3142.1273	3142.7412
3150.1505	3150.9491	3160.6200
3163.3168	3163.6571	3165.1652
3166.0162	3169.5684	3173.6100
3175.4273	3177.9741	3178.8838
3181.1776	3189.4039	3196.4949
3202.7991	3203.9972	3207.1692
3208.7182	3242.7156	3261.2595

R'_p -TS1-3

Zero-point correction= 0.705379

Thermal correction to Energy= 0.743635
Thermal correction to Enthalpy= 0.744579
Thermal correction to Gibbs Free Energy= 0.637427
Sum of electronic and zero-point Energies= -1784.966236
Sum of electronic and thermal Energies= -1784.927981
Sum of electronic and thermal Enthalpies= -1784.927037
Sum of electronic and thermal Free Energies= -1785.034188

Cartesian coordinates

C	-0.581558	-0.859589	1.722763
C	-0.857575	-2.242705	1.717216
C	-2.189013	-2.629865	1.899461
H	-2.414195	-3.691280	1.988869
C	-3.235176	-1.725069	1.780135
H	-4.262959	-2.081604	1.783009
C	-2.969827	-0.390733	1.466434
C	-1.646809	0.037460	1.597080
H	-1.424656	1.096862	1.479410
C	0.823374	-0.294496	1.971565
C	0.118401	-3.315799	1.275452
H	1.136432	-2.959059	1.420799
H	-0.015875	-4.208378	1.894734
C	-0.099850	-3.758999	-0.243653
H	-0.466127	-4.789305	-0.261734
H	0.875079	-3.759347	-0.744372
C	-1.072454	-2.868672	-0.980730
C	-2.422790	-3.192941	-1.107297
H	-2.744061	-4.221970	-0.949288
C	-3.405764	-2.199508	-1.224476
C	-3.038008	-0.840134	-1.253308

C	-1.683356	-0.570665	-1.442735
H	-1.374065	0.465455	-1.515841
C	-0.715542	-1.557000	-1.299318
H	0.333795	-1.266694	-1.273398
C	-4.800321	-2.652974	-1.067664
H	-4.936052	-3.748458	-1.184000
C	-3.915497	0.314083	-0.822104
H	-3.453989	1.235079	-1.192455
H	-4.923085	0.243974	-1.231442
C	-4.026297	0.425880	0.759475
H	-5.016783	0.070308	1.056105
H	-3.953606	1.486717	1.023247
O	1.776261	-1.075512	2.288531
O	-5.754778	-1.946843	-0.806508
H	0.686038	0.624405	2.588217
C	3.202810	1.414834	-0.566339
C	1.431856	0.682913	0.533508
N	2.718160	0.410456	0.209576
N	1.243503	1.882483	-0.056558
N	2.346790	2.367757	-0.755784
C	0.048718	2.673115	-0.099963
C	-0.414570	3.309134	1.053232
C	-1.628693	3.999064	0.967879
C	-2.342825	4.088609	-0.223059
C	-1.795141	3.510273	-1.373796
C	-0.595439	2.807636	-1.341056
H	-2.016345	4.480610	1.862306
H	-2.321049	3.606468	-2.320988
C	0.325096	3.272623	2.364684
H	1.365379	2.965171	2.243428

H	0.310206	4.264200	2.822900
H	-0.155137	2.581927	3.065816
C	-3.674119	4.789986	-0.286885
H	-4.482474	4.062613	-0.415275
H	-3.869979	5.354211	0.626726
H	-3.715998	5.477356	-1.135704
C	-0.006767	2.239866	-2.607486
H	0.777270	2.898965	-2.990123
H	0.452963	1.260708	-2.444805
H	-0.779244	2.136023	-3.371940
C	3.691789	-0.688186	0.284066
C	4.970455	0.125847	-0.115045
O	4.446699	1.217870	-0.975901
C	6.046753	-0.589696	-0.901214
H	6.839770	0.122133	-1.142248
H	6.477905	-1.385004	-0.289256
H	5.669791	-1.017720	-1.828541
C	5.553541	0.792441	1.126208
H	5.995084	0.033881	1.776827
H	6.328831	1.504228	0.835472
H	4.779452	1.320290	1.690824
C	3.172753	-1.857228	-0.569762
C	2.945102	-1.534706	-2.048985
H	2.406204	-0.591647	-2.192177
H	3.877713	-1.473223	-2.614191
H	2.340761	-2.325003	-2.505210
C	3.992625	-3.132585	-0.377270
H	3.458677	-3.983513	-0.810478
H	4.967209	-3.075539	-0.868368
H	4.151684	-3.340538	0.685042

H	3.765137	-1.015986	1.320207
H	2.190370	-2.039602	-0.113804

Vibrational frequencies

-155.2300	22.8172	35.1260
41.5951	43.2222	49.4150
50.4097	54.5016	56.3301
78.0865	87.0104	91.9403
96.3819	107.8235	115.7952
130.6203	138.3402	153.4062
157.4637	181.6614	191.5995
195.9899	203.8438	212.2056
214.0246	219.9852	227.8466
231.2081	237.1964	239.3580
253.3421	255.3064	264.6872
275.2418	281.6058	285.2834
293.2460	303.3359	304.5016
309.7385	312.2093	335.4688
337.4243	345.2628	363.6912
378.6160	383.1091	397.0068
407.5630	423.4823	427.5716
434.7951	444.5879	455.1692
463.0547	479.5993	493.3120
505.2876	520.6160	525.6696
538.1250	547.9930	555.1188
566.3384	572.9333	587.3359
606.0329	623.7393	646.0518
661.2902	664.9690	671.0801
682.4811	710.8848	737.7833
739.9178	746.7094	753.1429

759.1572	763.9096	780.8923
783.9996	796.1528	817.7033
821.3463	829.4431	847.8670
850.0548	878.2542	885.5687
888.1330	900.1653	910.5584
914.7287	915.0755	921.1545
930.5854	938.6294	950.6752
957.9048	965.3747	966.1766
975.1944	980.5343	982.2874
988.7087	989.8457	997.7046
1001.5568	1008.8736	1011.1775
1037.8252	1040.0953	1043.4811
1043.6194	1054.6165	1060.9674
1063.8612	1064.9359	1092.3964
1108.4238	1120.2661	1143.6145
1160.2661	1164.9189	1174.7311
1182.5056	1191.3815	1192.9183
1200.0126	1204.5175	1213.9194
1220.1224	1223.8901	1227.7549
1233.0571	1238.8855	1243.8682
1261.6113	1267.7548	1270.6638
1280.7451	1285.5782	1292.0158
1298.2483	1304.5767	1320.8484
1323.5172	1326.0642	1327.8224
1344.5964	1357.0432	1357.7975
1361.4454	1363.0092	1371.1243
1382.7733	1399.2565	1417.0942
1418.7416	1419.0450	1421.0007
1425.7296	1428.5630	1433.5413
1434.7933	1439.6350	1446.2287

1458.3790	1463.4096	1472.4842
1480.4620	1481.7621	1485.2842
1487.5925	1488.1540	1490.2808
1491.3182	1491.9610	1494.4467
1496.8912	1499.4458	1500.8468
1505.3038	1508.0024	1509.6817
1512.8450	1516.4310	1518.4072
1523.3258	1527.2953	1552.5484
1553.8912	1554.8512	1641.0413
1644.7567	1676.9702	1686.4417
1688.9544	1690.2892	1737.8332
1825.2778	2872.0536	2966.3876
3070.7706	3075.1893	3075.3354
3076.4830	3076.6203	3077.4277
3080.6280	3082.4428	3084.2897
3090.8274	3092.0538	3100.1404
3130.7802	3137.5349	3138.3579
3144.0745	3147.5347	3149.2290
3149.7432	3162.7667	3165.3813
3165.4853	3172.2219	3173.2840
3174.4260	3174.9255	3175.9987
3179.6160	3181.9407	3182.4720
3183.4264	3193.4741	3198.1205
3200.0303	3203.6888	3205.1345
3206.9070	3214.9607	3262.6490

R'_p -TS1-4

Zero-point correction= 0.705415

Thermal correction to Energy= 0.743802

Thermal correction to Enthalpy= 0.744747

Thermal correction to Gibbs Free Energy= 0.637343

Sum of electronic and zero-point Energies= -1784.965459

Sum of electronic and thermal Energies= -1784.927072

Sum of electronic and thermal Enthalpies= -1784.926128

Sum of electronic and thermal Free Energies= -1785.033531

Cartesian coordinates

C	0.523689	-1.606156	-0.651187
C	1.375594	-2.720374	-0.508788
C	2.461236	-2.815999	-1.385296
H	3.089138	-3.703247	-1.343461
C	2.871294	-1.737589	-2.159728
H	3.814629	-1.792932	-2.699816
C	2.193412	-0.522918	-2.065404
C	0.948784	-0.529181	-1.429215
H	0.376077	0.390111	-1.393911
C	-0.773548	-1.638719	0.137978
C	1.363582	-3.648315	0.688589
H	0.354364	-3.950855	0.974345
H	1.924273	-4.549774	0.423628
C	2.044157	-2.992923	1.964776
H	2.614871	-3.767510	2.486220
H	1.242437	-2.650358	2.621543
C	2.916157	-1.814170	1.601318
C	4.195340	-1.953550	1.066123
H	4.727360	-2.897629	1.180767
C	4.753988	-0.970889	0.233505
C	4.011083	0.189993	-0.080369
C	2.884407	0.437159	0.698910
H	2.306670	1.336865	0.507230
C	2.338712	-0.544113	1.519737

H	1.354682	-0.384827	1.956661
C	6.049992	-1.325499	-0.376335
H	6.432665	-2.316006	-0.051342
C	4.157745	0.986909	-1.363951
H	4.229216	2.057609	-1.141369
H	5.072945	0.699277	-1.876724
C	2.917921	0.779622	-2.331789
H	3.287694	0.841538	-3.360466
H	2.214042	1.606826	-2.189121
O	-0.782644	-1.762471	1.377250
O	6.705351	-0.653906	-1.149554
H	-1.581179	-2.121780	-0.453801
C	-3.717572	1.220937	-0.342890
C	-1.765452	0.162062	-0.287573
N	-3.102344	0.015342	-0.493521
N	-1.681102	1.480248	-0.041951
N	-2.893316	2.180033	-0.070795
C	-0.512361	2.214488	0.345279
C	-0.119627	2.164455	1.686991
C	0.981334	2.932657	2.064514
C	1.677365	3.719337	1.143273
C	1.241285	3.747677	-0.183195
C	0.134228	3.008885	-0.604767
H	1.309252	2.908436	3.100812
H	1.768591	4.364503	-0.907095
C	-0.882931	1.326996	2.678434
H	-0.894747	0.271008	2.381623
H	-0.436476	1.408582	3.671133
H	-1.922597	1.667445	2.740949
C	2.911539	4.473178	1.563243

H	2.824487	4.835910	2.589913
H	3.786325	3.814831	1.519055
H	3.101376	5.324604	0.906391
C	-0.369923	3.079113	-2.021893
H	-0.417298	2.086375	-2.481896
H	-1.382595	3.492273	-2.047770
H	0.280288	3.708987	-2.631310
C	-4.108885	-1.053392	-0.547550
C	-5.317500	-0.177147	-1.040817
O	-5.035812	1.164506	-0.476892
C	-6.708094	-0.562990	-0.585139
H	-7.420146	0.163272	-0.984118
H	-6.966550	-1.547710	-0.980186
H	-6.798576	-0.578063	0.499969
C	-5.260890	-0.038900	-2.558689
H	-5.518298	-0.992555	-3.026030
H	-5.976980	0.717565	-2.885801
H	-4.261066	0.252175	-2.892712
C	-4.159913	-1.777603	0.813829
C	-4.386715	-0.839622	2.002189
H	-5.342448	-0.311129	1.953349
H	-4.373131	-1.420496	2.927970
H	-3.587517	-0.095222	2.075837
C	-5.120755	-2.969890	0.813293
H	-4.883199	-3.624766	1.655310
H	-6.164221	-2.667906	0.920183
H	-5.027023	-3.559592	-0.104257
H	-3.859947	-1.772100	-1.333597
H	-3.147275	-2.179295	0.944902

Vibrational frequencies

-112.9752	24.9244	29.9988
36.8930	46.2631	51.5216
59.0840	64.3239	68.9351
79.5972	85.6785	88.8406
99.3802	112.5123	115.9732
119.0559	127.6301	134.8668
155.4060	160.1355	176.2303
181.8344	198.7996	204.2081
211.1279	217.6457	226.5416
235.1481	235.7777	247.6374
250.2136	252.3047	263.0712
273.1205	284.1848	284.9510
285.6018	302.8369	307.1192
317.6035	326.0275	335.0065
343.4830	345.3315	359.3720
372.0736	383.7270	392.3181
404.2927	414.4286	425.3569
435.7314	446.9842	463.8890
467.6599	474.6687	486.1193
505.4838	521.3288	530.3103
533.8599	543.5352	556.6935
569.5659	585.3156	588.9199
601.2473	606.5107	633.7304
646.3288	653.5974	670.1437
694.2853	704.1591	719.0391
733.2361	745.9417	749.2336
760.8206	767.7933	779.1759
791.7381	797.8425	813.5746
817.6520	838.2693	853.5568

858.0278	878.2087	881.7045
889.1669	906.4290	909.7980
915.5982	918.3128	923.6117
935.2666	943.9079	951.8455
962.5560	964.1970	977.3888
979.2231	981.8140	985.6321
987.9804	993.8529	995.1918
999.8439	1006.5828	1013.3529
1034.3381	1037.4981	1041.2306
1043.7084	1061.6338	1064.4471
1069.0839	1073.8410	1076.2412
1107.6299	1113.2296	1133.9366
1144.4629	1163.0937	1171.0612
1176.1446	1185.2566	1191.4459
1198.7475	1199.8642	1214.9485
1216.4886	1219.8930	1223.7703
1229.6133	1235.1541	1250.3405
1265.1524	1274.6595	1275.8874
1278.6556	1289.8577	1295.8973
1298.6821	1314.9479	1321.8128
1330.5176	1332.3989	1335.0630
1344.6749	1349.6196	1353.9705
1357.3728	1364.0168	1379.7702
1391.4636	1405.0504	1413.8572
1417.3850	1418.4526	1420.5140
1421.3523	1430.0283	1431.0755
1439.2827	1445.9369	1459.9104
1461.7033	1461.8746	1476.1739
1481.7980	1483.3692	1486.2233
1487.9558	1488.4278	1491.1064

1491.6331	1494.1400	1494.2961
1497.0307	1499.9387	1502.6569
1505.4482	1506.0405	1509.4264
1510.2823	1521.0644	1522.3076
1527.3821	1533.0157	1550.9115
1560.0775	1632.6035	1637.2208
1640.6093	1676.1983	1684.8164
1687.0680	1688.3409	1736.6546
1825.1164	2902.6210	2958.6236
3054.2620	3071.0221	3074.2526
3076.1025	3077.8677	3080.1077
3083.7263	3086.4787	3087.3659
3087.5713	3096.1637	3099.9978
3122.5624	3123.2308	3126.5509
3140.4592	3142.6043	3152.0271
3152.1905	3152.3107	3164.6793
3167.3302	3167.4832	3168.0741
3172.1315	3173.0233	3175.0981
3177.3090	3178.9280	3181.5677
3185.2833	3201.7621	3202.4361
3203.2728	3203.5380	3206.8580
3209.2259	3239.9574	3262.1896

S'_p -TS1-1

Zero-point correction= 0.705452

Thermal correction to Energy= 0.743684

Thermal correction to Enthalpy= 0.744629

Thermal correction to Gibbs Free Energy= 0.637420

Sum of electronic and zero-point Energies= -1784.971526

Sum of electronic and thermal Energies= -1784.933293

Sum of electronic and thermal Enthalpies= -1784.932349

Sum of electronic and thermal Free Energies= -1785.039557

Cartesian coordinates

C	-4.324250	-2.051442	0.261612
C	-4.236262	-0.875624	1.037928
C	-3.372942	-0.917098	2.131051
H	-3.308831	-0.053468	2.787775
C	-2.415330	-1.924468	2.258171
H	-1.632329	-1.805536	3.002149
C	-2.314651	-2.940070	1.306274
C	-3.376752	-3.066426	0.410985
H	-3.387399	-3.893762	-0.298528
C	-5.250231	-2.201956	-0.876714
C	-4.764509	0.460326	0.562241
H	-5.830574	0.423367	0.333314
H	-4.614510	1.182780	1.369715
C	-4.008589	0.981115	-0.734052
H	-3.836556	2.056141	-0.608978
H	-4.666826	0.843892	-1.595305
C	-2.706179	0.252838	-0.979234
C	-1.666470	0.346879	-0.051864
H	-1.670022	1.131359	0.703128
C	-0.687197	-0.634116	0.055868
C	-0.779732	-1.791871	-0.739973
C	-1.650786	-1.747889	-1.832724
H	-1.701896	-2.604204	-2.502082
C	-2.594494	-0.727896	-1.966766
H	-3.349179	-0.795786	-2.747304
C	0.319789	-0.500797	1.187071

H	0.908762	-1.434865	1.320662
C	-0.275950	-3.143451	-0.262338
H	-0.458418	-3.868407	-1.061522
H	0.799120	-3.162159	-0.069286
C	-1.003368	-3.649486	1.054604
H	-0.343920	-3.478698	1.911263
H	-1.140243	-4.731732	0.964553
O	-6.007635	-1.353994	-1.305857
O	0.040888	0.195492	2.196325
H	-5.207410	-3.200979	-1.359501
C	3.802565	1.281789	0.054791
C	1.781959	0.410427	0.283531
N	3.109615	0.126151	0.251095
N	1.779199	1.734082	0.080234
N	3.037199	2.316534	-0.073316
C	0.623078	2.571219	-0.044707
C	-0.044366	2.604003	-1.268019
C	-1.186398	3.402727	-1.356939
C	-1.647314	4.140303	-0.268022
C	-0.932338	4.089207	0.933879
C	0.215814	3.313692	1.068556
H	-1.736659	3.430625	-2.294434
H	-1.280533	4.667186	1.786822
C	0.404372	1.749449	-2.422138
H	-0.070923	2.075548	-3.348989
H	0.125364	0.703099	-2.244484
H	1.489819	1.790948	-2.552060
C	-2.889496	4.987845	-0.374122
H	-3.392348	4.835263	-1.331419
H	-2.645783	6.050829	-0.283808

H	-3.595024	4.746984	0.426446
C	0.989726	3.243535	2.355670
H	2.023074	3.570965	2.206320
H	1.003228	2.207950	2.708792
H	0.530246	3.877741	3.115987
C	4.040248	-0.990316	0.435619
C	5.345948	-0.338099	-0.150984
O	5.117725	1.116176	0.040870
C	6.582007	-0.690113	0.650173
H	7.436365	-0.117784	0.282449
H	6.806768	-1.753670	0.542217
H	6.432326	-0.465633	1.708274
C	5.553404	-0.511432	-1.647818
H	5.777040	-1.549357	-1.900310
H	6.400747	0.107236	-1.951107
H	4.671837	-0.190277	-2.208386
C	3.515918	-2.331951	-0.099462
C	4.567381	-3.433151	0.055428
H	4.981394	-3.454402	1.068092
H	5.393512	-3.309970	-0.651302
H	4.111102	-4.405972	-0.142271
C	2.911143	-2.310666	-1.505479
H	2.414387	-3.267766	-1.688357
H	3.664568	-2.185125	-2.284060
H	2.156715	-1.523794	-1.612875
H	4.197940	-1.110912	1.514856
H	2.700669	-2.578611	0.594183

Vibrational frequencies

-186.8601 22.2532 30.5117

36.0336	43.0045	50.7540
56.8698	65.6493	68.2286
73.0334	80.3600	84.6022
104.2936	115.3729	117.7178
127.7452	134.1438	146.7209
155.9233	166.5629	185.1764
198.3614	201.3274	209.5120
211.7964	217.0921	222.6306
228.7798	238.3761	244.3297
248.6465	264.0382	271.4686
279.1783	280.0199	284.1248
293.8036	298.0926	312.6570
328.1433	329.1443	335.5034
337.2977	347.3109	361.6218
368.8014	376.5789	379.6597
407.7041	414.1565	432.1354
437.5832	452.7779	467.3816
473.3556	481.9530	498.4290
510.7848	523.2401	528.9644
537.3436	554.1960	565.4739
567.6486	583.7886	589.5750
600.1579	623.8960	631.3750
659.8776	660.4188	667.8033
679.3017	705.6704	717.4237
735.8709	736.5385	752.9094
754.2460	760.6659	768.8686
785.5409	792.3655	801.6353
811.7718	829.8579	856.3448
858.6369	877.6943	883.0385
890.2645	911.1841	911.5095

