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SUPPORTING INFORMATION FOR

Insights into N-heterocyclic carbene and Lewis acid cooperatively catalyzed oxidative [3+3] annulation reactions of α, β-unsaturated aldehyde with 1,3-dicarbonyl compounds

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Part 1：The possible proton transfer processes for the formation of the Breslow intermediate

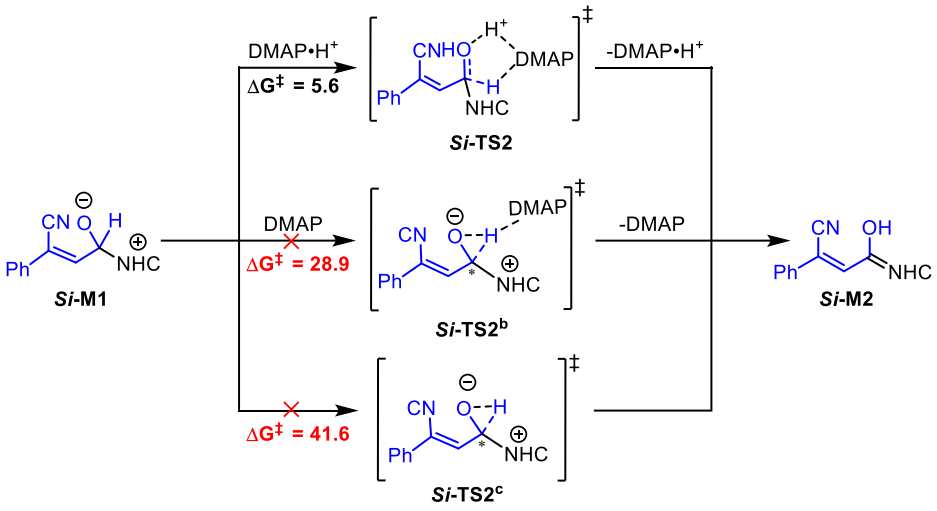

Fig. S1 The possible proton transfer processes for the formation of the Breslow intermediate (unit: kcal/mol)

Part 2：The relative Gibbs free energy profiles for formation of R2^{l}

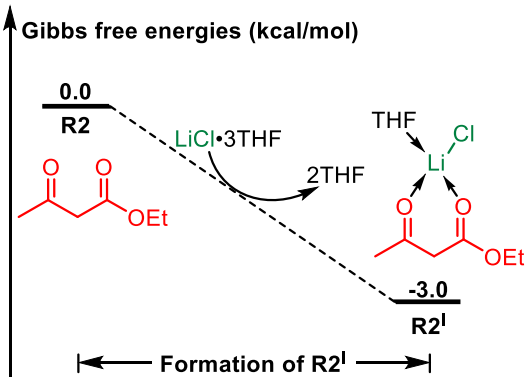

Fig. S2 The relative Gibbs free energy profiles for formation of R2^{l}

Part 3：NBO analysis for deprotonation of R2 with or without the presence of LiCl

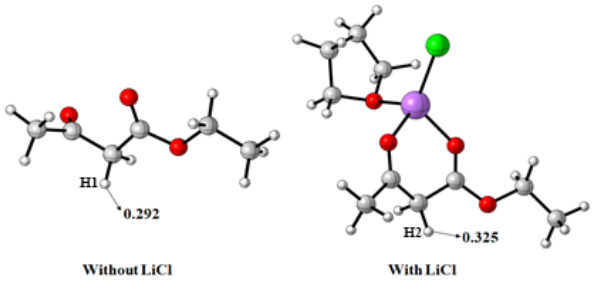

Fig. S3 NBO analysis for R2 and R2[l] (unit: e)

Part 4：Comparison of different coordination modes of LA

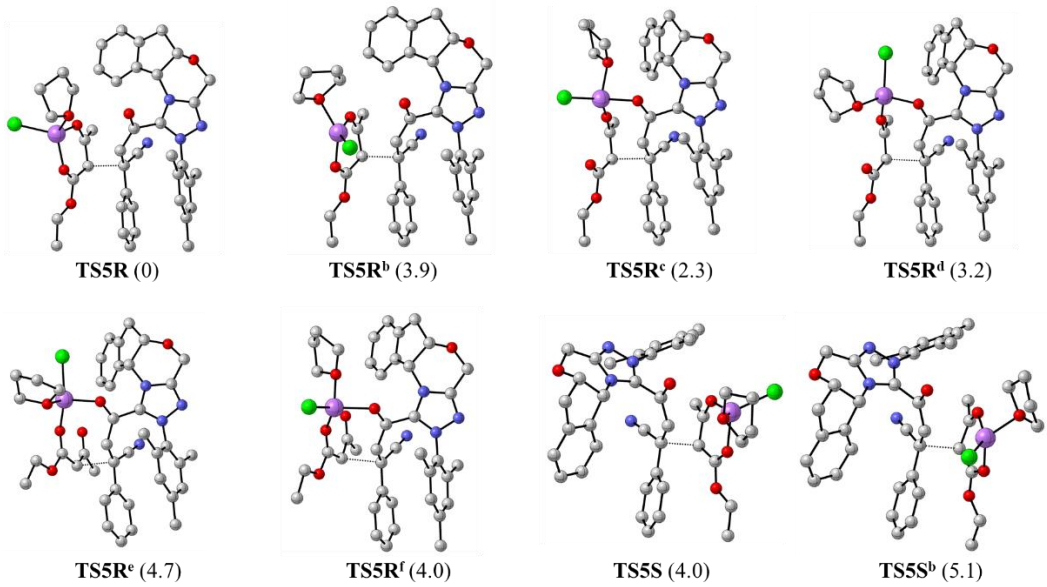

Fig. S4 Comparison of relative Gibbs free energies (ΔΔ*G*) of different coordination models of LA (unit: Å)

Table S1 Comparison of relative Gibbs free energies (ΔΔ*G*) of different coordination models of LA

Coordination model	SPs	*ΔG*‡(kcal/mol)
model A	TS5R	0
	TS5R[b]	3.9
	TS5S	4.0
	TS5S[b]	5.1
model B	TS5R[c]	2.3

	TS5R[d]	3.2
model C	TS5R[e]	4.7
	TS5R[f]	4.0

Part 5：The possible proton transfer processes for the formation of M7R

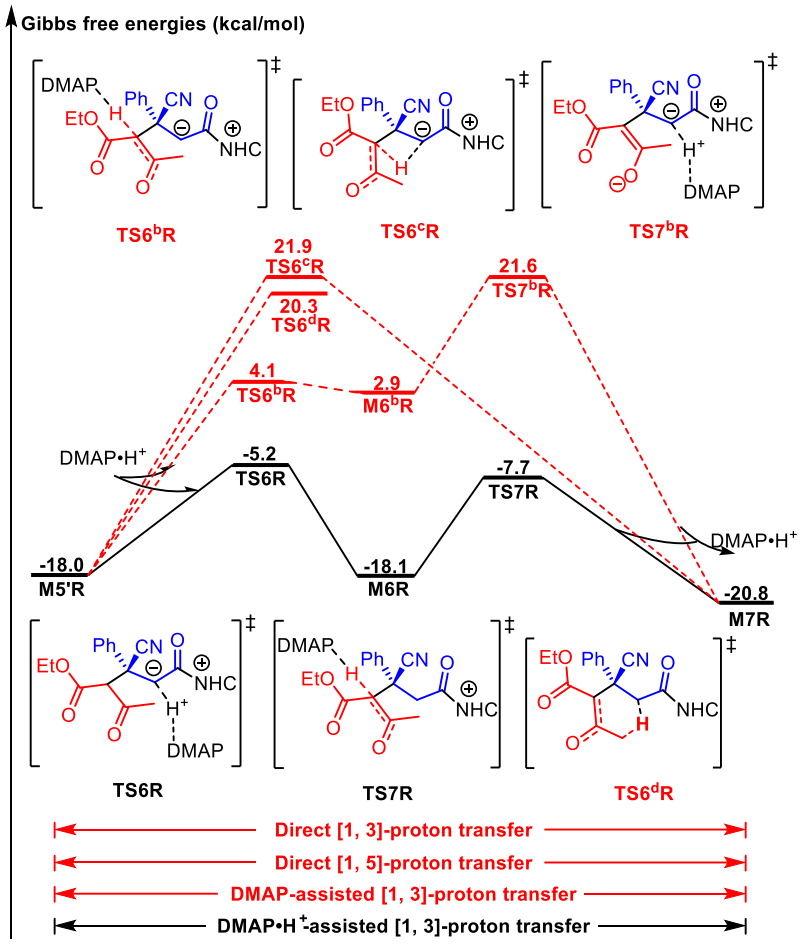

Fig. S5 The relative Gibbs free energy profiles for the possible proton transfer pathways

Part 6：Computational details of global reactivity index (GRI) analysis and Boltzmann distribution

For the global reactivity index (GRI) analysis, the relevant parameters of GRI, i.e., electrophilicity index ω[1], electronic chemical potential μ, chemical hardness η,

one-electron energies of the frontier molecular orbital HOMO (E_L) and LUMO (E_H), The HOMO energies obtained within the Kohn−Sham scheme,[2] nucleophilicity index N[3] was generally utilized to judge the nucleophilicity character.

Table S2 Energy of HOMO (E_H), LUMO (E_L), electronic chemical potential (μ), chemical hardness (η), global electrophilicity (ω) and global nucleophilicity (N) of SPs

	SP	E_H(a.u.)	E_L(a.u.)	μ(eV)	η(eV)	ω(eV)	N[a] (eV)	ω+N (eV)
[3+2]	**Si-M2**	-0.19021	-0.02458	-0.107	0.166	-	5.130	**6.759**
annulation	**R2[I]**	-0.29565	-0.04839	-0.172	0.247	1.629	-	
[3+3]	**R2[I-]**	-0.21623	0.06991	-0.073	0.286	-	4.422	**8.452**
annulation	**M3**	-0.31328	-0.13989	-0.227	0.173	4.029	-	

a E_H(TCE) = -0.37872 a.u. (calculated at the M06-2X/6-31G(d, p)/IEF-PCMTHF level).

In addition, the extent of enantioselectivity, in terms of enantiomeric excess (ee %), was calculated by using the Boltzmann distribution of diastereomeric transition states with the following equations:

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

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

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

Part 7：Quantitative NCI analysis for transition state TS5S

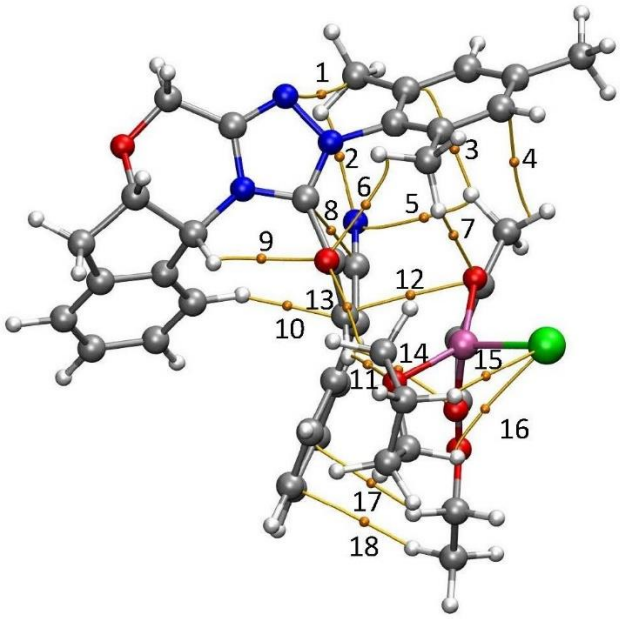

Fig. S6 Bond Critical Points (BCPs, color in orange) along the Bond Paths (color in yellow) for topological analysis of **TS5S**

Table S3 Summary of distance, type of interaction, electron densities (ρ_{bcp}), Lagrangian kinetic energies (G_b), potential energy densities (V_b), energy densities (H_b), Laplacian of electron densities (∇^2_ρ) at the bond critical points (BCPs) along the bond paths in **TS5R** (the bond lengths are in Å, others are in a.u.)

BCP index	Type of interaction	Distance	ρ_{bcp}*10^{-2}	G_b*10^{-2}	V_b*10^{-2}	H_b*10^{-3}	∇^2_ρ*10^{-1}
1	C-H···N	2.64	1.1878	1.0774	-0.8686	2.0884	0.5145
2	C-H···N	2.45	1.1606	0.8647	-0.7134	1.5134	0.4064
3	C-H···π	2.64	0.9248	0.6263	-0.5081	1.1817	0.2978
4	C-H···π	2.94	0.6816	0.4408	-0.3286	1.1221	0.2212
5	C-H···N	2.71	0.7613	0.5183	-0.4001	1.1820	0.2546
6	C-H···O	2.54	1.0938	0.9005	-0.7537	1.4681	0.4189
7	C-H···O	2.41	1.0604	0.8798	-0.7791	1.0063	0.3922
8	LP···π	2.98	0.9880	0.7144	-0.5585	1.5588	0.3481
9	C-H···O	2.46	1.1454	0.9428	-0.7949	1.4783	0.4362

10	C-H···π	2.51	1.0579	0.7939	-0.6558	1.3805	0.3728
11	C-H···O	2.36	1.2728	0.9882	-0.9541	0.3416	0.4090
12	LP···π	2.89	1.4017	0.9526	-0.8927	0.5987	0.4050
13	C-H···O	2.67	0.8602	0.7440	-0.6047	1.3926	0.3533
14	C-H···O	2.58	1.0299	0.7761	-0.6557	1.2043	0.3586
15	C-H··· Cl	3.10	0.5704	0.3459	-0.2580	0.8791	0.1735
16	C-H··· Cl	3.06	0.6615	0.4273	-0.3344	0.9294	0.2081
17	C-H···π	2.92	0.5988	0.3745	-0.2824	0.9215	0.1867
18	C-H···π	2.87	0.5762	0.3391	-0.2562	0.8286	0.1688

Part 8: Test results of the different computational methods

We have compared the relative Gibbs free energies (ΔΔ*G*) of Re/Si-TS1 and Re/Si-M1 optimized at the M06-2X/6-31G(d, p)/IEF-PCM$_{THF}$ (L1), B3LYP-D3/6-31G(d, p)/IEF-PCM$_{THF}$ (L2), ωb97X-D/6-31G(d, p)/IEF-PCM$_{THF}$ (L3) levels. As shown in **Table S3**, there are same trend and small energy differences between the stationary points (SPs), indicating the selected method should be proper and reliable in this kind of reaction system.