912.8433	926.6704	936.2704
939.6311	954.0299	957.5275
961.1636	964.5804	965.8646
979.8573	980.8894	981.7901
985.1414	994.6149	1003.0891
1008.1955	1013.2871	1022.2870
1026.0799	1035.1834	1041.6432
1044.1406	1062.5644	1063.1418
1071.5835	1073.3240	1091.3805
1106.4408	1116.1425	1148.1620
1156.4170	1156.7471	1170.6629
1173.0297	1181.9788	1188.0635
1198.5746	1200.3272	1214.7659
1219.5315	1221.3264	1226.2526
1231.4400	1237.5020	1257.5869
1263.1117	1275.5521	1278.4984
1284.2758	1285.9542	1292.2729
1307.5787	1315.3754	1330.6177
1332.0469	1336.5662	1340.8396
1347.9546	1359.1325	1361.9462
1364.4859	1366.0823	1382.0288
1387.8410	1400.2504	1409.3616
1414.9963	1415.8050	1419.0841
1425.1668	1425.6219	1435.1732
1440.2130	1441.3539	1462.4945
1462.9895	1469.5143	1473.8943
1479.8265	1483.4672	1486.4428
1488.1754	1488.9302	1489.0630
1490.1952	1490.7971	1495.4799
1497.4603	1498.0961	1503.0387

1506.5863	1507.8875	1510.7094
1515.7022	1519.1011	1522.8409
1527.1714	1533.5617	1551.9728
1561.5819	1587.6797	1642.7999
1648.8328	1681.3531	1685.6128
1689.1812	1691.1432	1736.7721
1828.0186	2904.2255	2958.7825
3056.4180	3061.2284	3072.5781
3074.1650	3074.2816	3075.6110
3078.9693	3079.7035	3081.4884
3090.0538	3093.2915	3095.9064
3097.2941	3130.1037	3132.5153
3142.1176	3143.8323	3148.2462
3149.2806	3152.4710	3154.8844
3161.4842	3164.8594	3166.3953
3169.8654	3172.4921	3173.0219
3177.7952	3179.9775	3182.2837
3184.9723	3185.9384	3188.6314
3196.6859	3200.4601	3202.7834
3203.2847	3204.6407	3220.6099

S_p'-TS1-2

Zero-point correction= 0.705300

Thermal correction to Energy= 0.743555

Thermal correction to Enthalpy= 0.744499

Thermal correction to Gibbs Free Energy= 0.637731

Sum of electronic and zero-point Energies= -1784.967784

Sum of electronic and thermal Energies= -1784.929529

Sum of electronic and thermal Enthalpies= -1784.928585

Sum of electronic and thermal Free Energies= -1785.035353

Cartesian coordinates

C	-0.372914	-1.482725	0.701396
C	-1.116653	-2.606618	1.121929
C	-1.732425	-3.379633	0.136260
H	-2.243149	-4.294714	0.428410
C	-1.873870	-2.911183	-1.169428
H	-2.485482	-3.466214	-1.877133
C	-1.416379	-1.637360	-1.502068
C	-0.557361	-1.007220	-0.594419
H	-0.153365	-0.033775	-0.854505
C	0.494675	-0.816048	1.765245
C	-1.493610	-2.819832	2.572846
H	-0.636232	-2.703003	3.239845
H	-1.864613	-3.842722	2.685395
C	-2.623901	-1.812983	3.073320
H	-3.385077	-2.397482	3.599695
H	-2.165295	-1.125713	3.785979
C	-3.244295	-1.013551	1.950479
C	-4.106066	-1.609099	1.030473
H	-4.574954	-2.563304	1.271064
C	-4.229756	-1.119038	-0.274210
C	-3.492764	0.013627	-0.678062
C	-2.910148	0.769939	0.338348
H	-2.386006	1.686776	0.080842
C	-2.775499	0.263834	1.630479
H	-2.137501	0.786807	2.336032
C	-4.978910	-1.971213	-1.213548
H	-5.540573	-2.794243	-0.723199
C	-3.058328	0.255932	-2.107188
H	-2.553797	1.227677	-2.134989

H	-3.901986	0.288579	-2.798783
C	-2.050819	-0.852757	-2.629431
H	-2.601799	-1.540512	-3.275117
H	-1.295749	-0.350409	-3.243745
O	-0.015369	-0.234014	2.737621
O	-5.014371	-1.851196	-2.423317
H	1.438155	-1.387593	1.923346
C	3.546732	1.091264	-0.398500
C	1.658524	0.456768	0.576749
N	2.942567	0.102672	0.317298
N	1.603857	1.681653	0.028486
N	2.780121	2.115296	-0.592506
C	0.462355	2.546548	-0.002106
C	0.007283	3.107123	1.196421
C	-1.106140	3.946240	1.132300
C	-1.737062	4.244035	-0.076723
C	-1.229417	3.685450	-1.251056
C	-0.129598	2.826735	-1.239707
H	-1.479247	4.390580	2.051703
H	-1.705678	3.914338	-2.201629
C	0.711029	2.840524	2.499592
H	0.561629	1.803230	2.817255
H	1.787272	3.012353	2.397361
H	0.328835	3.506049	3.275914
C	-2.964675	5.116157	-0.109414
H	-3.867304	4.503747	-0.011328
H	-2.961700	5.835126	0.712701
H	-3.037233	5.663733	-1.051641
C	0.404063	2.247885	-2.524056
H	1.308692	2.774232	-2.841211

H	0.675006	1.193353	-2.412192
H	-0.342076	2.330371	-3.317369
C	3.766282	-1.109124	0.312750
C	5.146531	-0.431894	-0.027490
O	4.777641	0.787022	-0.785375
C	6.120697	-1.204896	-0.889820
H	6.999833	-0.581188	-1.067798
H	6.442268	-2.108130	-0.367364
H	5.690639	-1.481797	-1.851580
C	5.808597	0.039195	1.262586
H	6.146271	-0.823741	1.841758
H	6.671503	0.664939	1.026384
H	5.109776	0.615874	1.875361
C	3.121487	-2.156102	-0.616128
C	2.829586	-1.637501	-2.025638
H	2.166282	-0.766682	-2.002386
H	3.737701	-1.359351	-2.567422
H	2.320226	-2.414980	-2.600869
C	3.875774	-3.488185	-0.627345
H	3.218995	-4.273010	-1.010225
H	4.758480	-3.459212	-1.269071
H	4.192812	-3.778137	0.379383
H	3.831773	-1.524392	1.323076
H	2.145493	-2.345058	-0.145352

Vibrational frequencies

-100.4645	21.7566	32.0384
38.4007	46.7942	53.2322
63.3537	66.7714	72.8226
75.9458	87.0659	92.8379

104.5650	109.8075	118.7352
131.9715	148.2587	157.1924
161.4164	165.1036	168.6520
188.1077	189.2838	195.7299
206.4043	216.0797	222.7160
232.2108	238.2746	248.0960
255.8950	260.9400	264.8687
269.7149	278.9030	283.3844
288.0146	310.3570	311.1217
316.8947	326.5820	331.2500
334.1494	360.5318	366.2576
372.4331	380.0489	386.8607
402.4040	416.7653	427.1384
432.5770	450.8960	458.9221
462.0925	472.0116	493.6200
511.2076	523.1194	528.0376
531.6539	553.3374	564.3289
572.0236	573.0562	587.9859
600.0212	602.8369	636.0580
653.4971	656.6788	673.7839
690.1141	701.2868	717.4571
738.0833	742.6238	745.4614
755.2995	761.9332	777.0176
791.9633	802.2824	805.9745
816.5178	828.3644	848.2720
853.6238	879.3610	881.7667
885.8662	907.6026	916.5064
918.8492	920.2104	923.0153
934.3193	942.9191	952.6974
953.9803	964.1684	970.0934

978.7525	980.2262	982.9005
984.9129	990.0438	997.8273
1002.8113	1005.4510	1010.9428
1036.8255	1040.2549	1042.4339
1042.5150	1060.7515	1063.1141
1068.7981	1073.8165	1074.4437
1103.7274	1112.0992	1135.5909
1149.6926	1163.6500	1173.0100
1174.2833	1186.4338	1194.7995
1201.6883	1202.4222	1217.2928
1219.0038	1222.4993	1230.0618
1234.3670	1234.9536	1256.2308
1259.6254	1277.0769	1278.9377
1280.6711	1289.2406	1290.4693
1299.5244	1310.4787	1320.9124
1327.8246	1335.8523	1336.7546
1345.9448	1348.4987	1354.6753
1360.0052	1364.0673	1376.8895
1395.2232	1406.4945	1412.3897
1418.0994	1419.4239	1420.3664
1421.0574	1429.0393	1432.4165
1438.6062	1438.9210	1460.6142
1462.6372	1463.4933	1472.2501
1475.4069	1480.0802	1481.7421
1485.4315	1489.2508	1490.5669
1490.9964	1493.0040	1495.1571
1495.6456	1497.3432	1498.8246
1502.2638	1506.0435	1507.9517
1509.4482	1519.7035	1520.6354
1528.5690	1529.7722	1551.6268

1558.8628	1634.9058	1641.5839
1641.9517	1676.0848	1683.1960
1686.0378	1688.8577	1737.5020
1823.4746	2871.6306	2957.5503
3049.4898	3064.2875	3074.8657
3077.5164	3077.7418	3080.6023
3081.6706	3082.2098	3085.2218
3089.8536	3095.4434	3099.4907
3115.6025	3138.7478	3143.4573
3144.1786	3145.7419	3146.4024
3150.5360	3155.4184	3159.9702
3163.4782	3164.5422	3165.5302
3167.5363	3167.9802	3171.9383
3173.2902	3176.8805	3177.8996
3181.9098	3188.4755	3202.9381
3206.0737	3206.1647	3206.1736
3223.1598	3235.4326	3241.1212

S'_p-TS1-3

Zero-point correction= 0.704984

Thermal correction to Energy= 0.743466

Thermal correction to Enthalpy= 0.744410

Thermal correction to Gibbs Free Energy= 0.635537

Sum of electronic and zero-point Energies= -1784.965917

Sum of electronic and thermal Energies= -1784.927435

Sum of electronic and thermal Enthalpies= -1784.926491

Sum of electronic and thermal Free Energies= -1785.035364

Cartesian coordinates

C	-0.649798	-1.073936	1.226072
C	-1.618229	-1.711245	2.031554

C	-2.237831	-2.850399	1.515379
H	-2.924038	-3.408656	2.148650
C	-2.149145	-3.173552	0.162436
H	-2.759088	-3.978897	-0.239870
C	-1.452072	-2.335830	-0.706709
C	-0.603884	-1.380921	-0.131391
H	0.019464	-0.769890	-0.777892
C	0.191712	-0.009936	1.920222
C	-2.191270	-1.058532	3.272093
H	-1.411508	-0.672137	3.932814
H	-2.752271	-1.815110	3.828568
C	-3.169653	0.151754	2.934646
H	-4.058229	0.051437	3.566005
H	-2.659399	1.077944	3.202424
C	-3.551159	0.207558	1.473013
C	-4.403333	-0.744778	0.915345
H	-5.030556	-1.352768	1.567462
C	-4.322279	-1.090035	-0.438257
C	-3.398253	-0.439694	-1.280947
C	-2.815176	0.723439	-0.780214
H	-2.162002	1.306061	-1.423935
C	-2.865126	1.034587	0.577870
H	-2.221988	1.822122	0.962174
C	-5.077456	-2.289392	-0.841809
H	-5.828634	-2.620337	-0.094005
C	-2.806772	-1.074256	-2.518434
H	-2.245625	-0.301658	-3.053069
H	-3.574814	-1.461303	-3.188728
C	-1.816558	-2.271966	-2.173477
H	-2.302146	-3.207275	-2.462251

H	-0.923063	-2.153308	-2.795890
O	-0.318652	1.047133	2.317634
O	-4.928986	-2.920068	-1.870996
H	1.029587	-0.460580	2.494457
C	3.662296	0.609828	-0.533085
C	1.673021	0.422435	0.435784
N	2.890381	-0.162824	0.279775
N	1.830905	1.547774	-0.274524
N	3.074556	1.703830	-0.898479
C	0.862023	2.594807	-0.412933
C	0.744522	3.537707	0.610988
C	-0.214799	4.538839	0.456347
C	-1.020436	4.614556	-0.680681
C	-0.836791	3.674931	-1.697779
C	0.104366	2.652338	-1.585305
H	-0.329116	5.281867	1.241821
H	-1.440485	3.738195	-2.600268
C	1.621513	3.465846	1.830733
H	1.299109	2.628260	2.456803
H	2.668075	3.310039	1.552214
H	1.549459	4.389206	2.408481
C	-2.078055	5.680418	-0.806808
H	-3.047858	5.298615	-0.471518
H	-1.835984	6.552779	-0.196069
H	-2.192615	6.003124	-1.844236
C	0.300341	1.641349	-2.684287
H	1.350773	1.581451	-2.982430
H	-0.001782	0.640008	-2.355495
H	-0.299251	1.901961	-3.558798
C	3.526394	-1.460670	0.512776

C	5.001247	-1.052257	0.142895
O	4.841529	0.069732	-0.811338
C	5.871077	-2.086529	-0.538043
H	6.837573	-1.632839	-0.769794
H	6.041423	-2.928668	0.135922
H	5.428018	-2.452503	-1.463503
C	5.690894	-0.480713	1.376707
H	5.877499	-1.278983	2.099273
H	6.644657	-0.032147	1.091913
H	5.069691	0.282079	1.855184
C	2.761372	-2.551136	-0.259538
C	2.580050	-2.253301	-1.749327
H	2.114139	-1.275961	-1.915845
H	3.524821	-2.273452	-2.299523
H	1.922042	-3.006925	-2.191125
C	3.309470	-3.958522	-0.011165
H	2.556179	-4.696436	-0.298153
H	4.207627	-4.163684	-0.596911
H	3.545556	-4.115534	1.046044
H	3.499086	-1.703674	1.579491
H	1.760327	-2.515003	0.191773

Vibrational frequencies

-92.6308	12.3584	20.8957
34.6409	41.6739	45.0007
51.8911	56.4692	69.8841
71.2328	85.5946	89.5878
95.5037	105.9367	117.5385
129.7537	134.4480	154.5871
158.5790	166.4425	174.0764

176.2461	189.7443	199.8299
204.8899	217.3479	222.1130
236.0065	241.9827	244.8773
254.6704	262.2871	266.7505
273.6224	281.0999	283.6868
285.2335	308.0180	314.0256
317.5233	327.6109	330.2003
333.9768	353.6737	366.6259
377.7105	379.6490	385.9047
400.9316	416.4272	421.8212
429.8928	448.8363	458.5175
462.5337	471.1706	491.2346
508.2307	520.0913	527.0581
532.0949	553.1587	560.1874
570.2079	572.9261	587.5023
601.4658	604.9432	637.9655
654.6043	658.8459	672.5723
686.5467	704.5567	718.7883
739.1264	743.0945	749.4996
756.7255	763.9421	777.2660
790.1197	800.8141	808.6130
814.0745	830.4720	849.7155
853.1339	879.3485	882.1824
885.4788	907.8122	914.2363
915.7817	920.3575	922.2018
934.3707	942.3723	950.7913
954.0293	963.3431	971.4324
979.6535	979.9397	981.8781
987.4361	988.7400	995.9210
1003.2424	1005.8111	1009.2978

1037.2002	1038.0613	1040.7135
1043.9006	1058.7811	1063.1387
1068.9647	1071.6948	1074.0458
1089.1858	1112.6803	1122.8471
1145.4826	1162.9656	1172.4845
1173.0422	1183.0789	1192.3889
1199.3129	1201.9694	1218.3511
1218.4664	1225.2717	1226.0536
1232.8355	1235.8137	1257.4401
1259.4248	1278.3756	1279.3683
1280.9856	1288.2950	1290.5301
1299.5065	1306.9333	1322.3069
1324.2222	1333.0127	1334.1554
1347.1667	1350.8724	1356.0871
1359.5717	1363.6131	1377.7801
1393.2035	1398.6460	1406.6273
1407.6736	1414.0789	1419.4079
1420.0106	1424.6606	1431.8446
1437.5053	1437.9046	1464.0152
1464.4707	1466.4367	1472.1943
1477.2740	1481.5427	1482.9130
1486.2435	1489.4460	1491.2602
1491.8199	1494.1032	1494.9740
1495.5013	1499.4944	1501.8206
1503.8539	1506.9002	1508.2387
1509.6023	1521.0924	1521.4348
1527.1080	1527.7514	1551.6149
1565.5800	1637.6955	1641.3793
1659.0197	1681.3871	1682.9381
1685.7462	1692.6714	1732.5446

1823.5179	2901.9197	2961.7113
3063.4630	3070.4315	3074.2839
3075.0282	3075.7073	3080.0337
3080.2753	3082.2746	3085.1475
3094.7442	3095.5371	3100.0160
3115.4044	3138.2334	3143.9311
3143.9540	3145.0692	3145.3525
3153.0918	3153.3185	3159.9275
3165.2651	3168.0362	3169.3781
3169.8717	3170.7031	3172.2555
3172.5374	3174.1119	3178.0892
3181.6102	3190.5239	3200.8227
3203.8416	3206.5196	3207.5615
3215.9303	3217.1384	3228.9385

S'_p -TS1-4

Zero-point correction= 0.705300

Thermal correction to Energy= 0.743655

Thermal correction to Enthalpy= 0.744599

Thermal correction to Gibbs Free Energy= 0.636677

Sum of electronic and zero-point Energies= -1784.966621

Sum of electronic and thermal Energies= -1784.928266

Sum of electronic and thermal Enthalpies= -1784.927322

Sum of electronic and thermal Free Energies= -1785.035244

Cartesian coordinates

C	1.063756	-0.408180	1.583336
C	1.872103	-1.368306	2.231478
C	3.257893	-1.181915	2.175692
H	3.897329	-1.861208	2.735345
C	3.843017	-0.292178	1.279501

H	4.922333	-0.290673	1.146300
C	3.034767	0.442900	0.413678
C	1.666607	0.480173	0.694537
H	1.039084	1.109572	0.076013
C	-0.440347	-0.436038	1.857719
C	1.365521	-2.705342	2.737244
H	0.474482	-2.602129	3.356039
H	2.158162	-3.151434	3.345947
C	1.009148	-3.716808	1.563948
H	1.428981	-4.695951	1.815596
H	-0.077310	-3.803852	1.521130
C	1.521938	-3.241777	0.225610
C	2.879661	-3.286016	-0.087160
H	3.542914	-3.930485	0.489578
C	3.450083	-2.370441	-0.977675
C	2.648047	-1.405546	-1.621134
C	1.267657	-1.596393	-1.543578
H	0.610156	-0.916663	-2.083874
C	0.712343	-2.479938	-0.619754
H	-0.357567	-2.451281	-0.431412
C	4.925329	-2.349005	-1.008158
H	5.395371	-3.237616	-0.537313
C	3.183457	-0.080982	-2.115206
H	2.410442	0.385297	-2.731898
H	4.073411	-0.209535	-2.731492
C	3.554747	0.912050	-0.926525
H	4.643330	0.997646	-0.884087
H	3.149650	1.899107	-1.177797
O	-1.038720	-1.537923	1.918822
O	5.623600	-1.466086	-1.466495

H	-0.719052	0.369171	2.568380
C	-2.806020	0.479539	-1.318907
C	-1.319922	0.512576	0.320973
N	-2.251274	-0.250446	-0.309512
N	-1.392109	1.664161	-0.372980
N	-2.315183	1.672489	-1.419729
C	-0.644531	2.862533	-0.129100
C	-0.877257	3.577831	1.048632
C	-0.109213	4.722047	1.269331
C	0.850795	5.153186	0.354106
C	1.026834	4.424377	-0.824360
C	0.285088	3.276110	-1.090701
H	-0.274257	5.295136	2.178125
H	1.761234	4.755892	-1.554547
C	-1.941076	3.158950	2.029032
H	-2.890612	2.976287	1.516890
H	-1.670728	2.238272	2.553801
H	-2.097020	3.939867	2.774837
C	1.693314	6.369893	0.635683
H	1.925544	6.910730	-0.284526
H	1.186048	7.051882	1.321286
H	2.643001	6.080346	1.096795
C	0.475748	2.500636	-2.365716
H	0.501914	1.424057	-2.166724
H	-0.353136	2.675473	-3.057109
H	1.407786	2.787946	-2.857271
C	-3.072551	-1.457492	-0.086947
C	-3.671692	-1.569313	-1.529545
O	-3.761978	-0.158193	-1.978447
C	-5.052697	-2.170686	-1.676388

H	-5.335606	-2.147372	-2.731352
H	-5.037064	-3.212589	-1.349110
H	-5.802860	-1.628275	-1.103030
C	-2.677322	-2.265861	-2.452868
H	-2.593648	-3.320333	-2.177705
H	-3.021632	-2.197599	-3.486837
H	-1.684139	-1.812349	-2.383931
C	-3.993026	-1.219327	1.126403
C	-4.880741	0.022873	1.014814
H	-4.289133	0.930996	0.858529
H	-5.610689	-0.044607	0.203802
H	-5.434555	0.155581	1.948036
C	-4.788020	-2.469489	1.513210
H	-5.173863	-2.351347	2.529137
H	-5.643898	-2.647867	0.859059
H	-4.153541	-3.361328	1.500198
H	-2.434213	-2.316340	0.121499
H	-3.270520	-1.046088	1.930977

Vibrational frequencies

-143.8011	17.2713	32.1961
37.7675	38.4505	43.5992
48.3316	67.3896	69.2626
74.7644	85.1962	95.1064
104.2367	106.9511	110.5946
123.4491	128.0532	140.4689
149.5854	160.2748	175.9290
181.7147	195.4705	198.7716
200.6318	219.4886	223.4806
235.7421	242.3881	249.2077

252.9315	258.5991	271.7950
281.9651	282.6641	287.2371
295.1687	307.7008	314.3061
319.4113	335.6458	341.2049
344.8690	347.6088	372.8894
375.0088	382.4391	408.0256
410.1565	418.3795	424.7000
429.5430	444.9522	461.7381
464.9858	470.2826	494.2847
504.5709	521.4648	525.0423
533.5186	548.7499	554.6474
571.9485	580.1999	589.4756
605.1477	608.9732	644.8756
655.7689	657.9745	672.5984
685.5919	709.8606	727.7960
737.8126	744.6519	749.0986
758.6519	760.1117	780.8382
791.6785	801.1459	804.8833
823.5420	825.9071	846.1728
852.1133	876.0628	880.5959
885.8024	908.5307	915.6656
917.1543	919.1814	920.0338
933.4380	941.4400	950.5663
953.0018	960.5843	964.1421
975.7181	980.1888	981.2506
982.3730	988.1220	995.2806
1001.3503	1006.4350	1009.7799
1033.9296	1036.6065	1041.0483
1043.5796	1058.1251	1063.0989
1063.9786	1067.2754	1086.9847

1102.4791	1117.9026	1136.6946
1144.3526	1159.6562	1174.6383
1177.3738	1183.7000	1191.6038
1201.5841	1203.5162	1213.0476
1220.8077	1223.0657	1224.1309
1228.0864	1235.5273	1239.5873
1261.6519	1270.2357	1277.8796
1281.5078	1284.7228	1290.3375
1297.0057	1307.3044	1321.3021
1322.4045	1331.5419	1332.7272
1344.1284	1349.9576	1353.3306
1358.5726	1361.5833	1366.1379
1387.3644	1389.9492	1405.3703
1415.3421	1417.4321	1419.0660
1419.6121	1426.9851	1429.6126
1436.6147	1438.9381	1453.6425
1460.7293	1462.5758	1472.8812
1477.2953	1480.4485	1481.6164
1484.0649	1485.9696	1487.0250
1489.0485	1490.0144	1491.5501
1494.9342	1495.0098	1497.0901
1502.1122	1503.7230	1505.5460
1509.6957	1519.2737	1520.9756
1526.3441	1533.9796	1551.2538
1556.6616	1586.6915	1637.9195
1642.5757	1679.1961	1684.4145
1687.2710	1692.7213	1739.2011
1826.8361	2918.0559	2966.5373
3074.0131	3075.2822	3076.2909
3077.3172	3079.4973	3079.8752

3083.1347	3083.7573	3094.5116
3099.8742	3107.6192	3109.6264
3142.2427	3145.1575	3146.1918
3147.5912	3147.6419	3151.7318
3161.1197	3161.3483	3165.2372
3168.4578	3171.1830	3171.2239
3172.3879	3173.7677	3175.1300
3175.5531	3176.1573	3177.1905
3179.6476	3180.3933	3189.7415
3202.0669	3207.7640	3207.9681
3210.0584	3227.1227	3274.5204

R_p -TS2-1

Zero-point correction= 0.732416

Thermal correction to Energy= 0.777214

Thermal correction to Enthalpy= 0.778158

Thermal correction to Gibbs Free Energy= 0.653943

Sum of electronic and zero-point Energies= -2069.444543

Sum of electronic and thermal Energies= -2069.399745

Sum of electronic and thermal Enthalpies= -2069.398801

Sum of electronic and thermal Free Energies= -2069.523016

Cartesian coordinates

C	1.485704	0.170413	0.312268
C	2.686714	0.345057	1.034431
C	3.877712	0.006431	0.386005
H	4.818920	0.212253	0.892892
C	3.897123	-0.743316	-0.788542
H	4.842329	-1.121632	-1.171807
C	2.695077	-1.188984	-1.337840

C	1.522407	-0.611992	-0.849566
H	0.566853	-0.917657	-1.277516
C	0.118134	0.611061	0.749889
C	2.739831	0.610480	2.526073
H	2.110323	1.450150	2.820335
H	3.775487	0.857210	2.781919
C	2.295835	-0.644532	3.396243
H	3.009026	-0.759686	4.218901
H	1.314280	-0.427060	3.821570
C	2.205597	-1.908670	2.573302
C	3.352410	-2.536149	2.086948
H	4.319552	-2.314231	2.538178
C	3.327840	-3.286882	0.907409
C	2.122507	-3.445350	0.190224
C	0.954009	-3.079656	0.856359
H	-0.006855	-3.199446	0.362996
C	0.987721	-2.314144	2.023049
H	0.056129	-1.892926	2.396805
C	4.640787	-3.693800	0.378025
H	5.481369	-3.520448	1.082826
C	2.074360	-3.687786	-1.303299
H	1.025327	-3.841834	-1.575884
H	2.633241	-4.578781	-1.594364
C	2.639278	-2.466192	-2.145593
H	3.646812	-2.720051	-2.483585
H	2.007138	-2.358030	-3.033670
O	-0.084396	0.863245	2.126547
O	4.860373	-4.171370	-0.718865
H	-0.774820	-0.406402	0.489747
C	-1.872088	2.981189	-1.103222

C	-0.436448	1.687191	-0.066243
N	-1.756735	1.994643	-0.175329
N	0.155084	2.534968	-0.934804
N	-0.742878	3.349269	-1.619037
C	1.555674	2.836914	-0.981809
C	2.296656	2.464877	-2.104139
C	3.662147	2.742721	-2.090796
C	4.271936	3.368753	-1.002379
C	3.483214	3.751366	0.083651
C	2.113757	3.495756	0.117299
H	4.265500	2.452000	-2.947389
H	3.944951	4.255940	0.928887
C	1.633666	1.802509	-3.280062
H	2.380673	1.447452	-3.992274
H	1.034604	0.948107	-2.952559
H	0.964817	2.500232	-3.793293
C	5.761363	3.592966	-0.988047
H	6.033753	4.416140	-0.323987
H	6.275646	2.693705	-0.632093
H	6.140021	3.813192	-1.988934
C	1.261685	3.912146	1.288148
H	0.435473	4.549936	0.953741
H	0.825122	3.047441	1.801591
H	1.855408	4.476398	2.009489
C	-3.068515	1.654143	0.393008
C	-3.951283	2.242752	-0.765702
O	-3.127548	3.342923	-1.324428
C	-5.300413	2.827573	-0.410209
H	-5.747040	3.249263	-1.313979
H	-5.956501	2.035859	-0.042831

H	-5.232236	3.609822	0.343383
C	-4.090919	1.195504	-1.867062
H	-4.751362	0.395543	-1.522471
H	-4.522060	1.649973	-2.761513
H	-3.120409	0.756999	-2.119835
C	-3.169285	2.179159	1.834416
C	-2.967985	3.688605	1.975179
H	-2.020840	4.007476	1.527363
H	-3.769180	4.277880	1.522905
H	-2.927284	3.949867	3.035962
C	-4.425054	1.655034	2.531103
H	-4.502028	0.571871	2.390531
H	-4.352942	1.850186	3.604376
H	-5.340146	2.131938	2.171056
H	-3.194092	0.569582	0.394969
H	-2.320973	1.694026	2.326553
C	-2.433740	-1.306812	1.503907
O	-1.698460	-1.237823	0.384159
O	-3.549870	-1.881699	1.437284
Cs	-3.292726	-3.233289	-1.170150
O	-1.974705	-0.762199	2.569673
H	-0.799976	0.191853	2.403948

Vibrational frequencies

-1323.8034	15.8495	20.1788
28.5409	34.4589	38.0680
40.0971	51.1049	54.5904
56.8514	60.3567	65.9449
71.8417	82.9145	86.6397
89.9730	103.8478	111.9798

118.3551	124.4412	129.9773
136.4037	139.5794	144.7362
154.2529	155.6903	171.8385
185.3007	194.9870	200.8833
205.2287	211.0946	222.9143
227.9973	233.2394	239.1944
239.8378	245.8876	248.4444
268.2173	273.3204	281.3302
282.6881	288.6448	296.4642
298.5346	302.0248	315.2977
318.6482	330.5235	335.3773
346.5275	352.0476	367.9012
376.7390	380.9422	394.2967
412.5882	425.6752	427.0180
436.3510	439.6521	460.4051
471.4267	486.0208	495.2906
509.4390	518.0633	528.0409
539.4784	547.2137	559.8040
570.2764	588.6218	591.6839
602.2716	618.9917	634.8206
653.1467	662.7962	674.5839
680.0130	698.4708	707.1127
714.2645	728.7051	737.9102
744.4639	754.0458	758.9999
765.4505	773.6472	791.8725
802.2681	806.8858	823.3870
833.8612	845.2124	857.2567
857.9672	868.7133	879.8798
885.9185	898.9524	911.1506
912.0371	917.2687	925.2937

929.6105	936.4383	948.5247
953.0606	956.2241	961.5031
963.3976	976.3630	983.5270
984.2463	996.8554	1000.5181
1005.0482	1007.5027	1013.6351
1038.3849	1038.9661	1039.6937
1044.0115	1061.6624	1062.1658
1067.4533	1071.9150	1073.6308
1084.2557	1090.2574	1103.8545
1120.6621	1138.4502	1157.1885
1159.7007	1174.4865	1181.6561
1185.3503	1195.4050	1198.9838
1205.8575	1207.6537	1218.6219
1220.9763	1222.1731	1227.7731
1233.9656	1238.6871	1257.7244
1275.5566	1276.6264	1280.7802
1284.3616	1287.7378	1297.7385
1305.5365	1313.2822	1325.9469
1335.1025	1336.0005	1343.5323
1349.2978	1357.9526	1360.1885
1363.0435	1377.8392	1387.5044
1406.4976	1412.8547	1414.5987
1419.2522	1420.3448	1422.9503
1430.3956	1432.0672	1440.8428
1441.8588	1450.2876	1452.6595
1464.7636	1465.1130	1473.6602
1477.7082	1481.5421	1482.0467
1483.2622	1485.6795	1490.6652
1492.3444	1494.3604	1495.4161
1497.7511	1499.7788	1503.9995

1507.4312	1508.6207	1514.8546
1519.5592	1522.5478	1523.4579
1532.7125	1543.6115	1551.4905
1552.3551	1566.1545	1591.2113
1613.7924	1639.1593	1643.1336
1679.7987	1684.3111	1685.1862
1693.2995	1722.4711	1738.9773
1825.6977	2762.0523	2959.3319
3061.1253	3073.7776	3076.8121
3077.4561	3077.8172	3079.0662
3079.1350	3082.0692	3089.4570
3092.8053	3102.5769	3125.5261
3127.0349	3143.4359	3144.9218
3148.4630	3149.6904	3156.2893
3157.1184	3158.4805	3161.5469
3163.1749	3165.0388	3167.9362
3170.1571	3170.5113	3170.8917
3174.5726	3175.0146	3176.2341
3177.7123	3180.3922	3182.3703
3202.1648	3202.7259	3204.2455
3206.0226	3219.3148	3222.6407

R_p -TS2-2

Zero-point correction= 0.732524

Thermal correction to Energy= 0.777025

Thermal correction to Enthalpy= 0.777969

Thermal correction to Gibbs Free Energy= 0.653967

Sum of electronic and zero-point Energies= -2069.442211

Sum of electronic and thermal Energies= -2069.397711

Sum of electronic and thermal Enthalpies= -2069.396767

Sum of electronic and thermal Free Energies= -2069.520768

Cartesian coordinates

C	0.646656	-1.352139	-0.271705
C	0.985109	-2.578930	-0.880163
C	2.188587	-3.177920	-0.492736
H	2.432185	-4.161611	-0.889209
C	3.157657	-2.479284	0.224882
H	4.136396	-2.926667	0.386715
C	2.945421	-1.138392	0.547863
C	1.651140	-0.644498	0.391922
H	1.443141	0.388399	0.666806
C	-0.682505	-0.659211	-0.477807
C	0.274304	-3.108761	-2.107876
H	-0.810297	-3.056947	-2.002497
H	0.556393	-4.158026	-2.240682
C	0.660233	-2.313954	-3.437380
H	0.960698	-3.046011	-4.194008
H	-0.236703	-1.802601	-3.788199
C	1.766332	-1.305326	-3.223258
C	3.090006	-1.724463	-3.088257
H	3.372440	-2.723071	-3.421618
C	4.024835	-0.979333	-2.363116
C	3.644337	0.236560	-1.756794
C	2.427555	0.778914	-2.167030
H	2.087907	1.721597	-1.745456
C	1.497838	0.024359	-2.884561
H	0.496761	0.424907	-3.014762
C	5.314427	-1.642013	-2.105349
H	5.460335	-2.578936	-2.683410
C	4.309209	0.772750	-0.507008

H	3.857885	1.745465	-0.286137
H	5.382463	0.919972	-0.638768
C	4.100884	-0.182898	0.742547
H	5.019562	-0.755537	0.893310
H	3.951271	0.447043	1.627146
O	-1.214053	-0.766909	-1.764186
O	6.181064	-1.262526	-1.340721
H	-0.439232	0.603751	-0.362481
C	-1.097183	2.436581	-1.351815
O	-0.215741	1.920900	-0.499661
O	-1.209691	3.684654	-1.433194
Cs	0.992668	4.492742	0.345877
O	-1.804547	1.622121	-2.066856
H	-1.443438	0.226260	-1.992560
C	-3.580061	-0.446667	1.626613
C	-1.713845	-0.809153	0.541210
N	-3.052890	-0.573746	0.371106
N	-1.571085	-0.910088	1.881594
N	-2.745904	-0.663196	2.585398
C	-0.367601	-1.157483	2.611686
C	0.306860	-0.064677	3.158162
C	1.525003	-0.312870	3.788926
C	2.059517	-1.599951	3.860523
C	1.324806	-2.667900	3.340347
C	0.098551	-2.470895	2.711793
H	2.083323	0.521915	4.206643
H	1.726939	-3.675970	3.407395
C	-0.238270	1.328920	2.993623
H	-1.230629	1.419002	3.444867
H	-0.339816	1.582256	1.929206

H	0.425372	2.056531	3.466409
C	3.431474	-1.833064	4.434940
H	3.734376	-1.017238	5.094835
H	4.164608	-1.898403	3.622514
H	3.477193	-2.770323	4.994775
C	-0.688488	-3.611337	2.125283
H	-0.668868	-3.568295	1.030657
H	-1.734549	-3.570882	2.443115
H	-0.265096	-4.568791	2.433615
C	-4.077960	-0.166900	-0.628155
C	-5.359714	-0.275865	0.275888
O	-4.847734	-0.079526	1.647110
C	-6.349650	0.845626	0.032293
H	-7.139395	0.804584	0.786041
H	-6.807691	0.741836	-0.952610
H	-5.852174	1.815981	0.090424
C	-6.023124	-1.646672	0.310501
H	-6.505085	-1.888622	-0.636641
H	-6.785095	-1.636994	1.093112
H	-5.295403	-2.427873	0.545213
C	-4.082042	-0.916189	-1.973661
C	-5.296190	-0.531625	-2.825454
H	-6.239023	-0.936028	-2.447261
H	-5.156924	-0.927500	-3.834847
H	-5.395503	0.555273	-2.908270
C	-3.876428	-2.429544	-1.896433
H	-3.560358	-2.792075	-2.878915
H	-4.784201	-2.972009	-1.622744
H	-3.084754	-2.684514	-1.185774
H	-3.885900	0.888898	-0.854065

H -3.217163 -0.514846 -2.494418

Vibrational frequencies

-1211.8149	13.4686	20.7188
23.9413	29.5585	34.9172
37.8822	41.0779	49.0790
56.6724	67.1960	71.5627
74.2091	77.2700	85.7625
97.0175	101.6926	111.2809
119.7801	132.4287	135.7416
145.1589	150.8475	153.3688
160.2984	166.6026	172.4538
199.4245	201.1965	205.3484
208.6815	215.0272	221.9667
227.3054	234.7107	242.4521
249.9740	253.0490	264.2471
276.7291	280.8918	284.3727
286.6778	298.3560	303.1012
305.7340	315.3706	320.7470
324.5905	330.0196	337.3046
347.5386	361.5164	373.7699
382.1388	389.8213	401.7974
411.2387	415.9695	425.0497
435.1445	437.0801	461.9983
475.5224	484.0870	504.7654
508.2744	519.5187	529.6983
537.2690	551.3065	565.0936
573.7477	574.3004	588.2779
604.1702	621.0353	639.8369
657.4974	665.5598	676.8775

683.1435	688.7072	711.6021
719.0960	728.4548	738.2308
741.0935	752.2495	755.6828
764.8581	774.7908	783.0412
800.2853	807.8569	820.3880
834.3533	841.6396	852.6977
854.8888	866.3577	876.5181
886.0456	895.3753	907.4320
909.2467	918.2303	927.5943
932.3177	938.5822	946.8108
956.5650	956.9229	963.6371
972.6958	976.7428	984.1053
984.7090	996.4803	999.2882
1008.6100	1010.0870	1017.4723
1021.9841	1037.7633	1041.4809
1043.0135	1057.8012	1061.8417
1068.7413	1074.6964	1085.0240
1093.6660	1107.7031	1113.4108
1138.2444	1149.1109	1161.5184
1162.2881	1174.7102	1184.0353
1187.8789	1193.9436	1200.5917
1201.7870	1210.6481	1216.3477
1224.2634	1231.8245	1233.9086
1237.8255	1238.7527	1261.8629
1274.9925	1278.3480	1281.8964
1284.5663	1285.7429	1292.7521
1307.9541	1327.0551	1333.5904
1336.3263	1337.7973	1343.7886
1348.2232	1350.9013	1358.0579
1362.8281	1370.2201	1380.0846