Table S4 Comparison of relative Gibbs free energies (ΔΔ*G*) of the *Re*/*Si*-TS1 and *Re*/*Si*-M1 calculated by using the different levels (L1-3) (unit: kcal/mol).

	***Re*-TS1**	***Si*-TS1**	***Re*-M1**	***Si*-M1**
L1	9.1	6.2	2.0	0
L2	5.1	2.9	2.0	0
L3	8.8	4.5	3.9	0

Part 9：Optimized geometries of some stationary points

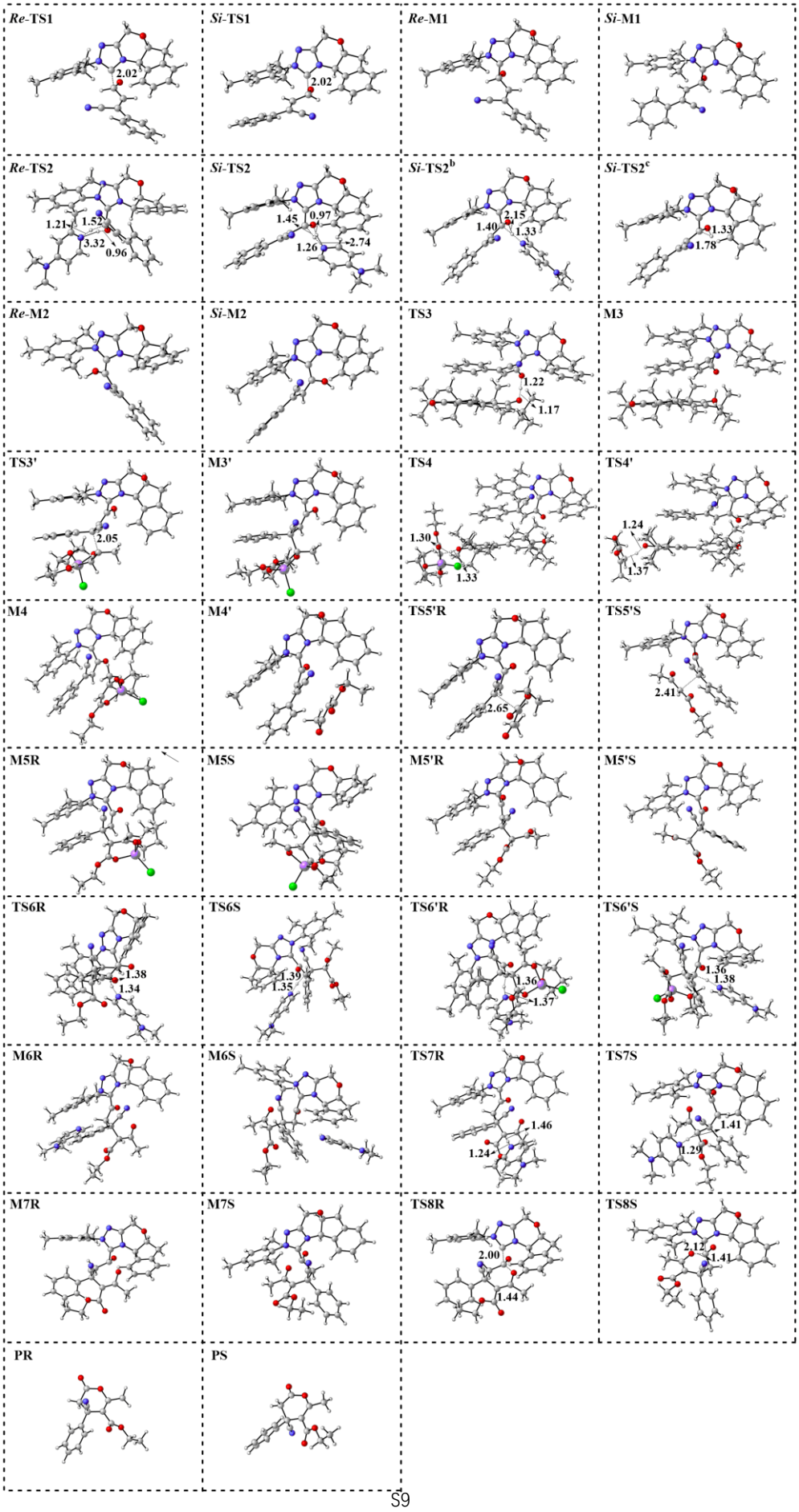
Re-TS1
2.02
Si-TS1
2.02
Re-M1
Si-M1
Re-TS2
1.21
1.52
3.32
0.96
Si-TS2
1.45
0.97
1.26
2.74
Si-TS2[b]
2.15
1.40
1.33
Si-TS2[c]
1.33
1.78
Re-M2
Si-M2
TS3
1.22
1.17
M3
TS3'
2.05
M3'
TS4
1.30
1.33
TS4'
1.24
1.37
M4
M4'
TS5'R
2.65
TS5'S
2.41
M5R
M5S
M5'R
M5'S
TS6R
1.38
1.34
TS6S
1.39
1.35
TS6'R
1.36
1.37
TS6'S
1.36
1.38
M6R
M6S
TS7R
1.46
1.24
TS7S
1.41
1.29
M7R
M7S
TS8R
2.00
1.44
TS8S
2.12
1.41
PR
PS

Fig. S7 Optimized geometries of some stationary points (unit: Å)

Part 10: Absolute single-point energies and Gibbs free energy (GFE) of the structures optimized at the L1 level

Table S5 The single-point and GFE (=*E*+GFEC) energies of the stationary points involved in the [3+3] annulation reaction of α, β-unsaturated aldehyde with 1,3-dicarbonyl compound (unit: a.u.)

SP	GFEC (M06-2X/6-31G(d, p)/ IEF-PCM$_{thf}$)	*E* (M06-2X/6-311++G (2df, 2pd)/IEF-PCM$_{thf}$)	GFE
R1	0.106510	-515.176790	-515.070280
NHC	0.333127	-1052.237451	-1051.904324
***Re*-TS1**	0.465869	-1567.421095	-1566.955226
***Si*-TS1**	0.469250	-1567.425617	-1566.956367
***Re*-M1**	0.468916	-1567.432334	-1566.963418
***Si*-M1**	0.467671	-1567.435542	-1566.967871
DMAP	0.130351	-382.220503	-382.090152
DMAP·H$^+$	0.145361	-382.670355	-382.524994
***Re*-TS2**	0.630656	-1950.109700	-1949.479044
***Si*-TS2**	0.632745	-1950.116679	-1949.483934
***Si*-TS2^b**	0.617132	-1949.629027	-1949.011895
***Si*-TS2^c**	0.465043	-1567.366544	-1566.901501
***Re*-M2**	0.466319	-1567.443713	-1566.977394
***Si*-M2**	0.470209	-1567.456684	-1566.986475
DQ	0.559982	-1241.364134	-1240.804152
TS3	1.054510	-2808.823884	-2807.769374
M3	1.060273	-2808.834832	-2807.774559
R2	0.120174	-460.320291	-460.200117
LiCl	-0.019950	-467.853140	-467.873090

THF	0.090046	-232.424631	-232.334585
LiCl·3THF	0.309706	-1165.177155	-1164.867449
R2[l]	0.229467	-1160.632578	-1160.403111
TS3'	0.734370	-2728.087171	-2727.352801
M3'	0.735337	-2728.088844	-2727.353507
TS4	1.313436	-3969.478023	-3968.164587
TS4'	1.199910	-3269.149967	-3267.950057
DQH2	0.585465	-1242.614309	-1242.028844
M4	0.705034	-2726.880597	-2726.175563
M4'	0.592994	-2026.541370	-2025.948376
TS5R	0.709501	-2726.871540	-2726.162039
TS5R[b]	0.712833	-2726.868690	-2726.155857
TS5R[c]	0.709735	-2726.868091	-2726.158356
TS5R[d]	0.710353	-2726.867247	-2726.156894
TS5R[e]	0.704093	-2726.858509	-2726.154416
TS5R[f]	0.709144	-2726.864795	-2726.155651
TS5S	0.708838	-2726.864068	-2726.155230
TS5S[b]	0.706975	-2726.860866	-2726.153891
TS5'R	0.596488	-2026.538686	-2025.942198
TS5'S	0.594776	-2026.536083	-2025.941307
M5R	0.711313	-2726.895454	-2726.184141
M5S	0.710542	-2726.886988	-2726.176446
M5'R	0.597212	-2026.575859	-2025.978647
M5'S	0.597882	-2026.567343	-2025.969461
TS6R	0.757795	-2409.241100	-2408.483305
TS6R[b]	0.744589	-2408.778196	-2408.033607
TS6R[c]	0.593427	-2026.508634	-2025.915207
TS6R[d]	0.593998	-2026.511625	-2025.917627
TS6S	0.756266	-2409.233381	-2408.477115

TS6'R	0.872964	-3109.555428	-3108.682464
TS6'S	0.871662	-3109.549860	-3108.678198
M6R	0.763119	-2409.267029	-2408.503910
M6R[b]	0.748656	-2408.784209	-2408.035553
M6S	0.759698	-2409.256086	-2408.496388
TS7R	0.757855	-2409.245201	-2408.487346
TS7R[b]	0.748123	-2408.753920	-2408.005797
TS7S	0.756940	-2409.231047	-2408.474107
M7R	0.598387	-2026.581514	-2025.983127
M7S	0.597700	-2026.585847	-2025.988147
TS8R	0.596917	-2026.573559	-2025.976642
TS8S	0.598234	-2026.574963	-2025.976729
PR/S	0.236134	-974.331832	-974.095698

Part 11: List of the Cartesian coordinates of all the SPs involved in the reaction

NHC

Zero-point correction= 0.383859
Thermal correction to Energy= 0.404669
Thermal correction to Enthalpy= 0.405613
Thermal correction to Gibbs Free Energy= 0.333127
Sum of electronic and zero-point Energies= -1051.536401
Sum of electronic and thermal Energies= -1051.515590
Sum of electronic and thermal Enthalpies= -1051.514646
Sum of electronic and thermal Free Energies= -1051.587132
Cartesian coordinates

C	0.240953	-0.163538	-0.878205
C	-0.510506	-1.498545	0.782625
C	-2.211311	-0.732558	-0.859723
H	-2.184120	-0.970603	-1.928536
N	0.752245	-1.356976	1.043432
N	1.180291	-0.540514	0.013307
N	-0.849850	-0.808836	-0.351907

C	-1.541064	-2.298827	1.516236
H	-1.364274	-2.254251	2.591567
H	-1.496801	-3.349847	1.196254
C	-3.138640	-1.729876	-0.120268
O	-2.820010	-1.754617	1.264400
C	-4.235287	0.379572	-0.291960
C	-2.898820	0.596022	-0.628361
C	-2.375168	1.876896	-0.733409
C	-3.222081	2.959385	-0.492097
C	-4.561264	2.751219	-0.159479
C	-5.078751	1.458586	-0.057527
C	-4.531884	-1.102485	-0.241671
H	-1.329520	2.020414	-0.989887
H	-5.206147	3.603511	0.029319
H	-6.118888	1.300940	0.212434
H	-5.018268	-1.438786	-1.164182
H	-5.159986	-1.400151	0.601324
C	2.549818	-0.125041	-0.007367
C	3.422292	-0.706636	-0.927808
C	2.961931	0.855902	0.901190
C	4.750340	-0.273814	-0.928063
C	4.296447	1.252989	0.868724
C	5.203749	0.699295	-0.038837
H	5.445948	-0.712639	-1.639268
H	4.635792	2.017734	1.563537
C	1.977849	1.464423	1.863959
H	1.636801	0.724420	2.594638
H	1.089721	1.823017	1.333379
H	2.428073	2.301773	2.399681
C	6.641305	1.152926	-0.046483
H	7.128692	0.923732	0.907103
H	6.708003	2.236602	-0.194220
H	7.206086	0.664048	-0.844804
C	2.937905	-1.757934	-1.890283
H	2.202133	-1.339561	-2.582939
H	2.447294	-2.578258	-1.357568
H	3.770089	-2.165796	-2.466657
H	-3.070542	-2.744064	-0.535537
H	-2.835683	3.971191	-0.561854

Vibrational frequencies

13.3874	28.4989	50.7851
67.1567	75.2047	99.6243
113.2791	147.3435	150.0695
159.6922	184.9366	197.6527