1393.9043	1403.6291	1411.4521
1412.3352	1416.8457	1421.0463
1428.9770	1431.1910	1438.2940
1439.2471	1444.2102	1451.9772
1463.7130	1466.0647	1473.0156
1475.1431	1479.9404	1482.8259
1487.2008	1487.9896	1491.0608
1491.8932	1493.1832	1495.6885
1497.2163	1499.2427	1499.3253
1504.9906	1507.3414	1515.2936
1518.0515	1520.8117	1523.4064
1525.8670	1545.4428	1551.4279
1555.3023	1578.6380	1606.0200
1637.6346	1639.5346	1642.7685
1682.5108	1684.1044	1687.2803
1693.8687	1736.7831	1766.4299
1825.9198	2423.4684	2960.7221
3049.4179	3067.2122	3071.8364
3074.3604	3076.8231	3081.1464
3082.9341	3093.4995	3093.8045
3094.8608	3096.0078	3099.9132
3128.6527	3139.1358	3139.9068
3141.0615	3151.3155	3153.0693
3156.6922	3158.5956	3161.4479
3164.4791	3166.5935	3170.4412
3172.4379	3173.2652	3173.7032
3178.6775	3178.7046	3184.7577
3192.2805	3193.8102	3199.8774
3201.7463	3203.3280	3205.6559
3212.5208	3217.1638	3235.7442

R_p-TS2-3

Zero-point correction= 0.731943

Thermal correction to Energy= 0.776621

Thermal correction to Enthalpy= 0.777565

Thermal correction to Gibbs Free Energy= 0.652932

Sum of electronic and zero-point Energies= -2069.437381

Sum of electronic and thermal Energies= -2069.392704

Sum of electronic and thermal Enthalpies= -2069.391760

Sum of electronic and thermal Free Energies= -2069.516393

Cartesian coordinates

C	-1.323993	-0.444163	0.236707
C	-2.201594	-0.099295	1.285674
C	-3.057518	-1.097486	1.762835
H	-3.684893	-0.888078	2.627131
C	-3.270985	-2.270165	1.041006
H	-4.036814	-2.969774	1.367032
C	-2.668581	-2.436946	-0.209169
C	-1.603086	-1.586258	-0.520915
H	-1.035409	-1.726600	-1.439751
C	-0.141184	0.403877	-0.191630
C	-2.481857	1.346915	1.656035
H	-1.623185	1.875693	2.088869
H	-3.256495	1.348418	2.429681
C	-2.992121	2.177631	0.416399
H	-3.581201	3.020850	0.794395
H	-2.122467	2.584581	-0.111307
C	-3.754638	1.317875	-0.573621
C	-4.820451	0.511942	-0.178342
H	-5.333739	0.712830	0.762207

C	-5.114109	-0.680093	-0.849596
C	-4.340002	-1.079136	-1.959773
C	-3.520053	-0.105630	-2.526911
H	-2.947644	-0.346848	-3.419123
C	-3.225402	1.073279	-1.843414
H	-2.432921	1.711465	-2.215347
C	-6.093973	-1.560237	-0.189489
H	-6.648572	-1.069264	0.638443
C	-4.136377	-2.526093	-2.343476
H	-3.586457	-2.546854	-3.288089
H	-5.082652	-3.048350	-2.487802
C	-3.301381	-3.329669	-1.253792
H	-3.975589	-4.032694	-0.758421
H	-2.542042	-3.911989	-1.784105
O	-0.340474	1.201380	-1.322891
O	-6.317018	-2.724721	-0.459548
H	0.748925	-0.445712	-0.581892
C	1.327867	-1.257976	-2.581648
O	1.580652	-1.264256	-1.277250
O	1.938189	-2.072104	-3.323500
Cs	4.012942	-2.945007	-1.445843
O	0.468885	-0.409332	-3.037181
H	-0.016030	0.585428	-2.103500
C	1.343544	1.715233	2.822947
C	0.478122	1.144952	0.890824
N	0.762897	0.685712	2.146099
N	0.973287	2.401531	0.886247
N	1.531157	2.773655	2.110070
C	1.061716	3.364983	-0.176349
C	0.313978	4.538464	-0.066104

C	0.446017	5.486197	-1.083638
C	1.303034	5.287718	-2.163977
C	2.060520	4.114234	-2.209572
C	1.963326	3.138376	-1.222025
H	-0.135300	6.402953	-1.022813
H	2.749316	3.955756	-3.035995
C	-0.572633	4.809929	1.120408
H	0.018126	5.177379	1.964967
H	-1.086760	3.907185	1.457832
H	-1.323165	5.562708	0.871812
C	1.408614	6.307090	-3.268615
H	1.020989	7.277439	-2.951378
H	0.835006	5.987496	-4.144430
H	2.446043	6.436036	-3.587541
C	2.779896	1.879211	-1.285962
H	2.158971	1.036903	-1.605429
H	3.200242	1.628187	-0.305997
H	3.602921	1.995308	-1.994288
C	0.487215	-0.433471	3.063762
C	1.392690	-0.003814	4.277933
O	1.572818	1.454248	4.097159
C	0.684468	-0.190468	5.604772
H	1.302950	0.200594	6.415502
H	0.506533	-1.253090	5.785593
H	-0.274566	0.331782	5.603768
C	2.802442	-0.574071	4.288589
H	2.794409	-1.648244	4.479335
H	3.361754	-0.085706	5.089484
H	3.312689	-0.383282	3.341701
C	0.648644	-1.832653	2.449083

C	0.326014	-2.915896	3.481115
H	1.090187	-2.991712	4.261039
H	0.271440	-3.886306	2.981470
H	-0.640871	-2.732606	3.960575
C	1.960645	-2.110314	1.708701
H	1.781837	-2.925387	1.002331
H	2.765850	-2.412452	2.382161
H	2.286201	-1.249809	1.115773
H	-0.562116	-0.341165	3.374214
H	-0.145962	-1.880133	1.699369

Vibrational frequencies

-1203.1468	12.1042	20.7070
28.4326	31.8017	37.1186
37.4706	43.8911	48.2413
53.4840	60.0598	61.8939
70.7243	75.8982	86.1078
96.0267	99.2641	108.5373
120.7726	127.6696	130.9366
137.5978	149.5463	151.9250
156.8232	162.8815	178.1806
185.6282	198.7619	210.7989
214.9691	220.0283	222.3340
228.5213	234.5885	242.1876
250.5075	258.2957	264.5066
268.9330	275.7192	278.7676
285.5458	293.7814	294.4617
311.0752	312.9873	320.0160
331.8935	332.5966	333.0545
340.7147	345.9617	356.3531

364.8838	373.2450	402.7285
416.5989	418.9213	432.9676
443.0769	451.0098	458.9202
464.9119	476.2877	488.7411
509.7380	521.6511	527.1747
538.4728	555.2317	563.4789
571.7399	578.2419	590.1430
602.0161	617.4513	632.2634
657.0467	665.3942	669.4547
684.4046	695.5036	707.9220
719.9931	724.0349	733.6387
737.6192	752.8873	760.2162
761.1335	775.6209	783.7748
796.9391	806.0645	816.3689
823.7168	847.9580	857.4861
864.0498	871.5957	884.6122
885.2036	895.3987	915.3509
916.3352	919.8575	928.4224
932.3406	943.9845	945.3661
957.2038	961.7797	966.6177
971.9151	981.1077	983.3997
984.3155	988.1642	1004.2382
1008.5294	1016.9668	1021.1922
1023.7839	1037.8504	1042.5428
1044.4959	1053.7072	1059.9238
1062.9382	1067.9396	1080.1588
1092.4587	1099.8546	1107.5129
1115.2843	1135.7430	1155.3459
1161.6263	1173.5261	1179.8375
1183.1585	1194.2998	1203.4066

1203.6381	1216.1393	1222.0336
1224.7588	1228.1924	1228.7914
1234.0897	1236.9536	1261.3446
1270.3506	1276.8064	1283.1411
1286.0781	1286.9888	1299.4809
1309.3650	1327.8327	1331.5439
1338.2577	1346.8731	1347.8760
1354.9822	1355.7472	1365.6892
1370.2692	1375.5651	1387.1674
1403.9014	1408.5610	1414.7320
1416.2639	1418.6777	1421.8268
1425.6017	1431.4867	1440.3687
1442.2409	1448.9055	1455.7187
1464.8310	1466.1839	1470.2153
1478.3254	1480.5501	1480.9017
1484.4969	1485.5581	1488.1010
1492.5738	1492.8447	1494.7987
1496.7065	1499.9615	1502.2061
1505.6428	1507.4641	1510.7042
1515.4980	1522.1268	1523.1430
1527.6476	1540.9147	1545.3333
1552.7245	1557.7905	1588.8385
1633.6991	1641.1576	1657.8322
1676.2201	1684.6570	1685.7478
1694.6312	1709.8695	1761.9818
1827.0886	2397.8608	2954.6245
3066.4987	3072.1289	3073.7930
3074.3716	3076.1831	3077.3371
3082.4950	3086.2737	3090.5260
3091.9534	3095.6501	3103.6684

3111.2687	3130.8401	3132.5838
3146.1719	3147.1841	3150.2775
3151.4326	3156.3105	3157.1923
3159.4684	3169.3223	3171.0824
3172.6795	3175.7044	3178.6136
3179.5906	3180.2019	3181.3162
3182.7204	3187.9389	3192.3634
3198.0357	3203.6373	3204.6092
3206.0954	3210.9012	3256.2584

R_p-TS2-4

Zero-point correction= 0.731972

Thermal correction to Energy= 0.776629

Thermal correction to Enthalpy= 0.777573

Thermal correction to Gibbs Free Energy= 0.653134

Sum of electronic and zero-point Energies= -2069.437352

Sum of electronic and thermal Energies= -2069.392695

Sum of electronic and thermal Enthalpies= -2069.391750

Sum of electronic and thermal Free Energies= -2069.516190

Cartesian coordinates

C	-1.324440	-0.443150	0.236505
C	-2.202052	-0.097594	1.285241
C	-3.058620	-1.095209	1.762432
H	-3.686028	-0.885294	2.626580
C	-3.272606	-2.267905	1.040780
H	-4.038892	-2.967024	1.366786
C	-2.670047	-2.435266	-0.209237
C	-1.603994	-1.585246	-0.520928
H	-1.036116	-1.726174	-1.439548
C	-0.141035	0.404195	-0.191602

C	-2.481496	1.348820	1.655378
H	-1.622486	1.877164	2.088059
H	-3.256085	1.350889	2.429070
C	-2.991370	2.179643	0.415636
H	-3.580169	3.023105	0.793527
H	-2.121532	2.586209	-0.112056
C	-3.754166	1.320101	-0.574347
C	-4.820537	0.514868	-0.179142
H	-5.333931	0.716258	0.761242
C	-5.114710	-0.677149	-0.850208
C	-4.340603	-1.076854	-1.960146
C	-3.519964	-0.103934	-2.527293
H	-2.947512	-0.345652	-3.419341
C	-3.224768	1.074929	-1.843961
H	-2.431819	1.712574	-2.215827
C	-6.095195	-1.556606	-0.190101
H	-6.649888	-1.065054	0.637423
C	-4.137789	-2.523993	-2.343591
H	-3.587972	-2.545254	-3.288251
H	-5.084371	-3.045744	-2.487717
C	-3.303131	-3.327827	-1.253816
H	-3.977619	-4.030585	-0.758444
H	-2.543961	-3.910434	-1.784054
O	-0.339725	1.202191	-1.322638
O	-6.318626	-2.721112	-0.459747
H	0.748593	-0.445692	-0.582095
C	1.327508	-1.257491	-2.582173
O	1.580070	-1.264334	-1.277748
O	1.937721	-2.071569	-3.324181
Cs	4.011256	-2.946600	-1.445969

O	0.468869	-0.408400	-3.037517
H	-0.015631	0.586284	-2.103445
C	1.344307	1.713421	2.823603
C	0.478608	1.144530	0.891195
N	0.762883	0.684616	2.146331
N	0.974675	2.400754	0.887142
N	1.532768	2.771973	2.111141
C	1.064082	3.364434	-0.175172
C	0.317282	4.538518	-0.064743
C	0.450253	5.486387	-1.082004
C	1.307248	5.287444	-2.162308
C	2.063860	4.113417	-2.208018
C	1.965707	3.137384	-1.220715
H	-0.130273	6.403632	-1.021009
H	2.752756	3.954641	-3.034297
C	-0.569307	4.810288	1.121709
H	0.021880	5.174706	1.967273
H	-1.085985	3.908274	1.457222
H	-1.317743	5.565418	0.873951
C	1.413147	6.306626	-3.267059
H	2.449768	6.430313	-3.590575
H	1.031723	7.278851	-2.948001
H	0.833995	5.990063	-4.140356
C	2.781404	1.877666	-1.284718
H	3.604392	1.993154	-1.993185
H	2.159869	1.035752	-1.604025
H	3.201737	1.626425	-0.304799
C	0.486353	-0.434703	3.063615
C	1.392596	-0.006384	4.277632
O	1.573393	1.451706	4.097708

C	0.685022	-0.193539	5.604736
H	1.303934	0.197220	6.415284
H	0.507197	-1.256228	5.785261
H	-0.274013	0.328701	5.604433
C	2.802009	-0.577496	4.287052
H	2.793380	-1.651800	4.477004
H	3.362125	-0.090068	5.087957
H	3.311802	-0.386386	3.339976
C	0.646387	-1.833782	2.448329
C	0.323582	-2.917266	3.480050
H	1.088274	-2.994177	4.259362
H	0.267776	-3.887358	2.979923
H	-0.642783	-2.733384	3.960330
C	1.957732	-2.112051	1.706990
H	1.777680	-2.925964	0.999596
H	2.762910	-2.415869	2.379750
H	2.284010	-1.251220	1.114946
H	-0.562818	-0.341530	3.374357
H	-0.148718	-1.880347	1.699122

Vibrational frequencies

-1202.7553	12.3233	20.8674
31.2355	32.6305	37.4412
37.5519	44.2878	48.2497
53.5930	60.2889	62.0795
70.8639	76.1311	86.1552
96.1456	99.4906	108.9410
121.0156	127.8519	131.1517
137.7668	149.7396	152.0059
157.1570	162.8825	178.1716

185.6830	198.8876	210.8430
214.9572	219.9885	222.5533
228.6737	234.9238	242.2359
250.6660	258.3252	264.6755
268.9969	276.0067	278.8732
285.6704	293.8244	294.5602
311.2329	312.9525	320.0931
331.9119	332.6225	333.0808
340.7281	345.9637	356.3342
364.8809	373.2691	402.7495
416.6256	418.9264	432.9619
443.0803	450.9705	458.9115
464.9080	476.2876	488.7490
509.7785	521.6541	527.1302
538.4770	555.2308	563.5064
571.7435	578.2561	590.1452
602.1131	617.4849	632.2920
657.0617	665.4031	669.4701
684.4156	695.5290	707.9444
719.9803	724.0386	733.6577
737.6415	752.8650	760.2359
761.1398	775.6142	783.7935
796.9449	806.0912	816.3906
823.7585	847.9881	857.4924
864.0523	871.5988	884.6045
885.1994	895.3883	915.3356
916.3211	919.8604	928.4243
932.3412	943.9780	945.4278
957.2265	961.7784	966.6479
971.9337	981.1224	983.4238

984.3386	988.2144	1004.2773
1008.5822	1016.9618	1021.2055
1023.7698	1037.9608	1042.5457
1044.4859	1053.7066	1059.9374
1062.9428	1067.9670	1080.1446
1092.4601	1099.7900	1107.4903
1115.3673	1135.7270	1155.3543
1161.6229	1173.5553	1179.8332
1183.1749	1194.3135	1203.4322
1203.6574	1216.1422	1222.0204
1224.7569	1228.1911	1228.8098
1234.0918	1236.9593	1261.3418
1270.3601	1276.8163	1283.1614
1286.0848	1287.0161	1299.4745
1309.3680	1327.8323	1331.5914
1338.1519	1346.8480	1347.8280
1354.9697	1355.7122	1365.7015
1370.2631	1375.5499	1387.1459
1403.9560	1408.5542	1414.7601
1416.2880	1418.7029	1421.8505
1425.6129	1431.5044	1440.3664
1442.3067	1448.9368	1455.7124
1464.8303	1466.1776	1470.2106
1478.3553	1480.6031	1480.9440
1484.5387	1485.6060	1488.1232
1492.6577	1492.9804	1494.8608
1496.7855	1500.0004	1502.2235
1505.6526	1507.4650	1510.7716
1515.5660	1522.1609	1523.1973
1527.6884	1540.9032	1545.3351

1552.7468	1557.7921	1588.8598
1633.6965	1641.1713	1657.8473
1676.2181	1684.6341	1685.7632
1694.6197	1709.8669	1761.9848
1827.0900	2397.5557	2954.6342
3066.5233	3072.1233	3073.8255
3074.3655	3076.0897	3077.1900
3082.4906	3086.3336	3090.5189
3092.0132	3095.6651	3103.6842
3111.2996	3130.8999	3132.7636
3146.0499	3147.1710	3150.3080
3151.4446	3156.3404	3157.2470
3159.4715	3169.2932	3171.1261
3172.6538	3175.6927	3178.5834
3179.5997	3180.2618	3181.3765
3182.7832	3187.9439	3192.4136
3198.0719	3203.6675	3204.6485
3206.0626	3210.9275	3256.2232

S_p-TS2-1

Zero-point correction= 0.732379

Thermal correction to Energy= 0.776774

Thermal correction to Enthalpy= 0.777718

Thermal correction to Gibbs Free Energy= 0.654854

Sum of electronic and zero-point Energies= -2069.443847

Sum of electronic and thermal Energies= -2069.399453

Sum of electronic and thermal Enthalpies= -2069.398509

Sum of electronic and thermal Free Energies= -2069.521373

Cartesian coordinates

C	-1.440808	0.506176	0.574154
C	-2.405346	0.960246	1.497082
C	-3.736772	0.990304	1.069015
H	-4.487375	1.417075	1.731280
C	-4.152875	0.331776	-0.086979
H	-5.215093	0.243698	-0.303194
C	-3.229101	-0.396506	-0.839295
C	-1.876509	-0.177269	-0.567657
H	-1.122056	-0.690102	-1.164052
C	0.056465	0.590612	0.770415
C	-2.109029	1.165716	2.967694
H	-1.200380	1.750294	3.117722
H	-2.947846	1.713169	3.408957
C	-1.930946	-0.205948	3.755717
H	-2.523269	-0.150624	4.674505
H	-0.878124	-0.296291	4.027700
C	-2.331659	-1.403485	2.925529
C	-3.671983	-1.679413	2.653831
H	-4.450378	-1.233594	3.273206
C	-4.054772	-2.348420	1.486186
C	-3.078466	-2.788901	0.566591
C	-1.758450	-2.783040	1.013317
H	-0.964573	-3.129018	0.357028
C	-1.382293	-2.089924	2.164995
H	-0.321091	-1.946046	2.358956
C	-5.498194	-2.356254	1.194701
H	-6.130404	-2.029404	2.047135
C	-3.349811	-2.965324	-0.912249
H	-2.450187	-3.398591	-1.360629
H	-4.182870	-3.644287	-1.101347

C	-3.668697	-1.595527	-1.648985
H	-4.746945	-1.538786	-1.815370
H	-3.179889	-1.624476	-2.628397
O	0.546764	0.552332	2.079182
O	-6.018821	-2.664105	0.139096
H	0.530461	-0.487390	0.239124
C	1.892595	-2.121983	0.837738
O	1.055185	-1.672769	-0.099114
O	2.626666	-3.106660	0.564406
Cs	1.734928	-3.705073	-2.155350
O	1.903809	-1.535742	1.984391
H	1.136773	-0.307783	2.105530
C	1.025190	3.117208	-1.630387
C	0.648074	1.649742	-0.043047
N	0.046387	2.399482	-1.007971
N	1.955203	1.959253	-0.163677
N	2.210483	2.893742	-1.169017
C	3.070079	1.432402	0.569103
C	3.865105	0.459190	-0.039199
C	4.982897	0.010461	0.663849
C	5.299571	0.506326	1.927938
C	4.484337	1.493382	2.488080
C	3.363363	1.980827	1.821285
H	5.615950	-0.749792	0.213151
H	4.732662	1.899518	3.465613
C	3.525597	-0.073652	-1.404750
H	2.541617	-0.553456	-1.369982
H	3.497963	0.732224	-2.144414
H	4.267342	-0.811009	-1.719336
C	6.489184	-0.021522	2.686930

H	6.183103	-0.817242	3.373323
H	7.238300	-0.437926	2.009932
H	6.958417	0.764790	3.283209
C	2.494517	3.056731	2.411335
H	2.408043	3.907319	1.726996
H	1.492608	2.654724	2.592048
H	2.911104	3.415510	3.354147
C	-1.260542	3.016727	-1.298459
C	-0.879725	3.621397	-2.692491
O	0.556936	3.956915	-2.542043
C	-1.590677	4.882824	-3.131961
H	-1.187013	5.194299	-4.098170
H	-2.656276	4.678292	-3.256844
H	-1.465397	5.699734	-2.423199
C	-0.979695	2.540114	-3.764043
H	-2.030180	2.300681	-3.946529
H	-0.533978	2.900624	-4.693288
H	-0.466094	1.625630	-3.453934
C	-1.657851	3.936127	-0.126463
C	-0.641326	5.035242	0.194398
H	0.345791	4.618978	0.421994
H	-0.521786	5.759367	-0.614798
H	-0.971691	5.580517	1.082122
C	-3.085763	4.466809	-0.268538
H	-3.777222	3.656706	-0.521424
H	-3.408188	4.894820	0.684295
H	-3.172575	5.248969	-1.025563
H	-2.024254	2.246164	-1.431948
H	-1.668959	3.255573	0.733732

Vibrational frequencies

-1228.2514	15.1667	21.3977
27.0363	31.1042	36.1706
45.1434	46.2673	52.1287
55.3411	69.6401	77.3690
80.4637	86.2025	91.0617
103.6447	108.1393	117.5019
120.1311	132.7431	144.1367
148.4702	152.2009	158.8051
170.7691	178.0094	186.7942
192.1591	196.0395	201.6645
208.6259	216.2633	223.9088
225.8727	231.6794	242.1641
246.1890	252.8762	255.9639
264.1209	273.2527	282.7195
283.6080	289.4119	295.3613
297.9438	314.3318	320.6165
321.3453	331.6150	334.5101
348.6531	367.5750	375.6218
377.2550	379.0588	401.4404
414.7930	420.5691	426.7541
434.5260	446.8146	457.0320
465.7567	473.3288	490.3234
510.4999	520.3164	527.0299
539.3231	550.5283	563.6609
575.7347	580.5119	589.3550
605.9859	621.9994	637.4941
648.4602	662.5443	676.3165
681.4498	690.3786	711.7757
721.2287	729.5276	738.3934

745.7079	752.8621	753.6369
763.2249	782.8709	792.5732
803.8090	814.9004	825.1402
834.7070	841.9468	855.1680
858.7537	861.3172	873.7683
884.5853	898.3125	907.6600
909.6069	918.6855	923.8779
927.1261	935.5432	941.4897
952.8208	956.6964	966.8159
971.3018	979.3908	982.4342
985.2131	992.9688	1000.0870
1001.0666	1008.3352	1015.4321
1034.5978	1039.8437	1042.5002
1045.1863	1062.1419	1066.1874
1073.3889	1080.8475	1081.3480
1088.6249	1104.8154	1107.6260
1131.3489	1138.5096	1158.4901
1163.5490	1172.0138	1185.5472
1186.9355	1198.0967	1201.9866
1204.6447	1218.6590	1220.4676
1223.3219	1227.2141	1232.1400
1234.0602	1237.2307	1242.4071
1276.4666	1280.3124	1281.4508
1285.9152	1289.7088	1295.0471
1307.2454	1313.7264	1327.9999
1334.3297	1335.5014	1341.0129
1348.5458	1350.1170	1359.4921
1362.2211	1364.9409	1379.3424
1397.4242	1399.5022	1402.4140
1412.2993	1418.1101	1420.3790

1423.5899	1429.9668	1439.2635
1439.5909	1444.8206	1456.8863
1465.4265	1469.5187	1472.9156
1476.6911	1481.1580	1482.6187
1486.8532	1489.1511	1492.2183
1492.6283	1493.9834	1496.3149
1498.5348	1500.2194	1505.8154
1507.8213	1510.3401	1512.3434
1512.6447	1520.5463	1526.7738
1527.4946	1544.8249	1551.3196
1552.7034	1576.9504	1602.5914
1635.8738	1639.7974	1643.1865
1680.3640	1682.2059	1684.8372
1694.4334	1729.3870	1751.2493
1824.1829	2423.4694	2959.2935
3066.2018	3071.7264	3078.7806
3079.5743	3081.4076	3082.7692
3084.4386	3084.4496	3086.7049
3092.3215	3095.4288	3101.6931
3142.7004	3143.5544	3145.2510
3147.8512	3149.3688	3151.1570
3153.6902	3156.8658	3162.8778
3165.0982	3167.1555	3169.3235
3170.1597	3171.7661	3172.7744
3174.9578	3175.7839	3177.3246
3179.8306	3182.6863	3190.6265
3204.3701	3205.6917	3206.5963
3209.5310	3215.5809	3219.3466

S_p-TS2-2

Zero-point correction= 0.732491

Thermal correction to Energy= 0.777143
Thermal correction to Enthalpy= 0.778087
Thermal correction to Gibbs Free Energy= 0.654326
Sum of electronic and zero-point Energies= -2069.443308
Sum of electronic and thermal Energies= -2069.398656
Sum of electronic and thermal Enthalpies= -2069.397712
Sum of electronic and thermal Free Energies= -2069.521473

Cartesian coordinates

C	0.523094	1.064524	-0.820828
C	0.689121	1.882688	-1.960124
C	1.747370	2.795799	-1.938794
H	1.849181	3.496023	-2.765373
C	2.770173	2.715936	-0.993008
H	3.649542	3.347462	-1.098191
C	2.767094	1.682265	-0.056234
C	1.578673	0.961030	0.089392
H	1.522526	0.163624	0.829572
C	-0.685838	0.185149	-0.582423
C	-0.035959	1.643280	-3.267125
H	-1.100511	1.466349	-3.112885
H	0.078295	2.537176	-3.888013
C	0.535651	0.393722	-4.073133
H	0.705072	0.706337	-5.108352
H	-0.232404	-0.381161	-4.067746
C	1.803256	-0.159193	-3.465661
C	3.016252	0.517699	-3.583914
H	3.137363	1.277085	-4.356450
C	4.016581	0.389814	-2.614622
C	3.820924	-0.451363	-1.498357

C	2.757692	-1.351074	-1.576601
H	2.588082	-2.069826	-0.777512
C	1.757489	-1.204830	-2.540032
H	0.859836	-1.811511	-2.453486
C	5.148541	1.323965	-2.734738
H	5.173277	1.875859	-3.698084
C	4.500136	-0.216340	-0.166260
H	4.221522	-1.043012	0.494795
H	5.588074	-0.206153	-0.253149
C	4.060973	1.147397	0.516235
H	4.853919	1.881591	0.356743
H	3.983724	0.968171	1.593976
O	-1.247731	-0.413111	-1.712769
O	6.006829	1.530926	-1.897721
H	-0.252697	-0.796336	0.135433
C	0.125257	-2.929802	-0.188466
O	0.293388	-1.911534	0.652438
O	0.814296	-3.971201	-0.016891
Cs	2.096373	-3.333290	2.537928
O	-0.739404	-2.807666	-1.135123
H	-1.119850	-1.421967	-1.535190
C	-2.716412	1.765111	1.955954
C	-1.690713	0.799592	0.273573
N	-1.505801	1.630310	1.340323
N	-3.004367	0.497948	0.325307
N	-3.667049	1.096844	1.396991
C	-3.766911	-0.393612	-0.503177
C	-4.420263	0.133854	-1.616761
C	-5.197644	-0.735089	-2.377900
C	-5.319715	-2.086855	-2.044134

C	-4.651866	-2.565340	-0.916239
C	-3.865353	-1.730581	-0.121790
H	-5.716822	-0.350750	-3.252589
H	-4.743816	-3.614148	-0.645196
C	-4.251581	1.584173	-1.974833
H	-4.553980	2.233048	-1.146716
H	-3.198717	1.797259	-2.189869
H	-4.844322	1.841529	-2.853998
C	-6.138183	-3.015185	-2.904330
H	-6.507799	-3.865992	-2.327701
H	-6.993426	-2.496205	-3.343665
H	-5.534046	-3.410544	-3.727305
C	-3.138813	-2.231765	1.095295
H	-2.056416	-2.126292	0.963911
H	-3.435416	-1.664452	1.983953
H	-3.362881	-3.286390	1.266597
C	-0.532138	2.556760	1.949557
C	-1.246531	2.714399	3.338141
O	-2.681023	2.564357	3.011833
C	-1.092469	4.030443	4.068789
H	-1.677852	3.987627	4.990224
H	-0.044794	4.184230	4.335640
H	-1.438517	4.876056	3.476530
C	-0.869045	1.544711	4.242546
H	0.173131	1.644950	4.555484
H	-1.504543	1.545223	5.130300
H	-0.985701	0.588236	3.724087
C	-0.308990	3.776060	1.037794
C	-1.593358	4.518853	0.662148
H	-2.091710	4.972451	1.522696

H	-1.354437	5.319296	-0.042805
H	-2.310818	3.854766	0.168225
C	0.788153	4.706634	1.562178
H	1.127318	5.351081	0.746835
H	0.448851	5.353066	2.373859
H	1.654499	4.133884	1.909148
H	0.422450	2.047004	2.099748
H	0.086106	3.339447	0.115313

Vibrational frequencies

-1206.9719	17.7090	22.7700
27.6814	33.0220	35.6139
42.5013	50.0774	50.2555
59.3649	60.9048	66.3286
70.4295	82.6891	84.1276
87.9155	106.0110	112.9655
123.5484	130.0829	135.3020
139.3339	144.8378	150.5834
157.4022	168.3995	181.1557
185.4095	195.9958	200.7376
203.9540	208.1896	212.7555
225.2558	228.9155	241.8690
245.6442	253.8048	259.0170
274.1201	277.3739	281.2367
285.2487	290.1306	295.4840
301.4973	313.7822	318.6695
319.2337	326.7976	337.4392
346.8702	360.3019	371.4548
374.7243	379.7614	403.2717
413.8491	419.3462	424.5997

435.4736	449.8096	457.6211
460.1256	466.6637	488.4406
506.1361	521.2837	525.5622
539.0149	553.2128	570.3025
573.1699	578.3229	588.8552
607.5745	623.9684	642.2568
649.9096	663.5966	677.6812
680.3051	689.8958	711.0709
718.5522	728.8254	739.6203
746.9704	750.1323	754.2043
764.7287	783.2874	790.6776
804.4884	813.4282	826.0958
836.0464	844.6843	856.5790
864.8841	874.3514	883.6804
888.5390	896.6919	908.7709
914.2308	918.6218	926.9429
933.8837	938.2318	941.3676
953.0151	956.3150	964.7289
973.6754	978.9705	982.3518
983.5622	994.9365	1001.6148
1002.7922	1007.2077	1014.1148
1036.6810	1037.5140	1040.9624
1043.2737	1059.3968	1063.1335
1064.3249	1073.6689	1080.9874
1085.3116	1097.8417	1106.5413
1109.3249	1138.0231	1157.3229
1164.5901	1171.4776	1186.1405
1186.7278	1199.8690	1202.7937
1203.7656	1217.4650	1219.4169
1224.3380	1229.4395	1232.2121

1233.6353	1238.2482	1243.4461
1275.7691	1280.4344	1281.9638
1287.0313	1290.7489	1292.5555
1305.5091	1312.6168	1328.9053
1334.2934	1337.0262	1342.0830
1348.9608	1350.1802	1360.6276
1364.2961	1370.9800	1380.6825
1398.8828	1406.6211	1412.7493
1418.0604	1418.8206	1421.6426
1427.2024	1432.0662	1439.4037
1440.9128	1453.6180	1457.2948
1462.8431	1466.1711	1473.2617
1475.0723	1479.5018	1482.3642
1486.0494	1488.8628	1490.4389
1492.0720	1494.7426	1495.7489
1496.6413	1497.6223	1501.3218
1506.6811	1507.7516	1511.0333
1512.2413	1521.4986	1523.6555
1526.7407	1543.7829	1552.4677
1553.9937	1576.8139	1589.5324
1633.6649	1638.2793	1642.8013
1681.0662	1685.1197	1686.7756
1694.7723	1711.8339	1760.4093
1824.5511	2584.2850	2960.7811
3068.4977	3070.5733	3076.8379
3076.8715	3079.4608	3080.1445
3083.0517	3086.1641	3092.5612
3097.5681	3102.6149	3130.1983
3135.3793	3141.7154	3142.7444
3146.3133	3146.3635	3149.0428

3151.4124	3159.5105	3160.9957
3164.6824	3166.9060	3169.6827
3170.4490	3173.7635	3174.7360
3175.9741	3176.4812	3179.8983
3183.2762	3188.6731	3190.8383
3203.4062	3204.2337	3206.6991
3207.7115	3213.7577	3224.4460

S_p-TS2-3

Zero-point correction= 0.732813

Thermal correction to Energy= 0.777202

Thermal correction to Enthalpy= 0.778146

Thermal correction to Gibbs Free Energy= 0.656274

Sum of electronic and zero-point Energies= -2069.452360

Sum of electronic and thermal Energies= -2069.407971

Sum of electronic and thermal Enthalpies= -2069.407027

Sum of electronic and thermal Free Energies= -2069.528900

Cartesian coordinates

C	0.565813	1.206582	-0.431862
C	0.942073	2.439553	-1.004549
C	2.114121	3.036671	-0.534751
H	2.379922	4.027408	-0.898504
C	3.034599	2.326135	0.233963
H	4.001612	2.769583	0.463043
C	2.804708	0.981634	0.525498
C	1.517037	0.490867	0.295846
H	1.272899	-0.535474	0.566803
C	-0.787804	0.566161	-0.673268
C	0.290284	2.983926	-2.255912
H	-0.795886	2.879459	-2.218719

H	0.529028	4.049017	-2.337889
C	0.795904	2.251508	-3.581053
H	1.106432	3.020509	-4.295519
H	-0.053365	1.712529	-4.004082
C	1.923851	1.277427	-3.326896
C	3.220110	1.720042	-3.069456
H	3.506110	2.737341	-3.336723
C	4.109191	0.961092	-2.300306
C	3.708206	-0.285568	-1.774972
C	2.549235	-0.842133	-2.316383
H	2.226643	-1.834816	-2.005147
C	1.668244	-0.074368	-3.079574
H	0.706382	-0.507418	-3.333156
C	5.359784	1.635127	-1.914017
H	5.536783	2.591455	-2.450332
C	4.283540	-0.860855	-0.499090
H	3.839131	-1.850848	-0.356076
H	5.367085	-0.980818	-0.550379
C	3.956013	0.033006	0.771341
H	4.849580	0.609637	1.022968
H	3.748253	-0.641576	1.609807
O	-1.242671	0.554967	-2.007862
O	6.165730	1.247200	-1.089256
H	-0.672078	-0.704352	-0.375808
C	-0.385065	-2.541575	-1.524608
O	-0.468703	-2.004742	-0.307590
O	0.167966	-3.665001	-1.651325
Cs	1.118591	-4.116945	1.079617
O	-0.882040	-1.888070	-2.517889
H	-1.131068	-0.427836	-2.291096

C	-3.868797	1.285835	1.013531
C	-1.853559	1.022514	0.196311
N	-3.174283	0.963514	-0.113281
N	-1.841983	1.441552	1.479879
N	-3.121265	1.605682	2.018551
C	-0.695959	1.612306	2.319521
C	-0.086284	2.867721	2.378752
C	1.078708	2.977942	3.133186
C	1.615308	1.883709	3.815143
C	0.941494	0.662686	3.769161
C	-0.221684	0.501107	3.018233
H	1.588772	3.937227	3.176931
H	1.339636	-0.189076	4.316045
C	-0.673707	4.038650	1.640378
H	-0.678497	3.850187	0.561949
H	-1.707183	4.216760	1.952487
H	-0.090534	4.942371	1.825459
C	2.925389	2.014637	4.545667
H	3.756828	1.926142	3.837102
H	3.014170	2.987599	5.034803
H	3.043639	1.233573	5.299788
C	-0.921362	-0.827174	2.910603
H	-1.989891	-0.725538	3.125565
H	-0.826321	-1.241102	1.897429
H	-0.496384	-1.542144	3.618869
C	-4.062229	0.312567	-1.085793
C	-5.407944	0.944025	-0.580321
O	-5.179066	1.164421	0.869745
C	-6.663125	0.108156	-0.703701
H	-7.501704	0.666719	-0.281177

H	-6.875368	-0.084562	-1.757525
H	-6.576153	-0.842062	-0.178458
C	-5.598622	2.319173	-1.210005
H	-5.825144	2.208464	-2.273272
H	-6.428781	2.836624	-0.724893
H	-4.694724	2.926784	-1.110884
C	-3.828205	-1.208073	-1.046252
C	-3.944330	-1.825774	0.348518
H	-3.234408	-1.371212	1.047792
H	-4.948189	-1.740997	0.775080
H	-3.692901	-2.888408	0.289743
C	-4.651634	-1.962183	-2.093897
H	-4.670718	-1.425140	-3.047556
H	-4.189438	-2.936217	-2.274469
H	-5.682596	-2.138505	-1.778947
H	-3.839958	0.683521	-2.087509
H	-2.780955	-1.316597	-1.349026

Vibrational frequencies

-1275.0008	22.7489	27.9156
30.2671	38.0312	40.7272
45.0337	54.2633	62.5684
68.3491	68.8194	71.7288
76.6951	79.2490	82.6162
89.3142	111.9867	115.2838
123.7558	131.7156	134.3796
135.5328	146.2668	155.6088
158.6284	163.1502	170.4988
188.6511	202.9290	205.1166
210.6241	221.3624	225.0652

227.6340	241.6628	247.0304
250.6851	256.1125	267.6494
270.3139	276.3642	280.8285
285.5686	286.2714	296.4791
301.0618	312.4353	319.7710
321.2127	327.6927	348.6593
351.6960	358.9616	369.3279
375.2692	376.7889	399.8348
414.2826	416.4288	423.3468
435.7275	438.8232	452.2647
465.0185	482.8480	496.9720
509.6204	515.0337	528.4556
538.0345	549.0582	566.4760
571.6484	580.9511	589.0490
604.5620	627.2597	643.0215
651.4686	662.3562	677.9213
680.7145	692.0249	707.8231
716.7208	730.0784	739.2274
744.6999	751.7524	760.6144
763.8555	775.5436	790.3385
804.1158	805.3154	826.2727
840.5951	848.5650	853.3718
861.1185	866.6526	880.7389
896.8207	899.5675	906.0290
912.2590	918.7659	927.1991
931.5727	942.2037	945.4175
953.9452	956.8914	963.2189
971.4334	977.1713	982.2402
985.2943	994.2366	1001.1691
1003.3467	1006.8559	1025.7194

1035.7186	1038.1093	1040.0642
1043.3136	1058.8616	1060.1125
1068.4600	1072.7406	1080.3312
1087.1848	1102.4354	1110.2080
1129.0001	1135.1151	1152.9346
1163.2093	1168.4729	1185.4215
1188.1669	1195.0489	1198.8165
1202.1902	1207.0746	1217.9678
1218.6590	1227.3295	1233.1292
1237.6095	1238.2957	1245.9728
1273.4064	1279.0775	1280.5646
1282.6489	1284.7948	1288.8167
1305.0112	1312.6366	1325.4769
1335.5611	1336.3864	1345.5144
1348.5111	1353.8530	1358.5111
1363.3317	1382.9321	1385.4369
1407.5388	1412.6648	1414.3427
1417.6266	1420.9952	1424.2374
1429.0546	1432.6000	1438.4714
1439.0226	1455.0744	1462.3469
1464.4409	1467.9515	1472.4137
1474.4853	1477.5824	1483.2662
1485.3042	1488.7835	1491.5037
1492.9737	1494.1414	1495.2994
1497.8245	1497.9117	1503.1979
1506.7515	1509.1958	1511.2361
1519.5861	1520.9380	1524.8604
1530.9586	1546.3667	1552.1861
1557.1549	1575.6005	1591.3237
1638.6072	1642.8919	1644.5712

1683.0760	1683.4491	1686.2762
1694.4036	1706.5489	1750.1012
1823.9604	2627.0876	2959.2296
3054.6632	3069.9468	3072.9634
3074.8251	3075.1532	3078.6562
3083.6371	3085.7683	3089.8089
3094.6252	3100.3528	3117.3978
3127.5614	3141.0114	3141.4071
3143.2777	3147.7488	3150.4050
3151.3776	3158.8228	3159.4494
3160.2853	3160.8305	3166.1945
3169.0552	3169.4842	3170.9296
3175.6226	3176.3371	3177.1383
3182.4599	3185.1762	3188.8673
3195.5413	3200.1323	3202.5164
3206.0928	3209.6351	3250.5342