210.0138	229.9164	235.7202
262.4069	278.4899	302.8932
312.6959	327.2254	357.4939
377.3214	408.8449	436.9825
470.5965	481.1991	495.5495
509.2897	524.0712	559.3578
563.4537	586.0426	589.0416
612.8904	631.4737	643.8600
676.3304	705.7943	727.5769
751.2108	760.3824	764.8636
788.7948	840.4905	858.7846
881.3280	888.2176	898.7562
918.6326	920.4225	952.2067
964.5206	976.7546	987.0043
995.4749	1020.3246	1021.2566
1036.4335	1041.3367	1046.1184
1061.2011	1062.2366	1066.4910
1068.5077	1070.0364	1079.6463
1085.5379	1112.9981	1172.0891
1174.1707	1189.4520	1194.6500
1210.7212	1228.4625	1249.3389
1251.1251	1273.8958	1284.7050
1289.7466	1298.3304	1312.9898
1330.4900	1336.6233	1349.6379
1357.0989	1375.7799	1383.6576
1399.8779	1412.4975	1416.6349
1419.6572	1430.7889	1446.1445
1468.0041	1472.6411	1483.0497
1485.2549	1487.8537	1494.0906
1496.8754	1499.6987	1500.8951
1517.0462	1525.3908	1535.9992
1568.4765	1683.0150	1686.6804
1692.2571	1699.6930	1704.6591
3057.0013	3057.8685	3067.4706
3075.8520	3077.4023	3087.4687
3105.7406	3124.9693	3135.2399
3148.0640	3151.0218	3154.2223
3163.2494	3166.2753	3168.7258
3191.2720	3198.8807	3205.4419
3205.8773	3213.7134	3224.4669

R1

Zero-point correction= 0.143508

Thermal correction to Energy= 0.153781

Thermal correction to Enthalpy= 0.154725
Thermal correction to Gibbs Free Energy= 0.106510
Sum of electronic and zero-point Energies= -514.867046
Sum of electronic and thermal Energies= -514.856773
Sum of electronic and thermal Enthalpies= -514.855829
Sum of electronic and thermal Free Energies= -514.904045
Cartesian coordinates

C	3.148010	-0.490010	-0.073632
H	3.453073	0.559862	0.090093
C	1.698062	-0.757678	-0.116638
H	1.408905	-1.789786	-0.286463
C	0.762875	0.202705	0.026627
O	3.969180	-1.371009	-0.210974
C	-0.699937	-0.020533	0.013624
C	-1.569325	1.037819	-0.275904
C	-1.229747	-1.288651	0.286339
C	-2.943152	0.826798	-0.314797
H	-1.168798	2.026618	-0.478381
C	-2.602697	-1.493355	0.250475
H	-0.573350	-2.110254	0.553121
C	-3.462537	-0.438250	-0.053564
H	-3.606473	1.652789	-0.547458
H	-3.004047	-2.476960	0.469931
H	-4.534732	-0.601930	-0.077894
C	1.191495	1.576088	0.197894
N	1.501957	2.682591	0.331757

Vibrational frequencies

33.3464	91.7796	112.2723
142.8419	169.6563	228.5987
299.6536	324.5149	354.0730
410.6589	451.8797	496.2952
520.0820	626.8500	671.2315
674.7174	707.2344	789.3875
805.6129	870.3233	899.8275
960.7472	983.2025	1006.4789
1019.4087	1034.7641	1039.4261
1071.9629	1127.8043	1161.1211
1183.7987	1215.3757	1272.2748
1319.5174	1355.8845	1368.8967
1437.7934	1502.8322	1549.8226
1668.0679	1692.9766	1703.8369
1838.0952	2406.8355	3055.5693
3209.0900	3213.9625	3218.6474
3226.7556	3232.1359	3234.9801

***Re*-TS1**

Zero-point correction= 0.529824

Thermal correction to Energy= 0.561373

Thermal correction to Enthalpy= 0.562317

Thermal correction to Gibbs Free Energy= 0.465869

Sum of electronic and zero-point Energies= -1566.412283

Sum of electronic and thermal Energies= -1566.380734

Sum of electronic and thermal Enthalpies= -1566.379790

Sum of electronic and thermal Free Energies= -1566.476238

Cartesian coordinates

C	-0.608116	0.228912	2.033012
C	0.583733	1.081432	1.700344
C	0.557384	2.216326	0.982227
O	-0.488816	-0.653197	2.907458
C	1.762684	2.986352	0.588731
C	1.780543	3.693920	-0.618152
C	2.917804	2.955528	1.378715
C	2.939879	4.340030	-1.038056
H	0.886859	3.728616	-1.235107
C	4.073488	3.601011	0.956120
H	2.906960	2.437458	2.332677
C	4.090586	4.291342	-0.255017
H	2.942077	4.881313	-1.978428
H	4.961692	3.572739	1.578583
H	4.993574	4.797008	-0.580934
C	-0.703632	2.641216	0.423141
N	-1.702211	2.993085	-0.047767
H	1.534713	0.705939	2.073271
H	-1.578584	0.733507	1.859960
C	-0.766215	-0.801915	0.297614
C	-0.649130	-2.829409	-0.606538
C	1.378580	-2.064593	0.628746
H	1.343835	-1.755224	1.681428
N	-1.850750	-2.419653	-0.887706
N	-1.893211	-1.165692	-0.317938
N	0.034605	-1.878167	0.101896
C	-0.009909	-4.156711	-0.886912
H	-0.226313	-4.477732	-1.906707
H	-0.412939	-4.904185	-0.188893
C	1.794744	-3.549182	0.512170
O	1.391420	-4.049221	-0.757205
C	3.618945	-2.164026	-0.140630
C	2.482192	-1.353129	-0.125633

C	2.485497	-0.097320	-0.715171
C	3.670591	0.369022	-1.286738
C	4.817398	-0.425307	-1.278106
C	4.796412	-1.703128	-0.715110
C	3.325629	-3.496843	0.511856
H	1.585174	0.508467	-0.740379
H	5.732791	-0.051725	-1.725976
H	5.684296	-2.328058	-0.734820
H	3.701168	-3.528094	1.540640
H	3.740838	-4.351294	-0.027857
C	-3.103891	-0.398051	-0.357798
C	-4.015293	-0.556012	0.689165
C	-3.313476	0.470936	-1.428743
C	-5.183042	0.204000	0.640098
C	-4.497968	1.204924	-1.436596
C	-5.437410	1.087870	-0.410614
H	-5.912585	0.099805	1.439415
H	-4.686733	1.890540	-2.258974
C	-2.280418	0.610371	-2.513260
H	-2.038583	-0.360742	-2.955379
H	-1.354394	1.027332	-2.103395
H	-2.635829	1.275291	-3.301898
C	-6.692102	1.922590	-0.423660
H	-6.518497	2.884395	0.069662
H	-7.506487	1.421646	0.104413
H	-7.017177	2.130564	-1.445671
C	-3.737865	-1.523196	1.810668
H	-2.806724	-1.281537	2.336963
H	-3.631164	-2.540751	1.420922
H	-4.556596	-1.515690	2.532081
H	1.368523	-4.167537	1.312319
H	3.694494	1.358539	-1.734573

Vibrational frequencies

-177.5581	24.3347	30.3115
32.1113	35.7009	41.8293
45.6930	53.2033	67.7489
77.7215	82.1265	86.5066
95.2920	122.2999	128.3205
134.0160	140.0275	152.4412
159.6679	166.7180	192.8680
201.1360	209.0920	231.4221
243.3921	250.7953	273.1313
283.8169	296.3660	298.9375
311.0808	326.7683	349.1531

360.5495	365.0726	390.8218
409.1860	416.6749	442.4194
445.8792	463.7402	483.5800
489.6400	494.1782	509.3613
518.1300	528.6001	551.2041
560.2573	579.2516	586.4739
590.9051	617.1251	628.6841
633.3047	645.0295	670.1467
675.6365	694.8811	713.3364
717.3069	727.6502	753.1852
758.1087	770.3036	784.2056
792.3696	808.1991	839.4686
863.5848	877.0980	878.5040
881.8677	901.6905	911.0052
920.5289	924.9314	954.5618
962.2389	967.0647	979.8347
985.6737	991.6979	1006.5859
1009.5845	1019.0000	1021.7947
1025.7085	1028.8730	1039.7932
1042.0708	1046.7504	1061.9371
1065.0468	1065.4800	1068.2885
1074.0623	1074.6950	1079.0175
1092.3188	1112.1100	1126.9741
1128.7116	1141.8560	1173.0836
1174.0675	1185.2750	1189.9875
1205.8698	1215.4268	1216.5817
1239.7150	1256.5649	1272.1473
1279.3001	1284.8704	1288.6374
1305.9099	1309.1518	1317.8598
1325.5301	1335.3115	1349.1545
1358.1089	1358.9302	1364.6599
1370.3073	1377.5009	1385.9776
1400.6280	1409.3717	1418.0746
1423.3987	1424.9020	1436.7150
1468.2287	1469.0246	1471.8975
1489.8142	1491.5990	1496.8414
1497.0104	1497.3746	1499.5871
1504.6387	1512.5097	1515.5595
1527.1075	1536.8609	1552.8241
1572.5924	1630.0675	1673.8218
1675.1292	1680.3710	1694.0618
1696.7880	1702.2389	1706.5958
1723.7484	2401.4017	2988.7737
3058.1516	3059.5179	3067.2939

3073.1741	3081.8217	3093.7617
3099.5698	3127.9485	3136.6632
3143.1740	3145.1585	3162.4235
3167.3248	3169.2268	3170.2764
3191.4311	3196.7234	3199.8945
3205.5666	3208.3983	3215.8164
3217.7068	3221.7807	3226.4814
3230.2408	3236.9017	3239.9035

***Si*-TS1**

Zero-point correction= 0.530358

Thermal correction to Energy= 0.561136

Thermal correction to Enthalpy= 0.562081

Thermal correction to Gibbs Free Energy= 0.469250

Sum of electronic and zero-point Energies= -1566.416486

Sum of electronic and thermal Energies= -1566.385707

Sum of electronic and thermal Enthalpies= -1566.384763

Sum of electronic and thermal Free Energies= -1566.477593

Cartesian coordinates

C	-0.359732	0.411029	-1.973616
C	1.108767	0.606137	-1.721229
C	1.644557	1.618193	-1.018141
O	-0.733851	-0.389366	-2.854160
C	3.080993	1.742713	-0.671839
C	3.465552	2.435168	0.481150
C	4.060442	1.113358	-1.448214
C	4.800901	2.467148	0.871151
H	2.714010	2.934133	1.086918
C	5.393195	1.150739	-1.058412
H	3.782390	0.601263	-2.363922
C	5.767334	1.818090	0.107682
H	5.083735	2.999090	1.773703
H	6.144789	0.661199	-1.669643
H	6.809265	1.841491	0.410563
C	0.752502	2.593619	-0.437178
N	0.058078	3.378178	0.058585
H	1.753158	-0.173118	-2.121387
H	-0.968792	1.301664	-1.724714
C	-0.781698	-0.528775	-0.231610
C	-2.037703	-2.110136	0.694647
C	-3.239816	-0.444934	-0.729600
H	-2.993183	-0.320450	-1.791432
N	-0.826886	-2.402241	1.066093
N	-0.070954	-1.409610	0.479501

N	-2.047817	-0.987989	-0.088627
C	-3.317652	-2.839222	0.970252
H	-3.350839	-3.171612	2.008530
H	-3.384002	-3.719657	0.315214
C	-4.431463	-1.417874	-0.551666
O	-4.407725	-1.968660	0.759620
C	-5.151868	0.807316	-0.088234
C	-3.757615	0.837761	-0.119692
C	-3.044235	1.933472	0.343679
C	-3.756954	3.026391	0.838097
C	-5.151826	3.008885	0.862161
C	-5.860340	1.897579	0.400994
C	-5.663021	-0.508991	-0.629855
H	-1.957896	1.941762	0.337762
H	-5.692541	3.865392	1.252377
H	-6.945615	1.882902	0.436667
H	-5.989724	-0.407865	-1.670639
H	-6.488808	-0.933858	-0.054338
C	1.361053	-1.473713	0.572066
C	2.029134	-2.312739	-0.326403
C	2.023306	-0.691562	1.515392
C	3.417319	-2.370318	-0.239682
C	3.415287	-0.790913	1.571670
C	4.124183	-1.624859	0.710067
H	3.962446	-3.010325	-0.929866
H	3.956295	-0.184572	2.293771
C	1.260300	0.249836	2.407115
H	0.448840	-0.266946	2.928010
H	0.804463	1.056500	1.820400
H	1.922238	0.700529	3.148692
C	5.623637	-1.739047	0.798348
H	6.041089	-0.963542	1.443979
H	6.080784	-1.642531	-0.190295
H	5.913878	-2.714323	1.202369
C	1.256585	-3.080999	-1.366816
H	0.663426	-2.402525	-1.993636
H	0.558491	-3.781098	-0.897678
H	1.933810	-3.646326	-2.009132
H	-4.424775	-2.224623	-1.295665
H	-3.218004	3.893171	1.207140

Vibrational frequencies

-180.0952	23.4475	28.4568
39.6444	43.3399	57.4008
68.8466	75.4935	79.7448

86.0809	87.2588	112.6214
126.4364	131.9189	149.9324
159.3547	164.4761	187.0830
201.5421	206.9547	216.4741
221.2532	226.1462	233.0073
252.2737	260.4002	277.1220
282.8021	300.1225	303.5000
313.9112	325.4860	345.7600
363.0625	368.3978	386.6377
407.0456	411.8838	441.7384
461.1198	462.1232	481.0770
492.6055	497.4904	508.2839
518.3888	531.7419	538.3318
557.8064	585.4039	588.4674
589.5112	614.5529	626.5262
632.1799	642.5293	668.3150
675.2144	701.6789	709.7382
726.7716	729.6613	752.8270
757.6031	766.1497	787.2772
791.3366	806.7344	841.0010
860.1765	867.5537	881.3708
884.3238	901.0331	908.9499
916.4812	921.0822	947.2235
961.0394	965.3703	982.0734
983.9593	990.5949	998.5832
1007.8208	1017.8044	1019.5813
1025.7782	1026.6061	1035.4845
1042.7468	1048.5044	1060.2899
1064.6243	1065.0453	1070.6794
1073.2872	1073.8668	1077.3833
1082.0339	1115.3506	1119.7504
1124.3076	1139.4255	1172.8134
1174.7635	1180.6114	1190.3433
1199.4371	1213.7037	1216.4857
1239.5366	1253.8922	1269.7358
1273.1008	1280.4346	1286.9146
1303.5369	1307.9597	1316.7135
1322.6881	1334.4240	1338.5173
1354.2598	1363.7524	1366.2567
1366.6723	1378.2509	1387.2151
1399.3437	1411.6924	1420.9483
1424.0450	1425.8000	1436.4307
1466.8563	1470.8511	1474.3584
1490.2531	1492.4762	1493.2329

1495.1486	1499.2054	1499.7577
1506.1641	1514.7907	1517.9097
1528.6920	1538.0453	1551.6943
1567.6217	1628.6538	1671.5600
1678.6272	1685.3381	1693.0317
1693.5674	1698.1351	1706.5026
1721.9767	2394.3302	2972.9097
3053.8977	3058.6132	3067.3938
3070.5461	3082.2369	3092.7486
3099.1176	3126.9792	3138.9260
3140.5961	3147.2830	3164.5356
3167.0354	3173.1860	3174.5628
3187.4816	3195.7085	3198.2313
3200.5922	3202.9148	3207.6179
3208.0474	3213.4399	3217.9821
3220.9075	3222.4812	3235.4716

***Re*-M1**

Zero-point correction= 0.531745

Thermal correction to Energy= 0.563117

Thermal correction to Enthalpy= 0.564062

Thermal correction to Gibbs Free Energy= 0.468916

Sum of electronic and zero-point Energies= -1566.418795

Sum of electronic and thermal Energies= -1566.387423

Sum of electronic and thermal Enthalpies= -1566.386479

Sum of electronic and thermal Free Energies= -1566.481625

Cartesian coordinates

C	-0.640788	0.048267	1.659346
C	0.498716	1.030314	1.413149
C	0.419884	2.219754	0.792156
O	-0.455988	-0.744134	2.708637
C	1.586528	3.092645	0.501583
C	1.581882	3.915441	-0.630211
C	2.725572	3.060361	1.314649
C	2.701469	4.676668	-0.953303
H	0.700785	3.952460	-1.264581
C	3.841463	3.823329	0.990138
H	2.732069	2.451552	2.213235
C	3.835386	4.630888	-0.146482
H	2.685735	5.305551	-1.837332
H	4.715937	3.793793	1.631764
H	4.706960	5.226672	-0.396592
C	-0.854963	2.643510	0.262056
N	-1.862435	3.007537	-0.181230

H	1.465150	0.693390	1.784847
H	-1.591772	0.632616	1.626099
C	-0.760356	-0.886797	0.418765
C	-0.481727	-2.709562	-0.767316
C	1.464200	-2.050578	0.654143
H	1.367229	-1.773507	1.712976
N	-1.702392	-2.334843	-1.018435
N	-1.853581	-1.192776	-0.274624
N	0.135271	-1.837901	0.086329
C	0.204997	-3.982583	-1.168638
H	0.109974	-4.146825	-2.243011
H	-0.283142	-4.814358	-0.641725
C	1.857690	-3.533433	0.478165
O	1.578455	-3.921177	-0.863876
C	3.738308	-2.170828	0.008361
C	2.614090	-1.341047	-0.037070
C	2.672945	-0.092242	-0.639198
C	3.895833	0.349537	-1.148656
C	5.027857	-0.459380	-1.069204
C	4.953129	-1.733136	-0.500759
C	3.380989	-3.509178	0.616675
H	1.790456	0.531991	-0.729214
H	5.971798	-0.104346	-1.470117
H	5.827832	-2.375965	-0.473434
H	3.660679	-3.558698	1.674803
H	3.833296	-4.359351	0.102308
C	-3.104246	-0.484538	-0.277557
C	-3.981298	-0.688022	0.789336
C	-3.377257	0.361226	-1.354421
C	-5.185926	0.013657	0.757577
C	-4.597210	1.030976	-1.342440
C	-5.506688	0.874889	-0.293581
H	-5.891517	-0.119068	1.572535
H	-4.838363	1.698383	-2.166108
C	-2.382410	0.532696	-2.469658
H	-2.230460	-0.406591	-3.009807
H	-1.411068	0.850366	-2.077764
H	-2.726452	1.289951	-3.175462
C	-6.800140	1.647188	-0.290321
H	-6.625265	2.682957	0.025353
H	-7.525140	1.204645	0.398732
H	-7.242550	1.678764	-1.290695
C	-3.636851	-1.637885	1.906842
H	-2.681456	-1.382764	2.385347

H	-3.544479	-2.659318	1.521404
H	-4.422901	-1.630766	2.663636
H	1.344327	-4.196924	1.184862
H	3.958102	1.330943	-1.609236

Vibrational frequencies

25.3436	28.7207	31.9521
39.7703	43.7602	48.6868
69.1766	74.9120	87.9200
97.6198	106.5530	109.6383
120.0834	141.0392	149.1264
152.3287	155.5823	163.3943
172.6763	195.7605	201.6969
213.4983	231.1667	241.2240
252.3798	277.9576	283.4572
288.1327	296.4824	308.2707
330.2545	333.7025	360.2037
374.3463	376.4567	411.8529
413.3025	443.6960	450.9108
459.3498	476.9902	488.6236
499.4350	508.6684	521.6272
528.5905	533.6359	559.1886
582.7585	586.2255	590.6471
608.0064	628.6111	638.1460
642.2794	660.5201	674.0238
700.5727	711.5077	717.9059
729.5427	748.3863	755.4514
766.3962	772.5832	786.8034
799.4683	818.6574	842.0513
876.7306	879.8710	884.1180
886.2943	902.1974	912.2400
922.3922	952.0307	962.8724
965.6650	970.4304	979.9115
985.3586	988.7197	1011.4779
1016.3615	1018.0522	1023.9710
1035.7268	1039.3719	1043.8328
1046.8256	1057.0891	1059.3799
1066.3780	1068.5762	1070.3627
1074.3175	1075.9680	1078.8597
1104.5400	1113.9336	1129.0249
1138.8716	1178.1935	1179.4431
1186.5010	1188.8435	1203.2367
1211.1460	1219.2166	1224.0995
1238.9354	1256.3343	1269.4495
1281.6140	1285.4811	1287.0658

1303.9038	1314.8938	1318.9321
1326.7386	1330.3891	1341.2837
1348.6834	1354.4945	1363.9543
1371.4466	1375.0389	1378.9604
1381.0973	1397.3989	1408.7138
1421.1443	1427.0956	1437.8136
1465.4011	1468.2128	1473.8007
1484.5484	1487.9015	1495.5253
1497.6893	1498.7552	1504.4087
1510.9371	1517.3811	1521.6066
1527.4522	1531.3630	1544.5464
1554.5226	1582.2730	1670.8992
1672.2211	1681.4979	1691.7423
1694.6959	1700.9389	1703.0473
1709.4144	2399.4943	2869.3948
3035.8961	3055.1068	3062.5021
3069.1232	3089.5716	3091.6742
3107.5806	3111.1687	3125.1496
3137.2378	3152.2760	3156.0221
3159.4496	3167.9106	3173.6774
3193.1406	3203.1857	3208.1013
3209.2565	3216.8123	3220.0698
3223.5583	3231.2315	3232.5229
3237.8399	3238.7599	3247.6734

***Si*-M1**

Zero-point correction= 0.531313

Thermal correction to Energy= 0.562773

Thermal correction to Enthalpy= 0.563717

Thermal correction to Gibbs Free Energy= 0.467671

Sum of electronic and zero-point Energies= -1566.422965

Sum of electronic and thermal Energies= -1566.391504

Sum of electronic and thermal Enthalpies= -1566.390560

Sum of electronic and thermal Free Energies= -1566.486606

Cartesian coordinates

C	-0.318843	0.341236	-1.463960
C	1.159796	0.686187	-1.322686
C	1.684172	1.694175	-0.603789
O	-0.633954	-0.277770	-2.597344
C	3.133353	2.000687	-0.488704
C	3.564231	3.275716	-0.108192
C	4.087705	1.011318	-0.752750
C	4.922794	3.561493	-0.010263
H	2.832788	4.049517	0.107631

C	5.443789	1.300413	-0.657640
H	3.768832	0.005198	-1.006932
C	5.866834	2.576495	-0.287053
H	5.241752	4.556360	0.282553
H	6.172785	0.522739	-0.863735
H	6.926075	2.798030	-0.207603
C	0.791729	2.541470	0.152437
N	0.099163	3.229905	0.777342
H	1.818076	0.062216	-1.923609
H	-0.885561	1.280576	-1.244764
C	-0.755060	-0.624875	-0.327498
C	-2.099076	-2.057514	0.646141
C	-3.207090	-0.338857	-0.800223
H	-2.888747	-0.175969	-1.838150
N	-0.903565	-2.448010	0.977714
N	-0.077586	-1.538011	0.364834
N	-2.050963	-0.937952	-0.135185
C	-3.415674	-2.723848	0.916320
H	-3.497931	-2.993591	1.970121
H	-3.473323	-3.639869	0.311746
C	-4.406546	-1.310190	-0.707481
O	-4.470927	-1.842726	0.612020
C	-5.148645	0.895264	-0.234680
C	-3.754794	0.915755	-0.154474
C	-3.081250	1.975856	0.433797
C	-3.829492	3.044582	0.929601
C	-5.220577	3.040877	0.832196
C	-5.891522	1.962002	0.252811
C	-5.621753	-0.393806	-0.868302
H	-1.999726	1.980875	0.529795
H	-5.788699	3.878988	1.223151
H	-6.976033	1.951642	0.198960
H	-5.848365	-0.255776	-1.931169
H	-6.499284	-0.828164	-0.384030
C	1.346261	-1.728246	0.444514
C	1.954165	-2.492301	-0.552573
C	2.037675	-1.169377	1.521046
C	3.329910	-2.702181	-0.439490
C	3.407551	-1.408743	1.589085
C	4.065608	-2.176444	0.623961
H	3.835447	-3.287514	-1.203270
H	3.976921	-0.976258	2.408120
C	1.319187	-0.332733	2.543445
H	0.526082	-0.906395	3.032620

H	0.847988	0.538836	2.075542
H	2.012233	0.023984	3.306277
C	5.548414	-2.417082	0.733883
H	6.067896	-1.504924	1.039545
H	5.967308	-2.754529	-0.216361
H	5.760698	-3.183337	1.486290
C	1.145047	-3.037648	-1.698975
H	0.610244	-2.231375	-2.219908
H	0.394091	-3.746178	-1.332944
H	1.790088	-3.558789	-2.408117
H	-4.349690	-2.122478	-1.442463
H	-3.319643	3.880546	1.397349

Vibrational frequencies

18.0914	24.8176	28.2915
36.2257	45.1275	52.5781
61.8812	70.0869	81.2274
89.9329	99.3762	107.7258
114.4432	134.3997	147.5445
148.4065	153.3648	167.2135
192.5221	198.8824	208.1161
213.7465	239.2851	244.4250
249.8856	274.6070	281.2222
290.8520	306.3610	307.4484
326.1564	335.3622	352.6057
375.3831	392.4717	406.7412
420.3761	425.6776	440.3706
461.3603	482.8668	494.7534
501.6454	502.2419	514.4564
527.4541	546.1285	556.9503
574.2711	585.1925	588.9975
617.1717	627.0562	629.3184
643.8625	656.4590	676.2246
691.6208	703.7010	718.0337
728.8293	750.2121	758.9645
766.5842	774.5337	794.4183
801.2995	812.1247	840.1403
868.6506	879.2107	882.3682
884.7881	902.6002	912.4258
922.8830	940.9705	960.5200
962.8485	966.3880	977.3627
984.2245	988.8789	1011.1618
1018.7308	1020.1128	1022.4550
1031.9603	1037.6428	1041.1492
1044.9218	1053.6939	1057.1887

1064.3575	1066.9675	1074.4701
1075.4323	1078.3126	1082.1319
1116.8458	1118.5123	1127.5415
1128.9887	1175.2049	1181.1948
1181.4355	1191.0347	1200.0959
1213.6452	1216.0181	1219.7434
1238.2917	1253.7554	1270.4567
1279.3962	1280.1880	1285.5634
1302.9762	1318.6401	1320.9450
1323.9471	1329.3862	1339.9442
1343.2221	1353.0721	1363.4899
1369.4781	1373.6944	1379.4960
1383.2823	1392.3609	1408.8468
1416.4658	1423.3190	1438.5111
1464.9491	1467.4728	1472.8092
1483.0762	1488.2909	1491.6065
1493.2086	1498.3008	1502.1346
1512.5474	1518.1395	1520.9654
1526.7420	1535.7128	1546.2698
1553.8234	1588.0938	1670.7844
1676.7182	1683.8456	1687.6982
1694.8359	1697.4261	1706.5249
1710.0208	2396.5178	2850.2387
3038.2852	3065.2676	3066.0038
3070.3606	3084.8421	3100.3784
3105.1628	3117.9142	3133.3807
3140.5694	3147.5923	3162.7878
3167.3105	3169.3368	3176.3684
3194.9400	3198.9254	3200.7409
3203.0636	3208.5035	3214.0481
3215.0541	3219.6143	3224.5619
3226.2114	3230.8359	3234.6745