S_p-TS2-4

Zero-point correction= 0.732500

Thermal correction to Energy= 0.776644

Thermal correction to Enthalpy= 0.777588

Thermal correction to Gibbs Free Energy= 0.656861

Sum of electronic and zero-point Energies= -2069.439373

Sum of electronic and thermal Energies= -2069.395228

Sum of electronic and thermal Enthalpies= -2069.394284

Sum of electronic and thermal Free Energies= -2069.515011

Cartesian coordinates

C	1.520468	0.524209	0.532987
C	2.253852	1.135880	1.578656
C	3.443694	1.783298	1.230710

H	4.067373	2.180257	2.029766
C	3.761591	2.101966	-0.089215
H	4.626077	2.724971	-0.303949
C	2.836958	1.817739	-1.097572
C	1.804601	0.932643	-0.780889
H	1.118574	0.624596	-1.571822
C	0.428951	-0.480211	0.754606
C	1.662308	1.402351	2.951674
H	1.432491	0.490632	3.501782
H	2.400875	1.975158	3.523737
C	0.336286	2.244809	2.851383
H	0.204381	2.785266	3.795325
H	-0.502784	1.546935	2.745747
C	0.342704	3.167977	1.647813
C	1.390268	4.058413	1.414423
H	2.053286	4.340655	2.232384
C	1.749645	4.431426	0.115195
C	1.034032	3.932211	-0.993823
C	-0.190830	3.328585	-0.716008
H	-0.806390	2.980779	-1.543689
C	-0.529656	2.941068	0.581315
H	-1.380111	2.281209	0.729298
C	3.020094	5.168659	-0.011610
H	3.436882	5.510736	0.959362
C	1.656218	3.748336	-2.359127
H	0.864616	3.435679	-3.046458
H	2.088814	4.674111	-2.739603
C	2.798952	2.641052	-2.365979
H	3.760857	3.143802	-2.492363
H	2.638192	2.007596	-3.244369

O	0.392710	-1.004571	2.074849
O	3.616557	5.407307	-1.043929
H	-0.897495	-0.034611	0.595188
C	-2.708182	-0.132120	1.780681
O	-2.089227	0.266581	0.661984
O	-3.945642	0.074209	1.876333
Cs	-4.449975	1.453187	-0.650987
O	-2.005715	-0.684270	2.700133
H	-0.585647	-0.872131	2.389196
C	1.767421	-3.248471	-1.190395
C	0.726764	-1.643264	-0.126240
N	1.945433	-2.085168	-0.516979
N	-0.114070	-2.554090	-0.630586
N	0.519084	-3.586863	-1.307861
C	-1.545589	-2.524002	-0.554718
C	-2.162827	-3.082925	0.567259
C	-3.546216	-2.967928	0.651086
C	-4.291935	-2.341422	-0.348717
C	-3.634713	-1.859386	-1.480804
C	-2.246323	-1.917335	-1.594088
H	-4.053296	-3.352540	1.532050
H	-4.210124	-1.410705	-2.288962
C	-1.352488	-3.761447	1.635672
H	-0.778295	-4.594176	1.215219
H	-0.650772	-3.049127	2.078362
H	-2.003996	-4.148982	2.420269
C	-5.770804	-2.139047	-0.159020
H	-6.263184	-3.056081	0.174158
H	-5.918538	-1.382890	0.620457
H	-6.256442	-1.802219	-1.078538

C	-1.520137	-1.276714	-2.744653
H	-1.053677	-0.341510	-2.410282
H	-0.728409	-1.920815	-3.136318
H	-2.209989	-1.039429	-3.556874
C	3.354613	-1.914704	-0.143999
C	3.965089	-2.820835	-1.272752
O	2.903506	-3.827182	-1.543318
C	5.230069	-3.587698	-0.957412
H	5.493779	-4.201179	-1.822093
H	6.046871	-2.886466	-0.773829
H	5.115305	-4.236509	-0.090091
C	4.121685	-1.993100	-2.543909
H	4.932930	-1.272561	-2.412805
H	4.359914	-2.646197	-3.385765
H	3.205633	-1.437926	-2.768458
C	3.510651	-2.250791	1.350699
C	2.997695	-3.641132	1.732938
H	1.930803	-3.747063	1.508114
H	3.535140	-4.449869	1.230503
H	3.111951	-3.784442	2.810371
C	4.925560	-1.969851	1.858261
H	4.924985	-1.972193	2.951210
H	5.648765	-2.719125	1.529058
H	5.269065	-0.984621	1.526124
H	3.663137	-0.878748	-0.314827
H	2.843606	-1.528716	1.840729

Vibrational frequencies

-1309.2906	21.0704	29.0791
32.9653	39.3194	41.3786

44.4289	49.2647	57.7305
68.4645	76.6302	84.5774
87.5872	94.4103	101.5276
103.3544	109.3554	120.4528
128.9159	136.7825	144.2987
150.2990	155.9828	161.9117
164.5582	177.2803	180.5288
195.8002	198.1153	204.2313
207.1899	208.4895	224.4040
229.9025	234.2528	242.7316
248.3302	252.3165	258.0577
269.0278	273.6503	280.1593
286.6239	291.1116	293.5082
304.4782	310.6822	319.2460
322.8886	330.5457	337.7596
349.1945	355.6855	368.7471
376.8305	377.3476	396.2459
411.0322	421.5807	432.1737
438.5831	450.8790	459.0021
476.7461	485.5532	494.5292
516.4594	520.6869	523.6101
542.3659	546.0791	551.2914
569.9527	589.9485	595.5893
603.9166	618.1773	634.4587
647.5881	664.9964	666.6627
677.2075	702.2169	716.7046
728.7457	732.9302	736.5093
746.8124	751.5005	761.5082
764.7266	781.6074	787.6472
804.8017	812.1180	817.3712

830.5900	850.7011	851.2763
857.8349	862.0221	880.8939
885.4685	902.4406	908.0216
917.4364	919.0567	919.9307
932.1802	945.1226	946.0363
952.4686	956.9458	965.3426
965.5184	977.9722	981.7481
983.5092	993.6137	998.3599
1001.0593	1007.1860	1017.1814
1035.9339	1036.4858	1043.0732
1045.5052	1057.4009	1062.9728
1068.8199	1073.6252	1077.9795
1093.4059	1109.6811	1111.7014
1116.4284	1129.5405	1139.2660
1159.6888	1169.3931	1180.1514
1182.6376	1192.5318	1195.6525
1202.2811	1205.0505	1213.7034
1220.6753	1221.3617	1228.5081
1236.0907	1238.3341	1258.7738
1272.7937	1276.1179	1278.9216
1283.5869	1288.5485	1300.5255
1311.8049	1315.0057	1330.3243
1337.3519	1345.0397	1349.6050
1351.8602	1356.8523	1363.9348
1366.7515	1371.2561	1384.5233
1401.9479	1407.9953	1411.6771
1413.1047	1419.9841	1421.1182
1427.6608	1431.1327	1439.8901
1443.3487	1448.1899	1453.4754
1463.4650	1472.7188	1474.9525

1479.8590	1481.0990	1483.2732
1486.2523	1486.4724	1490.8622
1491.7287	1495.3672	1496.4862
1499.7394	1500.5364	1502.1245
1506.8456	1510.1554	1511.3511
1520.7160	1522.0744	1529.1053
1534.5070	1540.6725	1543.9937
1555.5278	1576.4144	1603.4850
1621.9719	1633.9237	1644.0481
1672.7006	1686.2426	1687.1633
1696.4033	1727.7123	1729.7669
1828.0208	2519.7389	2960.2431
3060.5840	3068.6410	3070.1516
3072.7241	3075.9853	3077.9563
3079.9952	3080.5293	3081.8078
3084.4902	3097.7745	3100.3585
3124.8455	3130.2082	3135.0452
3143.7424	3145.9346	3148.6210
3150.2421	3153.5252	3158.4371
3162.2615	3162.8378	3165.2037
3170.3615	3172.0337	3172.1188
3176.4989	3177.1101	3178.9059
3182.0301	3182.6563	3184.7863
3185.4541	3188.2688	3209.1353
3210.8154	3211.3284	3214.2408

R_p -TS6

Zero-point correction= 0.739029

Thermal correction to Energy= 0.780160

Thermal correction to Enthalpy= 0.781104

Thermal correction to Gibbs Free Energy= 0.664988
Sum of electronic and zero-point Energies= -1899.453545
Sum of electronic and thermal Energies= -1899.412413
Sum of electronic and thermal Enthalpies= -1899.411469
Sum of electronic and thermal Free Energies= -1899.527585

Cartesian coordinates

C	-4.217723	-1.657910	0.093604
C	-3.242176	-2.435957	-0.562281
C	-2.252677	-2.999466	0.248726
H	-1.526328	-3.671843	-0.201078
C	-2.043212	-2.556437	1.552731
H	-1.160269	-2.890216	2.093335
C	-2.837101	-1.542450	2.093375
C	-4.009284	-1.228618	1.407881
H	-4.700919	-0.506560	1.831566
C	-5.377142	-1.098155	-0.654458
C	-3.049976	-2.462493	-2.065159
H	-3.965573	-2.732395	-2.592444
H	-2.296839	-3.224810	-2.283997
C	-2.545866	-1.073909	-2.654320
H	-1.755069	-1.290615	-3.379254
H	-3.375216	-0.606584	-3.188192
C	-2.053812	-0.137873	-1.574265
C	-0.905301	-0.440706	-0.846323
H	-0.194654	-1.169023	-1.242559
C	-0.712666	0.007189	0.460194
C	-1.706268	0.786315	1.078304
C	-2.690788	1.329309	0.239245
H	-3.432649	1.998888	0.670005

C	-2.866665	0.882738	-1.068457
H	-3.734936	1.209171	-1.636047
C	0.490628	-0.541611	1.211705
H	0.786912	-1.542012	0.833124
C	-1.941783	0.810962	2.579343
H	-2.783091	1.486679	2.765987
H	-1.078389	1.180665	3.133703
C	-2.302002	-0.615782	3.162580
H	-1.391157	-1.048762	3.581353
H	-3.020386	-0.476522	3.976861
O	-5.489192	-1.057966	-1.862574
O	0.715521	-0.231214	2.398813
C	2.922876	2.101665	-0.908459
C	1.877538	0.381164	0.013011
N	1.749896	1.673892	-0.369142
N	3.135850	0.111905	-0.357942
N	3.828050	1.175101	-0.949897
C	3.783781	-1.159208	-0.235838
C	3.932576	-1.942472	-1.383689
C	4.558695	-3.179859	-1.244405
C	5.022358	-3.628801	-0.005876
C	4.847294	-2.813726	1.113713
C	4.231707	-1.565007	1.024051
H	4.681328	-3.809989	-2.121900
H	5.201531	-3.155407	2.083191
C	3.421242	-1.458117	-2.714083
H	2.372724	-1.150802	-2.640370
H	3.987367	-0.586817	-3.055406
H	3.501207	-2.243260	-3.467392
C	5.722934	-4.957723	0.114908

H	5.367776	-5.661751	-0.640905
H	6.802127	-4.838380	-0.025555
H	5.565616	-5.399015	1.101572
C	4.048518	-0.683018	2.230573
H	4.458652	0.314678	2.042321
H	2.986606	-0.563356	2.475919
H	4.563758	-1.108494	3.093685
C	0.832347	2.796033	-0.170949
C	1.470228	3.775807	-1.219359
O	2.902413	3.382660	-1.256816
C	1.419994	5.259027	-0.924710
H	1.951412	5.793559	-1.715730
H	0.381143	5.596299	-0.923810
H	1.875243	5.509237	0.032306
C	0.897182	3.472761	-2.600211
H	-0.147095	3.792201	-2.643104
H	1.463476	4.010481	-3.363406
H	0.936978	2.400775	-2.815833
C	0.779730	3.129004	1.331139
C	2.141966	3.454223	1.949246
H	2.849941	2.631441	1.805195
H	2.592685	4.363628	1.544295
H	2.024864	3.593914	3.027077
C	-0.292518	4.167617	1.659573
H	-0.461731	4.188686	2.739717
H	-0.009438	5.176841	1.351103
H	-1.241592	3.910265	1.176735
H	-0.171815	2.523209	-0.510746
H	0.460330	2.180212	1.783389
O	-6.326439	-0.614373	0.163213

C	-7.451244	-0.025923	-0.491964
H	-8.113639	0.312568	0.301847
H	-7.133413	0.815136	-1.111371
H	-7.952797	-0.762608	-1.121958

Vibrational frequencies

-147.1505	13.7700	20.1992
24.0093	31.4585	34.4099
43.1625	46.7905	50.1676
65.2458	68.9912	80.6605
83.0409	89.2660	102.8727
110.4653	116.9839	124.2106
134.8958	144.6616	157.1484
166.2499	168.2592	183.5435
186.9792	189.9749	195.1710
204.5295	214.1984	217.4497
231.6427	237.2079	242.0275
257.2866	265.2469	276.6029
284.3637	287.3229	294.5204
298.9376	301.4737	311.2962
315.7918	325.3121	329.2571
331.9801	349.0330	363.5273
373.7094	377.7215	393.0859
396.3854	415.5430	417.7659
425.3049	439.5161	441.6248
467.5863	472.6793	489.1821
509.9832	517.7913	528.0954
528.2420	539.5077	548.8408
557.0120	561.5950	583.1577
588.4762	604.5546	615.7775

636.0823	653.2971	659.5469
675.5060	687.6233	701.7343
723.0522	728.6140	738.8784
748.4939	758.1716	773.4056
781.9459	791.8833	796.2532
804.3773	815.3777	823.7648
831.0947	849.3242	858.7435
879.6114	886.9076	892.5075
901.2160	917.0445	918.2198
918.5557	935.6198	941.1048
942.9414	952.5727	953.0838
962.2845	963.7278	978.1103
980.0583	981.7270	988.8080
989.4947	996.0022	1002.1820
1005.9182	1013.7710	1036.5776
1037.7186	1038.7560	1040.7855
1061.6322	1063.1302	1070.5597
1076.1613	1082.1865	1109.0477
1116.7977	1123.7760	1133.7100
1167.5632	1167.9127	1171.0458
1175.2885	1185.9248	1190.3101
1200.4770	1201.7341	1215.9978
1218.8854	1219.5767	1221.7420
1224.8809	1232.4740	1237.8892
1246.9733	1257.4978	1265.7240
1277.6679	1280.9249	1285.7726
1286.6840	1303.4117	1305.0044
1325.3469	1326.1582	1334.2493
1334.9646	1344.0325	1346.3426
1353.2923	1357.9976	1361.0097

1366.2276	1387.8251	1396.0469
1407.6091	1416.6131	1417.4399
1421.0562	1421.8920	1424.7866
1432.4574	1433.3325	1438.2970
1452.1223	1457.6061	1463.9891
1467.7321	1477.9223	1481.8881
1483.6366	1485.3484	1487.8515
1488.4351	1490.0432	1493.0078
1495.6441	1495.7548	1495.9449
1496.7120	1499.0302	1501.4605
1502.6901	1507.1012	1507.5001
1509.3494	1511.6249	1520.5478
1521.7353	1523.0367	1542.4836
1549.3154	1563.6025	1625.8506
1642.0035	1645.8347	1681.1559
1683.0614	1687.5870	1692.4428
1727.3765	1828.4380	2926.4180
3057.0204	3072.4394	3074.0009
3075.4648	3075.7664	3079.0755
3080.3612	3083.3033	3088.1706
3091.5724	3093.0765	3099.2001
3099.6078	3120.7340	3128.4792
3140.9792	3145.7327	3146.1220
3147.7296	3152.9976	3155.4021
3156.6246	3162.6834	3163.5401
3166.6911	3167.3163	3169.3470
3169.8715	3170.6739	3174.1261
3174.9917	3176.7403	3179.5352
3188.6693	3195.6013	3202.7021
3205.4738	3209.0221	3210.5735

3211.1387

3212.4096

3225.2745

S_p-TS6

Zero-point correction= 0.738991

Thermal correction to Energy= 0.780122

Thermal correction to Enthalpy= 0.781067

Thermal correction to Gibbs Free Energy= 0.664306

Sum of electronic and zero-point Energies= -1899.453820

Sum of electronic and thermal Energies= -1899.412688

Sum of electronic and thermal Enthalpies= -1899.411744

Sum of electronic and thermal Free Energies= -1899.528504

Cartesian coordinates

C	-4.216700	-0.483892	0.513442
C	-3.645043	0.805662	0.530342
C	-2.848585	1.116151	1.636009
H	-2.435791	2.119171	1.720078
C	-2.387140	0.125765	2.502595
H	-1.639925	0.379785	3.251092
C	-2.712939	-1.214225	2.283401
C	-3.746466	-1.470440	1.383748
H	-4.088501	-2.490668	1.241338
C	-5.167955	-0.873813	-0.565070
C	-3.586501	1.711766	-0.686446
H	-4.576987	2.001629	-1.038358
H	-3.054399	2.620347	-0.386479
C	-2.809334	1.058621	-1.905514
H	-2.230000	1.854187	-2.387618
H	-3.538142	0.689072	-2.630089
C	-1.914901	-0.078329	-1.462862

C	-0.893640	0.173498	-0.553537
H	-0.573206	1.203558	-0.385646
C	-0.403425	-0.803666	0.310850
C	-0.968086	-2.087832	0.291876
C	-1.780319	-2.402431	-0.809157
H	-2.182552	-3.410075	-0.891167
C	-2.248128	-1.420770	-1.679413
H	-2.994429	-1.679111	-2.428277
C	0.527779	-0.320580	1.405121
H	0.314156	0.739749	1.662682
C	-1.013343	-2.986644	1.516264
H	-1.525028	-3.910156	1.227105
H	-0.018528	-3.250799	1.877796
C	-1.798735	-2.334712	2.730075
H	-1.065391	-1.932523	3.432126
H	-2.353809	-3.130196	3.237614
O	-5.598783	-0.134127	-1.425743
O	1.037061	-1.076128	2.249692
C	4.243576	0.461156	-0.313384
C	2.095408	0.353734	0.211315
N	3.228147	-0.366295	0.047490
N	2.520727	1.589516	-0.082288
N	3.873945	1.699552	-0.424415
C	1.671728	2.741741	-0.069767
C	1.017004	3.103295	-1.251244
C	0.113375	4.162508	-1.189366
C	-0.132300	4.845935	0.005354
C	0.553912	4.457704	1.157340
C	1.468293	3.403361	1.143077
H	-0.416537	4.457379	-2.092214

H	0.371851	4.984482	2.090673
C	1.246925	2.326554	-2.519634
H	0.819944	1.320097	-2.431419
H	2.315072	2.212577	-2.723602
H	0.776947	2.825053	-3.369079
C	-1.104098	5.997316	0.037109
H	-1.977974	5.791231	-0.585957
H	-0.634869	6.908664	-0.346925
H	-1.443979	6.200217	1.054653
C	2.206642	2.972509	2.383169
H	3.287279	2.986371	2.213609
H	1.940214	1.949235	2.669775
H	1.976289	3.634864	3.218860
C	3.703849	-1.730980	0.234761
C	5.084939	-1.623662	-0.509409
O	5.401831	-0.167765	-0.465054
C	6.195155	-2.332823	0.237140
H	7.152326	-2.163484	-0.260764
H	5.997827	-3.407860	0.253703
H	6.258485	-1.971510	1.265645
C	5.059215	-1.979343	-1.986785
H	4.882948	-3.047553	-2.128080
H	6.028931	-1.727982	-2.422130
H	4.283547	-1.419232	-2.514450
C	2.649118	-2.783234	-0.143453
C	3.181019	-4.197454	0.092432
H	3.614034	-4.303469	1.092065
H	3.945097	-4.473004	-0.642414
H	2.365327	-4.919405	0.000799
C	2.002410	-2.642474	-1.524102