***Re*-TS1(L2)**

Zero-point correction= 0.524566

Thermal correction to Energy= 0.556273

Thermal correction to Enthalpy= 0.557217

Thermal correction to Gibbs Free Energy= 0.460476

Sum of electronic and zero-point Energies= -1567.141522

Sum of electronic and thermal Energies= -1567.109815

Sum of electronic and thermal Enthalpies= -1567.108871

Sum of electronic and thermal Free Energies= -1567.205612

Cartesian coordinates

C	0.303219	0.472397	1.832628

C	-1.174053	0.646296	1.608253
C	-1.763567	1.589125	0.840295
O	0.684357	-0.249035	2.797810
C	-3.229347	1.730855	0.647278
C	-3.739120	2.319056	-0.521545
C	-4.132616	1.252206	1.610722
C	-5.114402	2.406993	-0.731407
H	-3.056600	2.695340	-1.277100
C	-5.506364	1.341498	1.399016
H	-3.762127	0.825528	2.536781
C	-6.004237	1.917116	0.226330
H	-5.489357	2.857776	-1.645134
H	-6.189941	0.969821	2.156208
H	-7.075484	1.988980	0.065499
C	-0.923516	2.471103	0.076871
N	-0.265761	3.181718	-0.570253
H	-1.793444	-0.071603	2.135047
H	0.883474	1.373306	1.553587
C	0.818052	-0.548951	0.219890
C	2.172112	-2.130554	-0.567020
C	3.260979	-0.325955	0.793717
H	2.961455	-0.149331	1.833689
N	0.984166	-2.503855	-0.957593
N	0.159964	-1.500681	-0.452401
N	2.111246	-0.956404	0.143263
C	3.485228	-2.831530	-0.747087
H	3.575976	-3.221465	-1.762900
H	3.542942	-3.678280	-0.045327
C	4.496861	-1.266986	0.733928
O	4.553487	-1.920060	-0.540607
C	5.160946	0.957204	0.157095
C	3.762196	0.939609	0.130059
C	3.034284	1.986873	-0.423919
C	3.733489	3.076602	-0.953736
C	5.131711	3.106446	-0.920644
C	5.855763	2.044777	-0.365418
C	5.695018	-0.306589	0.795483
H	1.950749	1.960450	-0.463423
H	5.661768	3.957647	-1.337829
H	6.941861	2.064821	-0.354970
H	5.981795	-0.133987	1.840003
H	6.558568	-0.734844	0.279511
C	-1.263960	-1.601685	-0.602696
C	-1.973575	-2.334600	0.357562

C	-1.883076	-0.940171	-1.669864
C	-3.364429	-2.388269	0.225885
C	-3.274041	-1.029365	-1.761154
C	-4.029377	-1.740777	-0.821881
H	-3.940489	-2.944300	0.960918
H	-3.781098	-0.517460	-2.574458
C	-1.071836	-0.141016	-2.658318
H	-0.261226	-0.741281	-3.083686
H	-0.608703	0.725790	-2.174901
H	-1.699044	0.222508	-3.475165
C	-5.535253	-1.770338	-0.916925
H	-5.960097	-0.873244	-0.452936
H	-5.953617	-2.641228	-0.404639
H	-5.869148	-1.789612	-1.958695
C	-1.251273	-3.011722	1.496785
H	-0.679437	-2.289250	2.092148
H	-0.535908	-3.750475	1.119826
H	-1.956577	-3.522981	2.155838
H	4.486130	-2.014849	1.537224
H	3.182627	3.901647	-1.394966

Vibrational frequencies

-225.0420	18.7142	23.2595
35.1993	40.4452	43.3250
57.4590	62.1152	74.0125
76.6526	81.3431	85.6795
89.1795	98.3697	120.7299
127.6633	144.1214	145.7762
158.0376	182.6776	199.5696
205.0604	213.9317	225.4470
237.9866	245.0100	267.5117
285.7723	289.5143	298.0202
314.4937	326.5563	345.5760
360.8718	367.0686	387.3447
403.4258	414.5296	440.8264
457.8674	461.7662	479.5829
492.0172	496.3444	511.5751
516.6344	530.8157	541.5817
557.9444	580.2018	586.6536
590.6410	608.0085	629.2276
631.7008	639.5398	663.6755
673.9410	688.3572	706.3994
720.3546	722.0221	745.1956
753.2497	760.7184	778.2963
784.4204	804.1978	831.8104

848.0356	856.3286	869.5973
872.1766	889.8735	899.1307
909.4256	917.4395	936.3887
951.8459	959.9295	967.3303
972.8680	976.8665	979.1990
982.6242	1001.3497	1004.3723
1010.8141	1013.9429	1035.3666
1042.0117	1043.7207	1047.2734
1052.5476	1059.6571	1064.8868
1065.9743	1068.6439	1070.2922
1080.0058	1107.7208	1112.4105
1119.8365	1124.2834	1132.1810
1184.7804	1189.6681	1191.0422
1194.9206	1202.4186	1221.1371
1223.3220	1245.4109	1263.7702
1266.8505	1272.7589	1279.9341
1293.4980	1303.5899	1315.2536
1319.7721	1330.5186	1333.6475
1343.5790	1353.6216	1355.7906
1370.6088	1372.7751	1376.1358
1384.4104	1396.7270	1404.1064
1422.0273	1429.3795	1438.2212
1447.4307	1454.4490	1462.1524
1475.9322	1487.1835	1489.3304
1490.0850	1494.0216	1495.8132
1499.5197	1501.1671	1505.5831
1517.1556	1520.6563	1535.7965
1540.4320	1546.2620	1622.9961
1628.8727	1642.2524	1643.3207
1653.7765	1657.4102	1662.9335
1663.5824	2325.4050	2913.0604
3002.3579	3032.1041	3043.1979
3045.4113	3048.5288	3054.8189
3061.4608	3095.1770	3108.8248
3111.0095	3113.3984	3126.3261
3128.6788	3134.4754	3138.5736
3178.9031	3181.4602	3181.5091
3184.6739	3191.5890	3192.5913
3199.6954	3204.6926	3206.4003
3213.1956	3217.8755	3220.1386

***Si*-TS1(L2)**

Zero-point correction= 0.524297

Thermal correction to Energy= 0.556146

Thermal correction to Enthalpy= 0.557090
Thermal correction to Gibbs Free Energy= 0.459319
Sum of electronic and zero-point Energies= -1567.137172
Sum of electronic and thermal Energies= -1567.105323
Sum of electronic and thermal Enthalpies= -1567.104379
Sum of electronic and thermal Free Energies= -1567.202150
Cartesian coordinates

C	-0.655619	0.292191	1.909202
C	0.554108	1.122849	1.592536
C	0.583279	2.292314	0.915790
O	-0.572315	-0.552141	2.844504
C	1.836634	3.013210	0.571228
C	1.934198	3.726985	-0.634480
C	2.964453	2.935438	1.404645
C	3.138421	4.321746	-1.010556
H	1.069852	3.802863	-1.287289
C	4.165203	3.531592	1.026757
H	2.897951	2.417976	2.356184
C	4.259651	4.222245	-0.184483
H	3.198796	4.861744	-1.950516
H	5.027115	3.462518	1.683314
H	5.196483	4.686547	-0.476562
C	-0.639704	2.820974	0.376728
N	-1.607839	3.270121	-0.088775
H	1.489901	0.699965	1.945373
H	-1.609732	0.816885	1.710131
C	-0.785296	-0.795782	0.258931
C	-0.696317	-2.848803	-0.598451
C	1.348907	-2.084232	0.627577
H	1.304524	-1.749745	1.671295
N	-1.900591	-2.434389	-0.884139
N	-1.927015	-1.152313	-0.338856
N	0.007180	-1.885707	0.084562
C	-0.084520	-4.196374	-0.845743
H	-0.292353	-4.532428	-1.863704
H	-0.525727	-4.922873	-0.145665
C	1.738188	-3.585428	0.561862
O	1.326124	-4.133380	-0.696932
C	3.600347	-2.248955	-0.116256
C	2.478129	-1.412149	-0.128702
C	2.517567	-0.164348	-0.740627
C	3.719329	0.265736	-1.313131
C	4.850761	-0.555298	-1.280081
C	4.795742	-1.823566	-0.688935

C	3.274554	-3.562822	0.561554
H	1.636071	0.463591	-0.779169
H	5.778554	-0.211326	-1.727690
H	5.669921	-2.468461	-0.687237
H	3.647297	-3.584929	1.592871
H	3.674429	-4.438624	0.043518
C	-3.138009	-0.382032	-0.365515
C	-4.058930	-0.569188	0.675860
C	-3.343545	0.523476	-1.412764
C	-5.226817	0.197042	0.644418
C	-4.529208	1.263259	-1.400281
C	-5.476295	1.117843	-0.380685
H	-5.958046	0.071758	1.438827
H	-4.712389	1.973476	-2.202200
C	-2.308254	0.703186	-2.493549
H	-1.998706	-0.258281	-2.914819
H	-1.413981	1.188141	-2.088055
H	-2.692407	1.328480	-3.302445
C	-6.729138	1.960292	-0.367766
H	-6.567279	2.884679	0.199797
H	-7.562927	1.430917	0.102463
H	-7.029764	2.246980	-1.379467
C	-3.786555	-1.561418	1.780358
H	-2.860904	-1.322807	2.317967
H	-3.667376	-2.571420	1.373029
H	-4.609829	-1.577271	2.498041
H	1.301447	-4.164426	1.385576
H	3.768885	1.246384	-1.776349

Vibrational frequencies

-226.6613	21.5780	25.5933
27.7148	36.0768	38.9500
42.1139	49.4373	64.2904
70.1537	78.6815	84.3567
88.7205	114.4622	118.7297
124.4324	138.6960	151.0869
160.1089	184.7602	195.0673
198.7072	206.5703	227.9196
238.2930	246.1218	269.2890
285.4087	289.2406	294.3671
313.3636	327.9786	348.2891
360.1619	365.8668	389.1338
405.5376	415.5824	438.0674
443.7596	463.8357	478.6721
487.3810	494.2773	512.1063

517.5986	528.0940	545.4436
558.4264	579.6043	580.3178
586.9403	614.1597	630.7001
631.6329	639.4366	665.7336
672.8513	684.7451	705.5550
710.0286	721.2892	743.3199
751.3271	760.1901	776.5809
781.1061	804.7931	830.0564
850.0190	860.7756	870.0089
873.6123	889.8911	901.4654
908.4827	919.2228	940.2383
950.9733	960.2129	969.5910
973.8928	975.6005	981.6253
983.4532	998.6329	1006.3931
1010.4803	1013.5464	1034.1537
1042.2013	1043.6340	1045.1099
1051.2379	1059.9239	1062.4234
1065.3181	1066.6143	1070.5966
1079.1674	1105.2898	1114.4740
1118.4944	1126.0670	1136.7212
1183.3035	1189.3599	1189.7356
1195.2806	1202.8379	1221.5094
1222.1189	1243.8957	1260.1228
1267.4270	1272.7909	1279.0663
1293.1425	1301.3078	1312.9450
1322.7446	1330.2989	1331.8723
1344.8030	1352.2575	1356.6431
1369.8904	1373.1510	1376.4372
1379.1408	1398.0070	1403.6631
1420.7107	1423.6974	1438.3054
1447.8578	1453.1541	1458.9284
1474.8921	1487.0383	1489.7935
1490.8009	1493.4130	1497.6100
1498.2279	1500.9639	1503.3794
1515.2022	1518.7945	1536.0613
1539.1991	1549.3480	1620.6857
1629.6305	1641.7824	1642.7440
1654.0311	1657.6521	1662.5802
1664.0185	2329.4640	2924.9355
3005.3102	3036.4685	3039.5533
3044.4070	3048.9947	3054.7206
3059.9172	3097.1458	3101.6810
3111.6087	3114.5529	3127.3591
3128.2483	3134.4850	3137.9659

3176.4774	3179.8620	3181.8924
3184.9311	3190.9924	3193.7490
3198.3553	3201.4769	3205.6029
3206.4051	3213.9983	3230.6877

***Re*-M1(L2)**

Zero-point correction= 0.526249
Thermal correction to Energy= 0.557870
Thermal correction to Enthalpy= 0.558815
Thermal correction to Gibbs Free Energy= 0.462810
Sum of electronic and zero-point Energies= -1567.146862
Sum of electronic and thermal Energies= -1567.115241
Sum of electronic and thermal Enthalpies= -1567.114297
Sum of electronic and thermal Free Energies= -1567.210301
Cartesian coordinates

C	-0.292955	0.353448	-1.414119
C	1.191925	0.674852	-1.268458
C	1.746324	1.685461	-0.562246
O	-0.601808	-0.252569	-2.567631
C	3.202961	1.980175	-0.493978
C	3.659473	3.248328	-0.099563
C	4.151681	0.995100	-0.818579
C	5.024771	3.529787	-0.047328
H	2.944063	4.021779	0.163173
C	5.513799	1.281153	-0.771757
H	3.828966	-0.005598	-1.080228
C	5.958163	2.549367	-0.386185
H	5.356373	4.517896	0.256952
H	6.230661	0.507028	-1.028809
H	7.020948	2.767126	-0.344260
C	0.883553	2.529460	0.220166
N	0.205974	3.218140	0.871270
H	1.829615	0.043454	-1.877982
H	-0.845806	1.300416	-1.200518
C	-0.776019	-0.632169	-0.318408
C	-2.166557	-2.088837	0.580098
C	-3.228046	-0.289337	-0.812782
H	-2.892510	-0.107443	-1.841741
N	-0.980933	-2.521777	0.912793
N	-0.120602	-1.589652	0.347406
N	-2.087844	-0.931359	-0.150914
C	-3.496082	-2.746885	0.807736
H	-3.598715	-3.051848	1.851351
H	-3.552010	-3.647912	0.177697