H	1.078912	-3.227724	-1.534931
H	2.641296	-3.012817	-2.328603
H	1.724427	-1.605297	-1.738885
H	3.911773	-1.861343	1.304692
H	1.859312	-2.595871	0.596453
O	-5.523264	-2.167585	-0.502366
C	-6.430659	-2.598006	-1.517581
H	-5.984782	-2.466758	-2.505673
H	-6.619056	-3.651200	-1.320371
H	-7.358908	-2.025991	-1.467544

Vibrational frequencies

-120.6563	13.9488	18.5794
18.7250	27.4154	29.4734
32.9865	41.9732	50.1653
59.1949	61.3429	76.2741
92.9300	95.0682	109.0418
115.8086	127.0239	132.6415
138.2917	147.2216	149.1319
155.1286	167.4068	181.7616
191.7477	195.4309	201.6851
213.6091	219.5245	227.8935
235.2305	240.6281	250.3827
261.7646	266.2889	267.9680
279.6255	283.7946	289.4904
301.4727	305.9295	313.1099
315.7555	324.1141	329.3175
330.5870	351.4464	359.0387
370.6343	375.8164	384.8677
394.8098	413.1757	418.1452

426.6052	445.6001	457.1564
465.9570	474.8291	486.2011
504.4971	506.2911	523.9884
528.9801	540.7273	551.0110
560.4808	563.9677	569.8326
587.5020	598.1724	613.1243
641.6220	656.3016	657.9683
675.2320	680.6099	688.2391
719.7287	730.0581	737.9088
738.5797	752.7172	768.6829
775.9080	787.9988	791.6329
805.0907	806.6381	823.6931
831.0191	853.3316	861.7922
878.8650	886.3765	890.9822
906.6760	912.9289	916.9389
930.5749	945.3117	947.1262
948.0334	952.7593	956.5668
962.4946	964.4856	976.5706
979.1466	982.1839	991.6530
993.9294	1001.6393	1006.4404
1013.7331	1021.0100	1023.9016
1035.6473	1039.7538	1040.8267
1061.2926	1063.4201	1066.3708
1068.9727	1083.7743	1116.5205
1121.7927	1124.9573	1135.7783
1155.0118	1168.7132	1172.1599
1174.2498	1186.8920	1189.6089
1199.6708	1200.8256	1216.3231
1218.0526	1219.9166	1223.2729
1233.3504	1234.1168	1236.2408

1245.9375	1261.7748	1264.1885
1278.0739	1284.3764	1287.2718
1288.7581	1306.8344	1320.6104
1327.7563	1331.9889	1339.9346
1344.4442	1345.5849	1347.2920
1354.5570	1361.8007	1365.2368
1371.0655	1393.1018	1402.7532
1407.5591	1415.7442	1416.3016
1418.9630	1421.7639	1426.9916
1428.8081	1435.3730	1440.6331
1453.2092	1457.1589	1462.1374
1463.9565	1474.9390	1481.3811
1481.8613	1486.4190	1487.0830
1488.2462	1488.2804	1491.0834
1492.9250	1494.5142	1495.4230
1496.2657	1496.7440	1498.5405
1499.1713	1506.1539	1507.7184
1512.8941	1515.3844	1516.9467
1519.5089	1524.5270	1547.0437
1548.2579	1564.7307	1640.3528
1644.1597	1664.7507	1678.4969
1682.6692	1691.2412	1693.7169
1723.4924	1829.4334	2918.8873
3064.4807	3065.5034	3069.9343
3072.1106	3076.0344	3076.6515
3077.3902	3079.8757	3084.3691
3087.5224	3090.2859	3090.5392
3092.0516	3092.8234	3136.3867
3137.6079	3141.3467	3146.1747
3149.0512	3150.9510	3152.1093

3154.3595	3164.5221	3167.3855
3168.0256	3169.9358	3170.8035
3172.5209	3174.3527	3175.0081
3176.5449	3176.8328	3179.4687
3182.8066	3184.8875	3191.2128
3199.4950	3201.2655	3206.8816
3207.2168	3212.0091	3233.1658

R_p -INT6

Zero-point correction= 0.740819

Thermal correction to Energy= 0.781736

Thermal correction to Enthalpy= 0.782680

Thermal correction to Gibbs Free Energy= 0.668313

Sum of electronic and zero-point Energies= -1899.459683

Sum of electronic and thermal Energies= -1899.418766

Sum of electronic and thermal Enthalpies= -1899.417822

Sum of electronic and thermal Free Energies= -1899.532188

Cartesian coordinates

C	-4.121498	-1.397069	0.761476
C	-3.166870	-2.433672	0.738215
C	-2.185746	-2.393629	1.734089
H	-1.471433	-3.211644	1.795453
C	-1.957802	-1.244626	2.487060
H	-1.059672	-1.164391	3.094831
C	-2.737025	-0.102587	2.287921
C	-3.903057	-0.255059	1.540231
H	-4.580065	0.586245	1.425641
C	-5.265319	-1.393719	-0.189794
C	-2.974450	-3.387906	-0.423849

H	-3.896544	-3.905372	-0.691967
H	-2.245173	-4.140213	-0.108561
C	-2.424219	-2.673664	-1.732707
H	-1.675677	-3.336436	-2.179581
H	-3.250156	-2.572159	-2.439307
C	-1.846233	-1.308194	-1.437628
C	-0.702533	-1.185358	-0.648331
H	-0.078473	-2.068515	-0.503218
C	-0.455718	-0.066157	0.150576
C	-1.381410	0.990765	0.143542
C	-2.346083	0.984432	-0.873003
H	-3.023430	1.832860	-0.950747
C	-2.590017	-0.145211	-1.650270
H	-3.458656	-0.172892	-2.304588
C	0.744573	-0.149937	1.125606
H	0.872507	-1.255202	1.302555
C	-1.561548	1.957292	1.296753
H	-2.237336	2.752285	0.961247
H	-0.612877	2.400945	1.593563
C	-2.181726	1.270138	2.586220
H	-1.375980	1.176071	3.314572
H	-2.958872	1.927389	2.990565
O	-5.373932	-2.096282	-1.174343
O	0.747143	0.594186	2.219480
C	4.062224	0.161631	-0.480257
C	2.016000	0.172901	0.287104
N	3.145156	-0.560855	0.220680
N	2.326274	1.303847	-0.350936
N	3.624976	1.325499	-0.843038
C	1.526726	2.490922	-0.477342

C	0.747853	2.657414	-1.622941
C	-0.002678	3.828774	-1.716237
C	0.034732	4.804566	-0.718654
C	0.861801	4.607235	0.389450
C	1.624606	3.450144	0.534418
H	-0.629866	3.981146	-2.591124
H	0.911769	5.369719	1.162873
C	0.701456	1.603443	-2.694481
H	0.133231	0.731969	-2.349238
H	0.219210	1.993046	-3.592635
H	1.707923	1.265494	-2.958960
C	-0.819378	6.041507	-0.823712
H	-1.030977	6.290186	-1.865923
H	-1.778410	5.887249	-0.318109
H	-0.333580	6.899119	-0.352779
C	2.497433	3.206662	1.733274
H	2.130320	2.311044	2.250080
H	3.536251	3.034942	1.431850
H	2.470822	4.062908	2.409535
C	3.639202	-1.921171	0.479235
C	5.175152	-1.627940	0.270202
O	5.203013	-0.478944	-0.667252
C	6.024846	-2.712479	-0.354457
H	7.042566	-2.332143	-0.467688
H	6.056301	-3.584723	0.301154
H	5.654692	-3.011373	-1.334547
C	5.777372	-1.138207	1.581770
H	5.824315	-1.963894	2.295935
H	6.788132	-0.765485	1.405755
H	5.174993	-0.336269	2.018719

C	2.881076	-2.929725	-0.403588
C	2.839065	-2.544951	-1.883789
H	2.325392	-1.590039	-2.038977
H	3.838165	-2.469599	-2.322485
H	2.286142	-3.304632	-2.442212
C	3.335798	-4.375850	-0.182516
H	2.550791	-5.053811	-0.525550
H	4.241304	-4.617013	-0.741154
H	3.517747	-4.583787	0.876511
H	3.479150	-2.174692	1.530878
H	1.852972	-2.869881	-0.023218
O	-6.210425	-0.500215	0.149914
C	-7.320124	-0.419522	-0.745005
H	-7.977216	0.344905	-0.335628
H	-6.983779	-0.140298	-1.745495
H	-7.836647	-1.379590	-0.798858

Vibrational frequencies

17.2821	21.7717	25.3825
32.8389	35.4396	46.6364
48.8540	56.8214	67.3945
75.6044	87.7776	97.1952
103.1281	115.2302	120.5510
131.3643	140.0908	143.7470
151.0698	167.0510	169.7196
176.5972	178.6720	187.9893
191.0418	202.5838	214.6507
216.0578	221.1335	239.9407
244.3545	252.0089	262.9946
268.1648	277.2993	280.8043

283.6835	285.4404	288.9637
305.3008	316.1137	322.2975
326.4283	329.2387	331.0647
344.0290	362.7116	367.9048
376.7433	384.9830	392.4403
410.0369	420.5206	421.8986
434.6814	441.3250	450.7825
467.7762	478.8342	503.9592
516.9298	524.6980	527.9967
537.4070	543.4614	552.0060
570.2362	588.4838	589.1696
599.2551	614.8410	626.8116
653.5020	655.2894	672.4582
688.8407	711.3952	723.7565
726.1865	735.8857	743.4464
751.8226	774.4608	782.0004
789.4662	791.0526	793.7933
803.9884	820.5616	829.6057
837.4542	852.8943	855.7110
880.4228	885.7514	900.1871
903.2531	911.5190	912.6769
919.2115	930.0682	937.9069
944.1022	951.6038	954.9056
960.0187	964.8550	974.8878
981.0163	983.5404	993.2827
994.7313	1002.3133	1002.9000
1010.7677	1038.3917	1038.5188
1040.3104	1043.6051	1061.9852
1062.1834	1072.9268	1074.6017
1076.1016	1102.8354	1114.8279

1124.3470	1132.6383	1163.8470
1166.0739	1172.3607	1176.4778
1186.3310	1192.2916	1202.0904
1202.4915	1216.6322	1217.2472
1218.3663	1220.8940	1228.5993
1232.6012	1238.1538	1246.5928
1252.9075	1258.6788	1269.6078
1279.6573	1281.9151	1283.8608
1287.1334	1296.6734	1304.9138
1315.0445	1322.0447	1331.7825
1335.2301	1337.0772	1337.5183
1345.0581	1349.8659	1360.7435
1365.1853	1367.6602	1374.5210
1394.1712	1399.8228	1412.0493
1416.0392	1419.9095	1422.4660
1425.8158	1433.3957	1439.0600
1454.4821	1456.2325	1463.8127
1469.4848	1472.5413	1480.7635
1481.5899	1484.2925	1487.3131
1488.7684	1490.2731	1490.7228
1494.5799	1495.3093	1495.5687
1495.8808	1499.5677	1501.4449
1506.1658	1508.0517	1508.0947
1509.8425	1520.4234	1523.6013
1526.0305	1534.2984	1539.7028
1547.6407	1549.2754	1571.3659
1640.4693	1644.6939	1680.3895
1681.6516	1683.6855	1690.2755
1740.4898	1826.5456	2729.3209
3051.6943	3068.7679	3071.1932

3071.4456	3073.8966	3074.9099
3082.4817	3082.6379	3083.1296
3085.9501	3093.4191	3095.1950
3101.7894	3127.1749	3127.7946
3141.3227	3144.8512	3146.9798
3152.7171	3156.6676	3162.0497
3163.3393	3165.4567	3165.9967
3168.7067	3169.8930	3170.4781
3172.1061	3174.1565	3178.0722
3182.5748	3183.1872	3185.1368
3194.2825	3194.6665	3202.5664
3202.8445	3205.3128	3206.9346
3211.7854	3214.6430	3223.8461

S_p-INT6

Zero-point correction= 0.741391

Thermal correction to Energy= 0.782158

Thermal correction to Enthalpy= 0.783102

Thermal correction to Gibbs Free Energy= 0.669930

Sum of electronic and zero-point Energies= -1899.464992

Sum of electronic and thermal Energies= -1899.424225

Sum of electronic and thermal Enthalpies= -1899.423281

Sum of electronic and thermal Free Energies= -1899.536453

Cartesian coordinates

C	-3.952283	-0.391342	0.219526
C	-3.335700	0.740559	-0.352715
C	-2.578975	1.537155	0.510577
H	-2.136586	2.457267	0.132764
C	-2.194462	1.080062	1.770382

H	-1.494330	1.673664	2.355158
C	-2.531175	-0.210158	2.188607
C	-3.539176	-0.852782	1.472424
H	-3.901467	-1.818588	1.810288
C	-4.883346	-1.228878	-0.585143
C	-3.189886	0.945257	-1.849280
H	-4.151055	1.067027	-2.350227
H	-2.614886	1.866884	-1.991065
C	-2.419749	-0.242869	-2.564405
H	-1.780733	0.199639	-3.336181
H	-3.150354	-0.882185	-3.064699
C	-1.613050	-1.073780	-1.590539
C	-0.590736	-0.475757	-0.854829
H	-0.222212	0.499335	-1.175775
C	-0.174394	-0.959139	0.384872
C	-0.841129	-2.062719	0.941608
C	-1.651219	-2.816392	0.082951
H	-2.129016	-3.715404	0.467590
C	-2.030230	-2.340162	-1.172594
H	-2.778648	-2.880940	-1.748796
C	0.806160	-0.100421	1.205686
H	0.221312	0.825076	1.416320
C	-0.967880	-2.240958	2.444133
H	-1.580338	-3.130355	2.627729
H	0.006467	-2.370158	2.915925
C	-1.645893	-0.994508	3.138325
H	-0.839548	-0.339758	3.482034
H	-2.193749	-1.349813	4.017861
O	-5.279930	-0.966293	-1.702418
O	1.433251	-0.629228	2.259175

C	3.896195	0.607145	-0.612538
C	1.916519	0.411164	0.273379
N	3.033179	-0.269680	-0.036933
N	2.146424	1.644392	-0.180024
N	3.405001	1.802341	-0.750018
C	1.227943	2.743365	-0.105300
C	0.593521	3.166864	-1.275190
C	-0.339529	4.199238	-1.159108
C	-0.634359	4.784571	0.072725
C	0.047512	4.342016	1.210693
C	0.997513	3.324444	1.148461
H	-0.851201	4.546583	-2.053290
H	-0.159182	4.808208	2.170737
C	0.925753	2.565897	-2.615843
H	1.093336	1.487066	-2.552413
H	1.843545	3.008425	-3.014825
H	0.118375	2.750260	-3.327087
C	-1.691257	5.852044	0.183980
H	-2.654527	5.405372	0.451999
H	-1.821559	6.381065	-0.762198
H	-1.438403	6.579129	0.958826
C	1.771641	2.890010	2.368043
H	2.842618	3.055382	2.209662
H	1.642482	1.826033	2.600672
H	1.462714	3.475010	3.235739
C	3.708225	-1.521100	0.310234
C	4.986342	-1.376216	-0.595626
O	5.084622	0.089959	-0.859025
C	6.248834	-1.766571	0.144722
H	7.124977	-1.582040	-0.480519

H	6.214243	-2.831383	0.389276
H	6.343019	-1.196729	1.071361
C	4.897578	-2.018361	-1.969531
H	4.880479	-3.106762	-1.887697
H	5.779633	-1.728827	-2.544835
H	4.005413	-1.689457	-2.506742
C	2.796994	-2.753561	0.226428
C	3.550748	-4.010046	0.665927
H	4.044656	-3.866888	1.632033
H	4.308230	-4.310653	-0.066025
H	2.849261	-4.841975	0.767211
C	2.055822	-2.970684	-1.096563
H	1.159436	-3.566400	-0.901788
H	2.661670	-3.505660	-1.831627
H	1.717279	-2.028973	-1.539517
H	4.006636	-1.419080	1.360395
H	2.047591	-2.523986	0.995411
O	-5.267185	-2.345407	0.056375
C	-6.156903	-3.189803	-0.674097
H	-5.681416	-3.537346	-1.593773
H	-6.376321	-4.029180	-0.017548
H	-7.071958	-2.652017	-0.928684

Vibrational frequencies

25.6633	28.3873	31.5785
36.0743	38.4802	46.0403
50.7253	56.4171	61.4625
65.9712	78.9530	92.4724
106.9008	116.0088	134.1296
136.5195	145.7794	149.2208

153.9012	164.9795	169.1383
178.7997	180.6719	194.1272
205.3606	206.3326	216.6573
224.9818	230.6681	237.0919
244.7738	250.6933	261.0333
265.5320	275.9683	283.2970
285.4896	290.2436	295.7124
311.9498	317.3368	320.5495
325.0918	328.2898	333.6742
337.8881	356.0889	368.3324
371.1297	380.0505	397.7974
404.6091	420.5208	422.0407
454.1219	460.7547	467.7401
475.0695	478.9960	493.3572
503.1237	510.2882	529.4707
534.7332	543.0543	553.0285
563.4543	587.2391	592.5028
600.4128	602.3870	626.3620
653.5400	658.0561	667.1314
684.4288	712.6474	715.8268
716.6390	731.7762	745.1043
747.4098	757.3534	771.5024
781.9240	789.0335	797.2425
811.5808	826.7002	833.1735
839.3445	857.1024	865.2874
885.0472	886.1707	899.3372
904.1400	913.5830	920.7521
922.3619	938.3476	947.1937
951.0319	955.7165	956.2534
962.9180	965.0438	973.8079

982.4987	983.3747	996.2842
1000.0110	1006.5616	1014.5672
1019.4532	1023.0320	1039.3154
1039.7281	1043.0280	1061.5173
1063.8035	1066.1979	1077.9233
1092.6216	1108.5931	1113.0986
1123.7096	1133.7696	1155.5738
1162.7139	1168.0535	1174.4962
1185.5628	1186.0099	1198.0955
1204.6373	1215.7466	1217.6995
1218.9616	1222.8428	1225.2104
1234.1340	1235.0493	1240.4543
1249.5482	1261.4953	1268.8462
1281.8712	1285.2342	1287.2036
1290.1398	1302.8762	1315.0419
1328.1915	1331.2995	1334.0064
1338.1768	1345.6327	1346.7390
1349.7147	1359.9035	1364.0944
1367.1123	1370.3905	1378.9603
1397.6645	1404.7805	1417.6855
1419.7420	1422.1238	1425.2507
1431.7370	1439.2128	1439.9929
1450.2551	1454.9312	1461.0174
1466.4741	1471.5892	1480.8582
1481.3897	1482.9770	1487.4840
1487.6724	1489.7020	1493.1521
1494.1976	1494.7483	1494.7569
1496.3894	1498.2227	1501.6976
1506.9917	1507.6326	1507.6745
1514.1590	1518.2103	1519.2459

1523.6942	1535.9915	1545.8403
1546.8009	1556.2331	1574.3231
1640.2938	1642.9500	1677.2988
1680.0767	1682.9375	1687.4376
1730.3896	1827.3592	2891.6632
3060.3769	3065.4461	3073.4052
3074.6022	3076.1402	3078.2767
3080.0479	3080.4649	3082.5346
3087.5874	3089.0560	3091.4414
3092.0131	3094.6811	3126.1310
3134.4459	3142.8432	3146.8101
3148.0684	3151.9667	3152.0611
3156.3319	3164.5502	3165.0981
3170.8328	3171.8142	3172.5443
3172.9384	3173.6991	3176.3827
3178.8955	3179.6148	3181.0700
3182.2295	3187.3752	3189.3846
3198.5675	3203.0947	3205.9129
3209.0327	3210.5797	3228.9944