C	-4.453050	-1.241776	-0.777928
O	-4.551458	-1.847180	0.519021
C	-5.157889	0.972580	-0.242290
C	-3.760900	0.963892	-0.147849
C	-3.072847	2.006171	0.463234
C	-3.806974	3.082735	0.972809
C	-5.201031	3.105888	0.865260
C	-5.886890	2.047105	0.258473
C	-5.652139	-0.292310	-0.910191
H	-1.993559	1.992107	0.564536
H	-5.758164	3.947400	1.266299
H	-6.971179	2.057823	0.193632
H	-5.878991	-0.123748	-1.969882
H	-6.540666	-0.723659	-0.441749
C	1.299260	-1.781384	0.463356
C	1.946110	-2.520037	-0.535267
C	1.961090	-1.238621	1.573129
C	3.326725	-2.704874	-0.397398
C	3.336569	-1.453079	1.664001
C	4.033909	-2.180010	0.689827
H	3.858524	-3.267914	-1.159459
H	3.879874	-1.034857	2.507010
C	1.209273	-0.436593	2.603827
H	0.357834	-0.999332	2.999496
H	0.810665	0.486653	2.168940
H	1.859977	-0.162053	3.436330
C	5.528973	-2.347159	0.802948
H	6.030744	-1.383744	0.655155
H	5.916010	-3.047018	0.058270
H	5.813454	-2.708987	1.796276
C	1.174808	-3.065143	-1.710910
H	0.632652	-2.262678	-2.229305
H	0.428585	-3.795254	-1.377125
H	1.843290	-3.560411	-2.418525
H	-4.403629	-2.015029	-1.554755
H	-3.284962	3.902598	1.456456

Vibrational frequencies

20.9094	24.0390	30.2353
38.6328	42.9907	58.9314
69.0489	72.6136	82.5554
93.5777	102.7006	105.8356
114.8675	123.2544	133.7666
147.8857	153.4977	159.5838
192.8363	196.9941	205.7854

215.5117	239.2587	243.6911
253.8443	266.4296	285.3963
287.0066	304.8760	309.7875
330.9464	334.2170	349.3290
373.8730	390.8855	402.4836
415.2609	420.0012	438.8392
460.1618	482.2584	491.4902
498.5736	505.8453	514.4123
532.2006	544.6757	557.0183
573.2051	580.2659	585.8740
612.1122	625.8079	632.3229
641.3656	652.0905	674.7514
681.8896	686.9068	709.8098
722.1491	740.2149	750.1645
757.1142	763.9232	785.9899
788.9055	802.0231	833.0117
854.8266	864.6295	871.0399
873.6283	891.5045	900.8035
909.3356	923.9287	942.5618
951.0788	960.0627	967.3803
974.0354	977.1403	987.1415
999.9460	1004.2807	1009.7463
1014.5614	1031.1218	1040.1997
1041.5422	1047.2553	1053.0515
1060.3152	1061.1461	1064.1194
1064.3070	1072.5485	1075.2559
1088.6753	1109.4491	1109.9922
1121.7667	1129.0787	1174.3352
1182.7848	1187.4733	1190.6031
1195.1442	1203.7923	1217.6423
1225.8093	1242.9293	1262.1111
1267.8611	1274.3766	1292.9623
1301.1983	1312.1033	1314.2574
1317.1615	1318.3540	1332.6812
1341.5059	1347.1683	1347.5604
1360.5153	1372.9479	1372.9835
1373.6506	1374.3041	1398.4388
1421.0663	1427.4206	1439.6948
1442.7539	1453.7760	1466.0350
1475.9830	1481.4238	1488.0013
1489.8668	1490.2592	1491.6652
1500.8724	1502.2422	1510.6750
1517.2030	1519.6681	1530.8176
1538.9986	1541.4380	1623.2622

1627.9096	1641.2332	1642.0560
1650.8497	1655.0247	1656.9642
1663.9151	2321.5941	2797.7800
3008.6704	3013.3707	3042.2588
3047.7325	3049.2817	3053.0933
3060.2601	3083.4293	3102.5810
3108.8436	3115.7618	3126.6672
3132.3613	3134.0489	3143.2002
3182.3281	3182.5552	3184.2044
3184.2444	3191.2418	3193.7592
3200.0972	3205.9784	3209.8253
3211.5717	3223.7189	3226.2107

***Si*-M1(L2)**

Zero-point correction= 0.526108

Thermal correction to Energy= 0.557878

Thermal correction to Enthalpy= 0.558823

Thermal correction to Gibbs Free Energy= 0.461764

Sum of electronic and zero-point Energies= -1567.142699

Sum of electronic and thermal Energies= -1567.110929

Sum of electronic and thermal Enthalpies= -1567.109985

Sum of electronic and thermal Free Energies= -1567.207043

Cartesian coordinates

C	-0.647695	0.168148	1.520146
C	0.543947	1.083092	1.273300
C	0.539669	2.315684	0.717657
O	-0.522344	-0.578528	2.623351
C	1.762363	3.132189	0.491284
C	1.810740	4.064427	-0.558426
C	2.908461	2.951483	1.284431
C	2.979502	4.778271	-0.822262
H	0.933763	4.223080	-1.178567
C	4.074579	3.664607	1.017488
H	2.884388	2.262683	2.122265
C	4.117712	4.578347	-0.039260
H	2.998886	5.489406	-1.642544
H	4.949299	3.512240	1.642385
H	5.027258	5.134699	-0.243851
C	-0.699154	2.849226	0.218197
N	-1.685763	3.300992	-0.204683
H	1.487117	0.673623	1.620023
H	-1.568627	0.790941	1.443915
C	-0.794898	-0.841224	0.347630
C	-0.610623	-2.770997	-0.703161

C	1.389527	-2.086571	0.640912
H	1.305824	-1.745938	1.681581
N	-1.829813	-2.376505	-0.955936
N	-1.921641	-1.159139	-0.298599
N	0.062849	-1.853933	0.064996
C	0.015073	-4.098013	-1.024320
H	-0.097943	-4.329964	-2.085658
H	-0.510979	-4.872487	-0.445219
C	1.725370	-3.597876	0.571898
O	1.402127	-4.091178	-0.736473
C	3.661650	-2.334807	0.003632
C	2.568991	-1.461653	-0.083393
C	2.681187	-0.239465	-0.737902
C	3.922568	0.128205	-1.269178
C	5.023025	-0.725628	-1.154511
C	4.895969	-1.969642	-0.524359
C	3.255729	-3.625448	0.683489
H	1.828244	0.419252	-0.846397
H	5.980904	-0.429210	-1.571427
H	5.744357	-2.645168	-0.462672
H	3.551839	-3.637018	1.739511
H	3.665354	-4.521232	0.209658
C	-3.158995	-0.426769	-0.293197
C	-4.042316	-0.637220	0.774798
C	-3.422061	0.454267	-1.349680
C	-5.236157	0.089910	0.764630
C	-4.631590	1.151015	-1.313857
C	-5.544370	0.986968	-0.264673
H	-5.940505	-0.049793	1.580296
H	-4.862981	1.842300	-2.119664
C	-2.426207	0.647994	-2.464677
H	-2.115679	-0.309580	-2.893799
H	-1.527559	1.152905	-2.094608
H	-2.849066	1.263167	-3.261660
C	-6.824334	1.786744	-0.235464
H	-6.640142	2.794914	0.154590
H	-7.577047	1.318026	0.404113
H	-7.246201	1.899975	-1.238679
C	-3.706839	-1.609098	1.879467
H	-2.753325	-1.355901	2.361203
H	-3.605325	-2.625086	1.480194
H	-4.493750	-1.619027	2.636754
H	1.203796	-4.180684	1.341305
H	4.025472	1.084618	-1.772346

Vibrational frequencies

21.9111	23.7438	32.0550
33.9295	39.2283	45.3568
45.5993	71.2890	74.6402
85.1709	99.4270	105.5452
115.0328	128.0824	139.9009
144.3103	155.6328	167.4602
190.9109	195.0882	201.9993
210.9876	230.5378	238.7362
243.4641	269.6360	280.9420
287.4214	293.7076	306.6688
334.0112	335.4138	355.9664
375.1324	377.7353	407.3225
414.8199	441.7304	452.0120
454.2010	472.8799	488.1566
497.6480	511.2476	519.2976
529.8062	531.5404	558.8662
579.1517	581.9473	585.2507
606.3517	631.5951	634.4998
638.3383	654.4813	669.0603
685.4935	701.8067	709.3013
723.9720	731.5522	748.3632
752.3714	761.6290	776.5770
787.4386	807.1733	837.6851
859.0681	862.0637	872.1596
875.6506	893.1813	902.0791
908.9289	931.0851	943.1358
955.3473	960.6058	970.2340
975.3294	977.0099	980.9658
999.0556	1001.7108	1005.8482
1013.1839	1028.3860	1042.2194
1042.6635	1046.1436	1055.3669
1058.9465	1061.3329	1062.8676
1064.5589	1071.5051	1072.6604
1085.0253	1107.8602	1114.4864
1121.2563	1131.0734	1179.9874
1181.9292	1186.5084	1192.9172
1194.7208	1204.6310	1218.7817
1222.0165	1242.3084	1261.8768
1268.0568	1278.0498	1293.0798
1295.2248	1312.3330	1314.3416
1318.9989	1327.2849	1336.5074
1340.8511	1344.3389	1347.8783
1361.5956	1369.6544	1373.9295

1374.3383	1384.2881	1398.8160
1421.4637	1425.5081	1439.4303
1441.0161	1452.8672	1466.0617
1476.0996	1481.6005	1487.2388
1490.6643	1493.6896	1494.9540
1499.0785	1500.4338	1506.9155
1512.7527	1519.3934	1524.1154
1537.4586	1538.5840	1619.4539
1626.7417	1641.3333	1642.0145
1649.1700	1655.9251	1656.4353
1663.1978	2327.1097	2835.5297
3008.6041	3017.5652	3038.5869
3040.4880	3049.7194	3050.2271
3060.5634	3082.9040	3102.3271
3112.7114	3117.7006	3124.6512
3129.0558	3132.8491	3140.5902
3180.0296	3182.7302	3183.4612
3184.5462	3191.2563	3194.1148
3199.1416	3205.4801	3206.4586
3210.4490	3214.4174	3229.5332

***Re*-TS1(L3)**

Zero-point correction= 0.530735

Thermal correction to Energy= 0.562122

Thermal correction to Enthalpy= 0.563066

Thermal correction to Gibbs Free Energy= 0.466472

Sum of electronic and zero-point Energies= -1566.566461

Sum of electronic and thermal Energies= -1566.535073

Sum of electronic and thermal Enthalpies= -1566.534129

Sum of electronic and thermal Free Energies= -1566.630724

Cartesian coordinates

C	0.323785	0.545865	1.929742
C	-1.153007	0.671367	1.696437
C	-1.751945	1.575230	0.903324
O	0.732084	-0.159793	2.873261
C	-3.215551	1.667210	0.674767
C	-3.710357	2.220399	-0.510182
C	-4.120149	1.166938	1.617243
C	-5.077931	2.253723	-0.757554
H	-3.020895	2.611149	-1.252549
C	-5.486108	1.198242	1.367048
H	-3.759514	0.763220	2.557520
C	-5.970472	1.739801	0.178455
H	-5.445598	2.680990	-1.684706

H	-6.176073	0.807875	2.107971
H	-7.038203	1.766547	-0.012924
C	-0.919451	2.465394	0.136867
N	-0.264430	3.176966	-0.504948
H	-1.758718	-0.051847	2.233637
H	0.901589	1.425796	1.593014
C	0.815990	-0.535447	0.241158
C	2.139578	-2.133250	-0.553712
C	3.258633	-0.352469	0.788161
H	2.987686	-0.166171	1.833726
N	0.950215	-2.479698	-0.946988
N	0.152146	-1.472520	-0.440393
N	2.097578	-0.968732	0.162336
C	3.440688	-2.850166	-0.736284
H	3.515591	-3.259727	-1.744117
H	3.498920	-3.680735	-0.017414
C	4.481100	-1.300189	0.707095
O	4.509147	-1.949188	-0.557862
C	5.153042	0.912132	0.122835
C	3.758610	0.905511	0.115154
C	3.033977	1.954552	-0.430261
C	3.732691	3.033716	-0.970984
C	5.127230	3.052173	-0.956985
C	5.848045	1.989367	-0.410592
C	5.684524	-0.353417	0.753728
H	1.948523	1.937702	-0.454449
H	5.657028	3.897792	-1.383948
H	6.933873	2.001188	-0.415191
H	5.982813	-0.180095	1.793631
H	6.537558	-0.787761	0.227633
C	-1.268668	-1.537023	-0.606675
C	-2.008818	-2.243290	0.344193
C	-1.855976	-0.859328	-1.674805
C	-3.394603	-2.252686	0.201658
C	-3.244478	-0.907224	-1.781037
C	-4.027392	-1.593448	-0.853650
H	-3.995310	-2.785384	0.934499
H	-3.727766	-0.377562	-2.597544
C	-1.016188	-0.079848	-2.650987
H	-0.213653	-0.697464	-3.064663
H	-0.544488	0.779587	-2.163302
H	-1.626455	0.291950	-3.476263
C	-5.525971	-1.637137	-0.998648
H	-5.899773	-0.731645	-1.482097

H	-6.014061	-1.726620	-0.024989
H	-5.831938	-2.496033	-1.606190
C	-1.322910	-2.945045	1.487265
H	-0.724325	-2.249107	2.086409
H	-0.640182	-3.716015	1.116609
H	-2.053950	-3.421735	2.143194
H	4.477283	-2.048307	1.509577
H	3.184128	3.862236	-1.406965

Vibrational frequencies

-211.0109	9.2837	24.9460
32.0874	36.9976	44.7138
57.0390	62.2626	71.6298
74.8970	79.0849	87.0383
116.0277	116.4600	121.4069
138.4853	148.6651	152.6624
156.0973	185.3029	200.4762
213.8077	219.9399	226.6712
245.9418	252.3025	268.7148
286.4371	294.7219	298.7325
314.6034	327.9308	344.6090
360.8464	366.1520	387.1127
408.2005	418.1049	441.1433
459.4286	461.0940	482.1884
494.5107	500.1316	516.0780
519.3073	536.4442	542.8229
561.1441	587.0360	589.2096
591.3961	618.0398	633.5266
636.2079	645.4382	669.2323
680.1368	698.4605	715.0601
723.8647	730.6888	754.8438
764.5401	768.8315	787.5859
794.6488	810.7247	844.0810
859.6467	877.8072	880.2538
881.8280	899.5736	906.2227
912.4034	920.0652	953.2807
964.2419	968.4293	981.8058
985.0866	989.5846	1004.2839
1006.9082	1023.0860	1023.6718
1027.6507	1027.9597	1044.7251
1050.0284	1050.8042	1062.1534
1067.5476	1071.3435	1074.0770
1075.2674	1077.3025	1083.7448
1086.9028	1114.6427	1121.4633
1133.0794	1138.4210	1168.9533