R_p -TS7

Zero-point correction= 0.766305

Thermal correction to Energy= 0.813307

Thermal correction to Enthalpy= 0.814251

Thermal correction to Gibbs Free Energy= 0.684460

Sum of electronic and zero-point Energies= -2183.921313

Sum of electronic and thermal Energies= -2183.874311

Sum of electronic and thermal Enthalpies= -2183.873367

Sum of electronic and thermal Free Energies= -2184.003158

Cartesian coordinates

C	-1.068517	0.790171	0.406256
C	-2.018049	1.386975	1.260381
C	-3.278563	1.666264	0.720676
H	-4.000075	2.202299	1.334094
C	-3.696272	1.124625	-0.493420
H	-4.733313	1.230704	-0.802978
C	-2.848756	0.265006	-1.195421
C	-1.510404	0.228671	-0.798355
H	-0.807433	-0.396950	-1.348153
C	0.392789	0.588356	0.739821
C	-1.829130	1.500804	2.758698
H	-0.846917	1.902161	3.011676
H	-2.591176	2.185330	3.144559
C	-1.982071	0.103529	3.505425
H	-2.630829	0.251081	4.374609
H	-0.992641	-0.191842	3.858206
C	-2.529045	-0.974890	2.598715
C	-3.872040	-0.982612	2.224116
H	-4.595281	-0.414509	2.802069
C	-4.280319	-1.535831	1.004414
C	-3.333061	-2.119024	0.137838
C	-2.070699	-2.373060	0.678783
H	-1.309963	-2.846284	0.063835
C	-1.661801	-1.801863	1.881088
H	-0.611366	-1.865880	2.158500
C	-5.675660	-1.295406	0.554108
C	-3.495355	-2.219090	-1.365370
H	-2.678839	-2.845315	-1.737998
H	-4.437228	-2.688347	-1.652220

C	-3.416092	-0.809344	-2.094232
H	-4.425581	-0.527313	-2.399961
H	-2.810879	-0.935038	-2.998163
O	0.737618	0.422023	2.084001
O	-6.062239	-1.304714	-0.597898
H	0.706339	-0.543887	0.203693
C	1.676128	-2.421625	0.846248
O	1.028620	-1.800038	-0.140657
O	2.241289	-3.518597	0.598365
Cs	1.548999	-3.860625	-2.218790
O	1.683527	-1.878254	2.013784
H	1.151033	-0.536167	2.122622
C	2.054690	2.945335	-1.443215
C	1.248975	1.537557	0.034770
N	0.900647	2.407534	-0.953508
N	2.596077	1.602300	0.060399
N	3.123299	2.495104	-0.874904
C	3.512001	0.845963	0.864618
C	4.164404	-0.241073	0.279480
C	5.100535	-0.923516	1.055557
C	5.380657	-0.542176	2.367362
C	4.715964	0.563633	2.903617
C	3.778128	1.281910	2.165889
H	5.619030	-1.775887	0.623530
H	4.939729	0.880068	3.919488
C	3.870465	-0.646461	-1.139385
H	2.812659	-0.917197	-1.226743
H	4.082024	0.172651	-1.833379
H	4.479829	-1.508253	-1.420441
C	6.367723	-1.317907	3.200296

H	5.852916	-2.084259	3.788361
H	7.105445	-1.822699	2.572574
H	6.895012	-0.664681	3.899655
C	3.075143	2.484274	2.732164
H	3.210888	3.356933	2.084562
H	2.003761	2.274140	2.807885
H	3.463459	2.727445	3.722744
C	-0.234359	3.259678	-1.351101
C	0.398179	3.815547	-2.671858
O	1.846769	3.878284	-2.360999
C	-0.022769	5.195332	-3.129119
H	0.532907	5.449725	-4.034685
H	-1.087812	5.191647	-3.371583
H	0.168764	5.959546	-2.377630
C	0.222246	2.794857	-3.792060
H	-0.827710	2.757252	-4.092282
H	0.825179	3.086577	-4.654311
H	0.524277	1.794851	-3.468173
C	-0.586941	4.208365	-0.188484
C	0.567648	5.097421	0.281593
H	1.435982	4.504030	0.587399
H	0.898387	5.809880	-0.477700
H	0.246225	5.669274	1.155773
C	-1.874561	4.990735	-0.453617
H	-2.213272	5.454512	0.476561
H	-1.742000	5.787583	-1.188369
H	-2.668748	4.322429	-0.801438
H	-1.103968	2.644222	-1.595306
H	-0.812051	3.521150	0.636261
O	-6.509715	-1.045103	1.578175

C	-7.858360	-0.760243	1.207783
H	-7.899583	0.119438	0.562186
H	-8.296029	-1.608949	0.678886
H	-8.390309	-0.575798	2.138839

Vibrational frequencies

-1217.3393	12.3330	22.2875
23.7431	26.9670	29.5680
34.2152	42.2533	46.9740
51.3072	59.9325	62.8729
72.6343	75.4991	80.9697
87.2390	92.3175	103.6762
110.9043	123.8148	129.7755
135.7314	139.3558	143.5874
152.5945	161.0280	164.6759
167.4426	184.7083	185.7111
191.4569	195.9247	201.8408
203.8439	215.6284	219.0722
224.7956	231.9334	243.4407
252.2030	256.3166	264.5272
274.1025	279.8277	282.9792
288.5528	293.3465	295.5978
310.4906	312.7540	321.3104
330.6677	333.7998	337.0914
350.0600	362.0621	376.4604
376.9632	380.0437	395.6921
401.6359	415.0583	421.1633
428.0686	438.4429	447.6056
461.5311	470.4743	484.0834
509.7427	517.9988	523.6114

523.9094	544.3308	550.6436
563.7934	575.9865	579.2378
589.4434	605.1296	620.2594
635.8193	648.0522	664.3375
678.2265	686.8299	693.1080
712.6599	721.6191	727.2484
728.2220	745.4365	752.4139
754.9872	782.8048	791.1109
794.5884	800.5024	810.3201
824.8144	826.1132	836.8225
841.9639	855.4053	858.5654
861.5010	875.8257	887.1681
897.6708	908.3539	910.0261
918.4527	920.8901	931.8642
938.8287	941.6152	951.6396
952.7776	965.0282	965.5998
973.2671	982.3170	984.6561
992.4963	998.8572	1001.8587
1009.8559	1018.3841	1034.0007
1039.0201	1041.0124	1044.4408
1062.4220	1064.8446	1072.6270
1079.3109	1081.2540	1088.5319
1103.9281	1107.6458	1120.6155
1130.6554	1145.8086	1163.2463
1172.1526	1177.6810	1186.7010
1187.3950	1198.3536	1202.9061
1204.2559	1218.1847	1219.2671
1222.0111	1225.0653	1226.2549
1231.7522	1234.1367	1237.8418
1242.4896	1251.2805	1280.2044

1280.8918	1283.8076	1289.4598
1293.8312	1305.8384	1314.7614
1317.4127	1333.1485	1334.7666
1336.8813	1340.4400	1347.1462
1349.2805	1360.9207	1362.2462
1365.3031	1380.2302	1397.0984
1399.9265	1402.5971	1411.6351
1417.9926	1420.0487	1423.6352
1429.9526	1440.0953	1444.6973
1456.6721	1463.1873	1465.2040
1469.7771	1476.7494	1482.1786
1482.5430	1486.2151	1488.3637
1489.1155	1490.7454	1492.5870
1494.4664	1495.6519	1497.8878
1500.8046	1501.1915	1506.8655
1507.7164	1508.1934	1509.9064
1511.8896	1513.2158	1520.7252
1526.1361	1527.7717	1544.7085
1550.8842	1552.3777	1577.3826
1602.0466	1635.9812	1640.4554
1646.3151	1680.4339	1681.9598
1683.5115	1693.7375	1731.3051
1750.9306	1825.1971	2420.2623
3067.0661	3070.0765	3078.4392
3079.1922	3080.5485	3082.0852
3083.9118	3085.9516	3087.1177
3093.6246	3094.0593	3095.0912
3101.7463	3143.0636	3143.0937
3143.8713	3149.1818	3150.2094
3152.9713	3153.2284	3158.0714

3163.8606	3168.3096	3168.7118
3169.3366	3170.6352	3170.7733
3173.6573	3173.7897	3173.9271
3178.4900	3179.1494	3182.8864
3189.1901	3203.8632	3204.3402
3205.7173	3207.7072	3211.9266
3213.7201	3217.9231	3223.8929

S_p -TS7

Zero-point correction= 0.766669

Thermal correction to Energy= 0.813863

Thermal correction to Enthalpy= 0.814807

Thermal correction to Gibbs Free Energy= 0.684486

Sum of electronic and zero-point Energies= -2183.922869

Sum of electronic and thermal Energies= -2183.875674

Sum of electronic and thermal Enthalpies= -2183.874730

Sum of electronic and thermal Free Energies= -2184.005051

Cartesian coordinates

C	0.415786	-0.718768	0.373820
C	0.603598	-2.013090	0.902516
C	1.715828	-2.223016	1.718902
H	1.839959	-3.188223	2.205794
C	2.759395	-1.294913	1.773434
H	3.675700	-1.547285	2.303004
C	2.712947	-0.148061	0.981202
C	1.483155	0.176613	0.397170
H	1.381419	1.097643	-0.173101
C	-0.902362	-0.315830	-0.276662
C	-0.198288	-3.184162	0.384652

H	-1.248340	-2.910808	0.248277
H	-0.150047	-4.003484	1.108321
C	0.330861	-3.717394	-1.025660
H	0.506012	-4.793827	-0.933991
H	-0.465966	-3.559049	-1.754224
C	1.585173	-3.017131	-1.496776
C	2.823088	-3.314779	-0.931033
H	2.949433	-4.235131	-0.368746
C	3.854616	-2.368215	-0.901297
C	3.649844	-1.084965	-1.448690
C	2.535402	-0.931558	-2.278090
H	2.357898	0.023287	-2.770157
C	1.517719	-1.880810	-2.307288
H	0.602753	-1.632054	-2.831547
C	5.065631	-2.667652	-0.094490
C	4.359395	0.164570	-0.968564
H	4.050546	0.982511	-1.626759
H	5.445511	0.078168	-1.020704
C	3.975204	0.546287	0.523252
H	4.803400	0.262936	1.175734
H	3.864542	1.635884	0.569645
O	-1.307142	-1.085657	-1.375033
O	5.864113	-1.851837	0.322273
H	-0.703302	0.898424	-0.761796
C	0.049792	1.562854	-2.668277
O	-0.310051	1.948457	-1.438895
O	0.875106	2.271930	-3.302327
Cs	1.474809	4.341096	-1.325326
O	-0.470576	0.489935	-3.146861
H	-1.041556	-0.494863	-2.171352

C	-2.968646	0.265444	2.603611
C	-1.936297	-0.212952	0.726759
N	-1.747717	0.206997	2.006639
N	-3.269301	-0.415279	0.649145
N	-3.939158	-0.111471	1.840475
C	-4.044627	-0.952156	-0.430794
C	-4.598240	-2.224564	-0.267640
C	-5.384721	-2.725221	-1.305358
C	-5.619217	-1.989143	-2.466597
C	-5.055972	-0.716408	-2.577628
C	-4.263680	-0.170875	-1.569265
H	-5.821617	-3.715425	-1.201841
H	-5.239280	-0.128388	-3.473828
C	-4.370458	-3.025793	0.987193
H	-3.328289	-2.967892	1.316316
H	-4.986259	-2.647049	1.808047
H	-4.622684	-4.074449	0.820773
C	-6.444784	-2.560478	-3.590450
H	-7.093534	-3.364544	-3.236502
H	-7.067590	-1.790749	-4.052829
H	-5.798950	-2.972506	-4.372463
C	-3.647095	1.191493	-1.718065
H	-3.660161	1.741636	-0.772248
H	-2.603588	1.109367	-2.042709
H	-4.193036	1.774543	-2.462926
C	-0.735471	0.863627	2.838667
C	-1.474021	0.690789	4.213488
O	-2.911487	0.721493	3.847317
C	-1.261123	1.747720	5.275052
H	-1.892276	1.510684	6.134696

H	-0.219671	1.733068	5.603397
H	-1.511114	2.748072	4.925617
C	-1.184075	-0.701767	4.765399
H	-0.145819	-0.753834	5.102347
H	-1.841238	-0.907961	5.612539
H	-1.334647	-1.469808	4.000961
C	-0.429181	2.257898	2.261224
C	-1.646474	3.178610	2.148397
H	-2.443226	2.718329	1.554665
H	-2.067041	3.459725	3.116481
H	-1.354357	4.098666	1.634367
C	0.763072	2.909923	2.962567
H	1.062149	3.813084	2.423069
H	0.537167	3.207360	3.988659
H	1.619004	2.226840	2.979296
H	0.182311	0.267821	2.851425
H	-0.111888	2.046089	1.231328
O	5.207809	-3.982042	0.151993
C	6.335449	-4.331297	0.953496
H	6.270340	-3.854022	1.933586
H	6.305394	-5.414306	1.054227
H	7.261149	-4.017700	0.467462

Vibrational frequencies

-1322.1504	18.9217	19.6530
24.5233	30.3564	33.1656
33.6723	37.6860	39.7261
52.2887	57.8965	63.6599
66.0728	68.6877	76.0429
82.9006	89.7107	97.3234

105.0674	124.9678	132.5843
135.0813	137.8442	141.5025
142.2945	150.5560	167.1357
172.1633	174.7064	178.6602
182.8200	185.4528	194.6398
204.4817	210.7875	211.4824
230.0554	230.6038	241.5994
246.8745	249.7791	269.9019
278.3332	281.6463	287.9128
288.4067	291.8740	299.3592
309.0691	310.0444	320.8059
329.5105	330.8048	343.0379
346.2774	356.3504	368.5866
374.7401	379.5641	390.0055
403.5989	412.3315	419.4253
424.2780	445.0446	449.6504
461.2584	470.7915	478.7467
506.9210	515.4750	522.6113
526.5798	538.9009	552.7043
561.8145	575.3302	584.1324
589.0584	607.4119	623.2563
645.2809	651.3430	666.7715
684.0611	686.8610	695.1218
705.1572	714.6001	725.1020
728.7017	743.5788	752.0416
766.8599	784.7919	787.7871
795.8800	801.7392	809.1865
822.9820	826.2858	842.6432
846.4014	853.4286	863.8517
870.0509	883.8680	895.5103

896.5968	908.9854	915.4888
916.9573	930.4998	935.8042
940.0030	948.7719	954.1391
964.4585	965.3991	972.1848
980.2580	980.9209	984.7622
994.0022	1000.4728	1002.6551
1007.0316	1013.8272	1036.2887
1037.1066	1041.7282	1043.3955
1056.8324	1062.3440	1062.8918
1066.9140	1076.9574	1083.6508
1097.9923	1106.7820	1111.4828
1125.9226	1140.4470	1166.4136
1172.0436	1173.5418	1180.8595
1187.4438	1192.3118	1200.4884
1202.3946	1218.1196	1218.5325
1220.1340	1222.7376	1225.7076
1233.6824	1236.2804	1239.8471
1249.1057	1249.8162	1275.2602
1280.2522	1284.1291	1285.0732
1286.4109	1303.7159	1314.5555
1316.1615	1332.9114	1333.9375
1338.8541	1344.9760	1349.1822
1352.1867	1359.0066	1364.5806
1381.3749	1389.9737	1408.1804
1413.6212	1417.2917	1417.8771
1419.9054	1421.9751	1428.6986
1431.5150	1439.7282	1454.5798
1458.9131	1462.7281	1465.7903
1466.8347	1474.2765	1478.7697
1482.7817	1484.3831	1488.2120

1488.9782	1489.6218	1492.5681
1493.6502	1495.1288	1495.7334
1495.9015	1498.0411	1500.6068
1503.1372	1506.8383	1508.0596
1510.5838	1519.8001	1520.9706
1523.8093	1530.6206	1544.9693
1549.6832	1550.9649	1565.5008
1580.7094	1640.5537	1641.7846
1645.3474	1681.6996	1682.9964
1684.3932	1692.8368	1705.1611
1754.8168	1825.2293	2673.0519
3072.3858	3075.8587	3077.6544
3077.8484	3078.3020	3078.6071
3081.2965	3082.7776	3083.3623
3092.1355	3094.3289	3094.7225
3102.7983	3126.6408	3139.4455
3144.5387	3144.8821	3146.9756
3147.5268	3149.3662	3152.4693
3164.4384	3164.9158	3165.0598
3165.4713	3168.7081	3169.5935
3173.3281	3174.4749	3175.2282
3178.2457	3182.7920	3188.4354
3195.7219	3204.1664	3204.2600
3206.3544	3208.5464	3212.2304
3216.0484	3226.8196	3265.2990

BP

Zero-point correction= 0.364655

Thermal correction to Energy= 0.385234

Thermal correction to Enthalpy= 0.386178

Thermal correction to Gibbs Free Energy= 0.315960
Sum of electronic and zero-point Energies= -1074.295966
Sum of electronic and thermal Energies= -1074.275388
Sum of electronic and thermal Enthalpies= -1074.274443
Sum of electronic and thermal Free Energies= -1074.344661

Cartesian coordinates

C	-1.774665	-0.129608	-0.896821
C	-1.022016	0.963736	-1.368708
C	0.173873	0.654342	-2.024189
H	0.743888	1.459507	-2.480812
C	0.750510	-0.608691	-1.925100
H	1.758900	-0.766652	-2.300045
C	0.131432	-1.614063	-1.177871
C	-1.196900	-1.401097	-0.813621
H	-1.749034	-2.188863	-0.309425
C	-3.112294	0.075764	-0.276752
C	-1.281291	2.406350	-0.985824
H	-2.317233	2.699063	-1.160437
H	-0.642207	3.032155	-1.615076
C	-0.943141	2.715746	0.536867
H	-0.410038	3.670453	0.572720
H	-1.883998	2.831364	1.077608
C	-0.131475	1.614015	1.177846
C	1.196868	1.401106	0.813610
H	1.748996	2.188908	0.309460
C	1.774651	0.129618	0.896766
C	1.022028	-0.963749	1.368626
C	-0.173877	-0.654424	2.024105
H	-0.743864	-1.459618	2.480711

C	-0.750547	0.608598	1.925019
H	-1.758965	0.766507	2.299921
C	3.112252	-0.075681	0.276620
C	1.281426	-2.406341	0.985763
H	0.642567	-3.032229	1.615154
H	2.317455	-2.698867	1.160158
C	0.942981	-2.715859	-0.536877
H	1.883729	-2.831806	-1.077735
H	0.409598	-3.670416	-0.572499
O	-3.537563	1.127605	0.155439
O	3.537326	-1.127369	-0.156140
O	-3.828486	-1.058221	-0.227971
C	-5.108801	-0.943732	0.396894
H	-5.545875	-1.939270	0.362146
H	-4.999210	-0.608004	1.429837
H	-5.733134	-0.231561	-0.145352
O	3.828650	1.058203	0.228467
C	5.109011	0.943749	-0.396327
H	4.999430	0.608786	-1.429521
H	5.546396	1.939121	-0.360825
H	5.733039	0.230992	0.145493

Vibrational frequencies

31.6531	32.5177	56.3355
85.2849	92.3879	116.9950
140.2955	143.4027	159.3533
166.5600	168.1900	193.4420
196.9267	221.5177	263.9326
294.0490	295.7188	312.1843
326.6328	335.0321	363.8275

369.9825	384.8177	398.4868
417.0084	426.4610	439.1266
477.9426	515.6777	528.1183
540.5181	553.9957	610.6442
657.0238	679.9749	693.7314
725.8014	725.9692	732.8559
793.2894	793.6073	794.1087
804.3005	810.1349	828.0333
838.3442	858.8379	892.7290
901.2508	920.5883	940.8381
940.9416	950.4100	959.0223
986.2492	994.8020	1002.7209
1014.9092	1037.4753	1038.4726
1123.5302	1132.3662	1167.5676
1174.5160	1186.3302	1186.4176
1193.7810	1202.6813	1216.7443
1219.1551	1221.9165	1222.6126
1224.2465	1235.1586	1244.4881
1256.4847	1285.7918	1291.2344
1308.4896	1317.2907	1334.5214
1337.8046	1344.2777	1348.2166
1363.1305	1367.1508	1458.7347
1460.5975	1482.8798	1485.4031
1487.9507	1488.0423	1495.3936
1495.4073	1501.5696	1503.7931
1508.0606	1508.0749	1550.0216
1550.2898	1643.2692	1646.7090
1682.5067	1684.9736	1825.8502
1828.0210	3092.5845	3092.6455
3094.5038	3094.5366	3101.7585

3102.5580	3158.6299	3158.6640
3171.4191	3171.4683	3176.2475
3176.2567	3199.4850	3199.5534
3213.6960	3213.7204	3214.6077
3214.6836	3224.3984	3224.6658

Part 9: References

1. C. Y. Legault, *CYLview*, 1.0b, Universit'e de Sherbrooke, 2009, <http://www.cylview.org>.