1186.8368	1194.2152	1198.7088
1207.7375	1221.7026	1230.6192
1239.1854	1261.4164	1281.9073
1285.2090	1290.2891	1298.0243
1308.2455	1313.2541	1327.1806
1328.7836	1341.1301	1345.5652
1355.7798	1361.1834	1374.2391
1381.7912	1382.1879	1393.2386
1395.7965	1422.8953	1428.2498
1429.1126	1435.1368	1452.6439
1465.0061	1472.6731	1477.8252
1494.2174	1495.0781	1498.7743
1500.4313	1501.5517	1505.6245
1506.9571	1516.1606	1518.0025
1529.9349	1535.0744	1558.1725
1571.0809	1626.5506	1664.2298
1667.7556	1675.2555	1682.9597
1693.7786	1695.4727	1697.4701
1720.3905	2372.0846	2971.9698
3036.3004	3063.5215	3063.9559
3072.2579	3073.3247	3088.8218
3091.4226	3134.1551	3139.5877
3144.6907	3155.3535	3167.8094
3169.8498	3170.8400	3173.6270
3203.1049	3211.4051	3212.8393
3214.6375	3218.3616	3225.1887
3227.6001	3229.3792	3236.4719
3242.7487	3244.3446	3244.7176

***Si*-TS1(L3)**

Zero-point correction= 0.530987

Thermal correction to Energy= 0.562222

Thermal correction to Enthalpy= 0.563166

Thermal correction to Gibbs Free Energy= 0.468139

Sum of electronic and zero-point Energies= -1566.561042

Sum of electronic and thermal Energies= -1566.529807

Sum of electronic and thermal Enthalpies= -1566.528863

Sum of electronic and thermal Free Energies= -1566.623890

Cartesian coordinates

C	-0.664465	0.253452	2.036200
C	0.512061	1.108477	1.676359
C	0.470958	2.280050	1.020149
O	-0.544013	-0.601818	2.933794
C	1.682310	3.030785	0.600600

C	1.687461	3.734160	-0.608462
C	2.854306	2.981019	1.362391
C	2.849203	4.352499	-1.059200
H	0.782008	3.786502	-1.206072
C	4.013385	3.599339	0.909586
H	2.857889	2.466124	2.317769
C	4.017043	4.282687	-0.304334
H	2.840304	4.886917	-2.003431
H	4.915746	3.552390	1.510234
H	4.923179	4.764496	-0.656297
C	-0.799589	2.790815	0.575623
N	-1.808163	3.224463	0.199973
H	1.476812	0.701501	1.967387
H	-1.643583	0.718990	1.820114
C	-0.746584	-0.848238	0.289188
C	-0.592506	-2.882287	-0.592473
C	1.415795	-2.071308	0.638124
H	1.378452	-1.760706	1.689103
N	-1.796086	-2.493506	-0.894144
N	-1.860511	-1.230927	-0.336320
N	0.069714	-1.915785	0.113599
C	0.064321	-4.204127	-0.846246
H	-0.146347	-4.549567	-1.858876
H	-0.333190	-4.943650	-0.135654
C	1.867791	-3.546933	0.534188
O	1.463225	-4.081652	-0.719887
C	3.656405	-2.118811	-0.134707
C	2.501950	-1.336094	-0.116673
C	2.473577	-0.081852	-0.706901
C	3.642358	0.410993	-1.286345
C	4.807175	-0.355114	-1.281654
C	4.819819	-1.630768	-0.714260
C	3.397338	-3.456427	0.519433
H	1.561869	0.504953	-0.723527
H	5.710772	0.039301	-1.735540
H	5.723194	-2.232885	-0.736110
H	3.782480	-3.478917	1.544979
H	3.830230	-4.302184	-0.019529
C	-3.072400	-0.471881	-0.396460
C	-4.026610	-0.673130	0.603942
C	-3.236646	0.453615	-1.428049
C	-5.190435	0.090968	0.543610
C	-4.418424	1.190375	-1.448648
C	-5.400784	1.025681	-0.471232

H	-5.949484	-0.045337	1.309590
H	-4.570319	1.918942	-2.240703
C	-2.161040	0.654983	-2.461125
H	-1.876078	-0.291570	-2.929516
H	-1.261615	1.077513	-2.001245
H	-2.496152	1.341198	-3.240938
C	-6.650348	1.867838	-0.495117
H	-6.477178	2.825754	0.006833
H	-7.477707	1.370318	0.016922
H	-6.961024	2.086351	-1.520090
C	-3.791289	-1.676715	1.702720
H	-2.880655	-1.445509	2.267461
H	-3.667847	-2.682620	1.289146
H	-4.632319	-1.692193	2.398482
H	1.469281	-4.161478	1.351034
H	3.640092	1.399083	-1.735894

Vibrational frequencies

-213.4914	21.5930	34.3092
35.2376	43.1025	46.1818
50.5153	69.1075	71.5487
73.1911	84.3221	91.6164
117.5122	124.4487	127.4633
138.9778	152.2541	157.2483
163.2488	188.5231	200.3388
204.4067	212.6855	230.9409
243.8095	253.2635	273.5022
287.8748	293.4148	296.1750
313.6213	331.3960	349.7103
359.9068	368.6021	388.1332
411.1536	418.7803	437.4130
447.9174	465.8536	483.6012
492.8777	500.3210	516.7413
523.3466	535.6802	543.5816
562.7172	581.2789	586.9412
594.0665	620.1743	635.0663
636.9300	648.2202	673.2764
680.7989	693.6280	712.9957
719.4760	731.1124	754.9712
763.2620	775.8034	786.4439
799.2222	811.4480	844.0591
864.9210	876.0413	885.2728
892.7673	903.2072	918.6929
924.0832	927.4174	957.6290
965.9344	969.7496	982.1141

986.3466	993.7051	1006.2470
1007.4011	1023.7321	1026.3640
1030.1335	1036.1469	1045.6504
1048.6418	1049.9008	1061.5246
1069.5612	1069.8763	1074.9687
1077.3409	1079.8827	1083.7868
1089.3173	1106.2242	1117.3286
1124.7188	1145.3430	1168.0208
1186.3820	1193.4618	1193.7113
1207.3391	1219.1269	1219.2321
1238.7939	1258.9923	1272.7932
1281.0804	1291.8208	1298.2408
1307.9935	1313.3057	1319.0648
1325.6515	1339.7446	1347.6409
1355.1195	1361.2339	1367.5870
1370.1316	1379.9939	1394.2253
1414.6111	1418.1083	1428.4037
1433.2399	1434.3207	1446.6981
1471.3842	1473.5773	1476.4660
1495.7984	1498.6232	1499.3378
1501.0145	1502.7556	1504.4865
1507.2322	1514.8199	1517.5208
1527.6756	1534.8064	1550.8044
1571.4582	1633.9810	1662.6981
1666.3133	1675.2195	1683.4574
1690.1965	1696.3374	1698.3622
1722.8992	2376.6296	2975.2569
3037.2771	3059.9475	3066.0228
3072.2974	3078.1137	3090.5052
3093.8087	3130.7604	3140.5251
3145.0737	3155.5186	3160.1307
3168.9552	3171.7611	3173.3331
3197.6339	3204.4852	3210.8925
3214.1210	3219.9257	3226.6123
3228.2744	3232.3895	3237.6231
3239.1291	3248.2374	3248.6574

***Re*-M1(L3)**

Zero-point correction= 0.532575

Thermal correction to Energy= 0.563842

Thermal correction to Enthalpy= 0.564786

Thermal correction to Gibbs Free Energy= 0.469565

Sum of electronic and zero-point Energies= -1566.574924

Sum of electronic and thermal Energies= -1566.543657

Sum of electronic and thermal Enthalpies= -1566.542713

Sum of electronic and thermal Free Energies= -1566.637935

Cartesian coordinates

C	-0.304136	0.345251	-1.432008
C	1.180127	0.672670	-1.300492
C	1.735875	1.647498	-0.560555
O	-0.624950	-0.257960	-2.574172
C	3.190581	1.948520	-0.493322
C	3.638608	3.198249	-0.053514
C	4.136476	0.987189	-0.867651
C	4.998947	3.486058	-0.002765
H	2.920277	3.954116	0.249641
C	5.493922	1.279600	-0.824200
H	3.816291	-0.004341	-1.168470
C	5.931796	2.529808	-0.391317
H	5.327764	4.461549	0.340454
H	6.213219	0.523670	-1.122992
H	6.992985	2.752357	-0.350466
C	0.873945	2.457487	0.261065
N	0.192665	3.110362	0.937739
H	1.813975	0.068571	-1.942981
H	-0.854858	1.292711	-1.211404
C	-0.768580	-0.630059	-0.323101
C	-2.143579	-2.056887	0.613967
C	-3.212600	-0.301636	-0.806910
H	-2.880754	-0.129068	-1.838468
N	-0.958759	-2.477831	0.945216
N	-0.111360	-1.567344	0.356014
N	-2.072314	-0.921892	-0.140745
C	-3.468211	-2.713415	0.857801
H	-3.569639	-2.990295	1.907891
H	-3.518388	-3.628278	0.249983
C	-4.423072	-1.262335	-0.754569
O	-4.517839	-1.831065	0.546974
C	-5.150322	0.946299	-0.264753
C	-3.758620	0.952283	-0.160230
C	-3.087927	2.004170	0.444721
C	-3.834999	3.074817	0.936372
C	-5.223819	3.083505	0.816974
C	-5.892403	2.015464	0.216874
C	-5.625706	-0.330371	-0.917560
H	-2.008441	2.004379	0.556489
H	-5.791340	3.923318	1.204926
H	-6.975595	2.015568	0.141807

H	-5.837241	-0.177819	-1.981580
H	-6.515748	-0.760428	-0.453249
C	1.306833	-1.752840	0.465903
C	1.952672	-2.477600	-0.536303
C	1.965459	-1.209298	1.571071
C	3.331362	-2.651251	-0.404871
C	3.339008	-1.409906	1.655196
C	4.035635	-2.124854	0.677678
H	3.865073	-3.206514	-1.171413
H	3.881911	-0.989624	2.497350
C	1.211919	-0.427767	2.612226
H	0.417140	-1.032133	3.059559
H	0.739853	0.458632	2.176079
H	1.882154	-0.095530	3.406445
C	5.529523	-2.280620	0.783319
H	6.020133	-1.310102	0.653138
H	5.917081	-2.962494	0.023301
H	5.817577	-2.661987	1.767106
C	1.184956	-3.024677	-1.709921
H	0.630730	-2.226977	-2.223200
H	0.453954	-3.769518	-1.377954
H	1.859913	-3.503961	-2.421436
H	-4.362771	-2.053071	-1.512060
H	-3.326589	3.904304	1.416779

Vibrational frequencies

17.8354	24.8249	28.7258
40.8370	44.1808	62.6119
76.2494	82.6337	84.5253
94.3878	106.8060	114.8596
120.0667	120.5921	134.1140
141.9938	153.5889	165.4023
194.0708	199.2726	208.5604
213.5947	239.4615	245.1305
252.6239	274.0804	286.8272
289.1410	308.0729	312.2814
335.3058	337.2878	353.5372
377.9742	395.9854	408.1075
419.3106	425.7468	442.5942
464.9827	487.5119	498.0702
504.6553	508.0066	517.1712
535.8177	550.9339	560.9682
580.4153	586.2626	591.9173
620.2190	631.2480	638.3477
648.6644	660.5911	681.9366

695.3012 700.7970 714.9807
733.2651 751.1246 764.5124
769.8553 776.3642 793.3850
801.9092 813.3923 843.7518
870.1543 872.3341 884.2297
886.8718 905.2337 916.5591
925.2326 945.9163 960.4377
965.7170 969.0744 979.1494
987.2377 991.2030 1003.9513
1021.3173 1024.0417 1025.1631
1025.7198 1042.2246 1047.3563
1049.4419 1058.0485 1064.5093
1067.5304 1072.6963 1074.2100
1078.9853 1082.1873 1092.1400
1116.6647 1121.4941 1130.2218
1132.2767 1176.8103 1187.4704
1195.1545 1196.6775 1205.7528
1219.4266 1222.0929 1230.1321
1237.7275 1261.3416 1281.1978
1287.7540 1290.5552 1294.4265
1307.9733 1323.3979 1328.0468
1330.8691 1335.1320 1343.6036
1348.6443 1357.6629 1364.2241
1378.1226 1381.1722 1383.7889
1392.6443 1395.0778 1421.7823
1428.5902 1433.3818 1447.2697
1469.0851 1474.6228 1486.6773
1489.2398 1492.2245 1494.9182
1496.2139 1503.2116 1504.4494
1516.9476 1517.4999 1520.8107
1532.2177 1535.5443 1549.4555
1557.8450 1586.3120 1665.5955
1668.7270 1676.9734 1680.6737
1690.8264 1692.0250 1698.1284
1708.6380 2367.7194 2815.5708
3022.2621 3041.8098 3066.3524
3074.3863 3077.2402 3082.2424
3094.0451 3113.2611 3140.9104
3145.4463 3159.5494 3166.5262
3166.7460 3167.0048 3178.5312
3210.4488 3216.8023 3217.0968
3218.1083 3222.7098 3223.6136
3225.5013 3233.2686 3240.0033
3242.6753 3247.4380 3250.2576

***Si*-M1(L3)**

Zero-point correction= 0.533078

Thermal correction to Energy= 0.564156

Thermal correction to Enthalpy= 0.565100

Thermal correction to Gibbs Free Energy= 0.471040

Sum of electronic and zero-point Energies= -1566.569716

Sum of electronic and thermal Energies= -1566.538638

Sum of electronic and thermal Enthalpies= -1566.537694

Sum of electronic and thermal Free Energies= -1566.631754

Cartesian coordinates

C	-0.687337	0.092661	1.607075
C	0.467998	1.055504	1.373893
C	0.424539	2.265434	0.791241
O	-0.544153	-0.679834	2.677821
C	1.641054	3.075373	0.513483
C	1.756232	3.775454	-0.691756
C	2.714859	3.080561	1.408924
C	2.933290	4.447011	-1.006098
H	0.927391	3.782943	-1.393749
C	3.889257	3.754069	1.093052
H	2.625539	2.566020	2.360410
C	4.004795	4.434426	-0.116895
H	3.013221	4.977578	-1.949204
H	4.713529	3.752221	1.798641
H	4.922902	4.958469	-0.361359
C	-0.827001	2.779097	0.298889
N	-1.819241	3.223208	-0.107823
H	1.431325	0.688887	1.720518
H	-1.629777	0.685673	1.538690
C	-0.785899	-0.877746	0.397019
C	-0.522734	-2.741639	-0.726142
C	1.431818	-2.047701	0.655838
H	1.340991	-1.751748	1.709250
N	-1.742302	-2.371039	-0.987517
N	-1.881868	-1.198473	-0.284546
N	0.103785	-1.844853	0.091942
C	0.152776	-4.030096	-1.088556
H	0.046806	-4.229078	-2.155744
H	-0.340609	-4.841458	-0.534331
C	1.826216	-3.534646	0.521335
O	1.528018	-3.974634	-0.799696
C	3.703351	-2.178298	0.006993
C	2.578938	-1.352238	-0.050541

C	2.634895	-0.116309	-0.676705
C	3.853117	0.318182	-1.199296
C	4.986415	-0.487375	-1.109176
C	4.914979	-1.748878	-0.515104
C	3.351175	-3.503424	0.643157
H	1.753152	0.506107	-0.772662
H	5.927999	-0.139084	-1.521389
H	5.790683	-2.389714	-0.477824
H	3.640529	-3.533294	1.699498
H	3.801097	-4.364189	0.143894
C	-3.119580	-0.475240	-0.303959
C	-4.034702	-0.705020	0.725850
C	-3.340045	0.428968	-1.343743
C	-5.221008	0.024955	0.691942
C	-4.543329	1.128639	-1.334807
C	-5.488182	0.944370	-0.324029
H	-5.953681	-0.127622	1.479917
H	-4.742460	1.843706	-2.128183
C	-2.306869	0.636269	-2.417952
H	-2.083203	-0.300124	-2.937589
H	-1.371147	1.010111	-1.989725
H	-2.653015	1.365862	-3.151659
C	-6.760562	1.751246	-0.314073
H	-6.596723	2.716357	0.176978
H	-7.556750	1.234952	0.227738
H	-7.109736	1.954497	-1.329576
C	-3.737344	-1.698592	1.818156
H	-2.790886	-1.467859	2.323982
H	-3.647023	-2.708197	1.402996
H	-4.538716	-1.705920	2.559080
H	1.327085	-4.172707	1.260375
H	3.911256	1.291354	-1.676459

Vibrational frequencies

24.4090	30.3374	37.9279
41.5444	47.4551	53.4550
75.3743	81.2853	89.9555
101.6071	104.3370	106.9815
124.2169	140.7282	148.9513
155.8695	162.9758	171.0986
196.2192	202.2644	208.1684
220.5306	235.1933	247.9323
250.4670	275.3931	280.7088
289.4148	294.8878	310.2236
336.8807	337.7268	363.4722

377.1582	380.9006	413.2109
420.6773	447.6368	453.2826
458.1928	476.0002	493.2407
503.5890	515.0520	524.0125
538.4443	541.3177	564.0739
586.4727	589.4943	591.7399
613.3065	634.8751	642.4285
645.6517	664.5403	678.8311
698.0509	713.6155	724.3547
734.4430	747.9007	763.1550
764.8879	774.6337	785.4647
803.8816	822.0135	846.9451
879.1349	882.6058	887.3156
891.0053	907.2953	921.3581
924.7571	953.2705	965.8800
969.5373	971.1432	983.5091
988.2912	993.7224	1010.2416
1018.7026	1023.5081	1027.7215
1035.2933	1043.2413	1044.2054
1054.3988	1061.0296	1067.5153
1070.4419	1074.1910	1075.9793
1079.0360	1080.4832	1093.2016
1102.2752	1119.6077	1124.8755
1138.9031	1175.8770	1188.6231
1193.2210	1193.7639	1206.8938
1216.1193	1222.5561	1232.3604
1239.7937	1257.6613	1274.5284
1287.9895	1294.2087	1297.5383
1306.8164	1321.5019	1324.5725
1331.3198	1335.6293	1347.5536
1348.8326	1360.7681	1364.0309
1372.3994	1380.8838	1384.9502
1388.7997	1409.6345	1415.2964
1429.4939	1434.4419	1449.5999
1470.8735	1476.5741	1481.4458
1491.3611	1496.7083	1501.5134
1501.8803	1503.1754	1507.1483
1516.3476	1520.9774	1522.6751
1529.8048	1534.1973	1547.4653
1553.6407	1580.0829	1661.5031
1664.0996	1675.6554	1682.8631
1690.9069	1693.5898	1698.2479
1707.3763	2373.6046	2846.2128
3041.7135	3042.5224	3067.1612

3070.4882	3071.5906	3081.4397
3092.6106	3118.6303	3141.7646
3143.0555	3157.9078	3163.7240
3165.7807	3171.1365	3174.0207
3205.0841	3210.9419	3212.4762
3218.3540	3219.2362	3222.5799
3224.0434	3230.4241	3234.8799
3238.7847	3248.7409	3262.5244

DMAP

Zero-point correction= 0.163817

Thermal correction to Energy= 0.172277

Thermal correction to Enthalpy= 0.173222

Thermal correction to Gibbs Free Energy= 0.130351

Sum of electronic and zero-point Energies= -381.936949

Sum of electronic and thermal Energies= -381.928489

Sum of electronic and thermal Enthalpies= -381.927545

Sum of electronic and thermal Free Energies= -381.970416

Cartesian coordinates

C	-1.947173	1.130360	0.000984
C	-0.563594	1.197377	0.002408
C	0.185377	-0.000547	0.000705
C	-0.564188	-1.198047	-0.000257
C	-1.947781	-1.130292	-0.001594
H	-2.516968	2.057890	0.002306
H	-0.081755	2.166582	0.006016
H	-0.082865	-2.167475	0.000866
H	-2.518052	-2.057529	-0.002704
C	2.270166	-1.258434	0.001480
C	2.268237	1.259200	-0.003118
H	2.034365	-1.855827	-0.887164
H	3.339815	-1.055107	0.001611
H	2.034553	-1.856591	0.889467
H	2.024423	1.856283	-0.889637
H	2.038718	1.857249	0.886867
H	3.338120	1.057632	-0.011745
N	1.548094	-0.000313	0.001505
N	-2.664752	0.000198	-0.001437

Vibrational frequencies

64.8189	97.3021	162.9976
227.9481	253.5068	290.1659
389.4165	417.2946	483.8453
546.5316	552.2094	679.9548
755.9872	777.7993	825.3240

841.6084	987.6619	991.4435
1010.0720	1018.4285	1096.2050
1105.6347	1147.2974	1151.6009
1154.9546	1214.1802	1263.1216
1283.9650	1354.9524	1390.3959
1429.5477	1455.4090	1490.3367
1492.8976	1496.7522	1500.8707
1525.2426	1539.8105	1583.9355
1631.5437	1691.3599	3048.5524
3056.6967	3109.2493	3110.3954
3178.2142	3180.9779	3184.3857
3190.3278	3236.9914	3237.2895

DMAP·H$^+$

Zero-point correction= 0.178411

Thermal correction to Energy= 0.186881

Thermal correction to Enthalpy= 0.187825

Thermal correction to Gibbs Free Energy= 0.145361

Sum of electronic and zero-point Energies= -382.377724

Sum of electronic and thermal Energies= -382.369253

Sum of electronic and thermal Enthalpies= -382.368309

Sum of electronic and thermal Free Energies= -382.410773

Cartesian coordinates

C	1.877312	1.178441	-0.004259
C	0.513869	1.215971	-0.005146
C	-0.235607	-0.000296	-0.001575
C	0.513611	-1.216477	0.003771
C	1.876946	-1.178731	0.004822
H	2.485154	2.073427	-0.008421
H	0.026881	2.180262	-0.009046
H	0.026725	-2.180815	0.010174
H	2.484631	-2.073828	0.007673
C	-2.304794	-1.262581	-0.007471
C	-2.303331	1.263394	0.008469
H	-2.085458	-1.843887	0.892742
H	-3.370148	-1.048326	-0.031174
H	-2.049825	-1.854591	-0.890586
H	-2.041637	1.856003	0.889527
H	-2.089127	1.843786	-0.893393
H	-3.368775	1.050345	0.039795
N	-1.569438	0.000038	-0.000869
N	2.540897	-0.000445	0.001231
H	3.553336	0.002145	-0.001487

Vibrational frequencies

94.8310	129.2605	163.2601
211.5568	250.2239	310.8687
391.8906	438.5057	491.2751
516.3025	553.0898	652.5468
716.5048	730.9503	777.9566
832.0660	846.3925	976.7692
1011.1573	1012.1409	1016.1971
1076.7458	1096.1133	1141.7134
1142.2713	1160.6309	1217.2612
1236.2263	1267.4594	1294.2382
1376.0192	1454.5058	1456.1778
1464.8798	1489.4083	1499.1479
1510.2900	1510.5072	1534.5090
1596.8232	1636.2488	1650.0071
1732.2008	3078.4827	3084.3764
3153.2021	3154.3863	3203.2934
3217.0807	3264.3790	3264.9974
3294.7588	3295.7542	3635.3517

***Re*-TS2**

Zero-point correction= 0.706048

Thermal correction to Energy= 0.747397

Thermal correction to Enthalpy= 0.748341

Thermal correction to Gibbs Free Energy= 0.630656

Sum of electronic and zero-point Energies= -1948.815891

Sum of electronic and thermal Energies= -1948.774543

Sum of electronic and thermal Enthalpies= -1948.773599

Sum of electronic and thermal Free Energies= -1948.891283

Cartesian coordinates

C	-0.207809	-0.201627	-1.186903
C	-0.636944	1.154493	-0.841167
C	-0.442653	1.796925	0.337126
O	-0.521068	-0.443515	-2.565462
C	-0.932735	3.162601	0.644901
C	-1.250041	3.510343	1.963255
C	-1.114228	4.113051	-0.367263
C	-1.751950	4.773876	2.261196
H	-1.108385	2.784050	2.759239
C	-1.618070	5.372915	-0.066875
H	-0.843704	3.874541	-1.391289
C	-1.941914	5.708541	1.247071
H	-1.995625	5.025144	3.288387
H	-1.749735	6.100186	-0.861349
H	-2.332749	6.694045	1.477430

C	0.204650	1.079941	1.397245
N	0.755013	0.512619	2.247709
H	-1.091417	1.712723	-1.659589
H	1.276835	-0.020573	-0.895811
C	-0.869663	-1.311871	-0.436513
C	-2.342992	-2.870550	0.042104
C	-3.261831	-0.925864	-1.209237
H	-2.814376	-0.462414	-2.095190
N	-1.213461	-3.315108	0.515236
N	-0.312255	-2.340485	0.210080
N	-2.182039	-1.640168	-0.523577
C	-3.646555	-3.606266	-0.075631
H	-3.929505	-4.036709	0.886126
H	-3.507635	-4.421722	-0.799266
C	-4.358065	-1.938280	-1.612659
O	-4.675256	-2.735251	-0.477578
C	-5.381701	0.046824	-0.833427
C	-4.056761	0.072289	-0.386968
C	-3.663049	0.918285	0.637915
C	-4.606553	1.791930	1.182529
C	-5.917272	1.801568	0.709702
C	-6.318051	0.917844	-0.294741
C	-5.571688	-1.043301	-1.865856
H	-2.652613	0.895502	1.027378
H	-6.639492	2.486891	1.141254
H	-7.349250	0.899511	-0.634070
H	-5.538606	-0.646871	-2.886669
H	-6.501037	-1.603544	-1.743656
C	1.063977	-2.541177	0.582517
C	2.017703	-2.786910	-0.411565
C	1.361471	-2.578504	1.950270
C	3.328727	-3.015330	0.003955
C	2.691147	-2.800446	2.307762
C	3.686868	-3.010773	1.352232
H	4.089874	-3.198801	-0.750765
H	2.950055	-2.816467	3.363076
C	0.295896	-2.441465	3.004343
H	-0.183221	-3.409587	3.179153
H	-0.477343	-1.729593	2.711197
H	0.737245	-2.096297	3.940238
C	5.123311	-3.212589	1.754968
H	5.218219	-3.360840	2.832038
H	5.721303	-2.338099	1.477958
H	5.555308	-4.077728	1.245551

C	1.695374	-2.806533	-1.882495
H	2.019980	-1.868052	-2.349240
H	0.631347	-2.953194	-2.079952
H	2.242934	-3.612990	-2.373984
H	-4.064125	-2.568375	-2.460963
H	-4.310636	2.464656	1.981291
C	3.243445	0.202080	0.212897
C	4.525628	0.694402	0.225930
C	5.004234	1.450326	-0.878282
C	4.092510	1.660853	-1.950199
C	2.831063	1.127128	-1.874864
H	2.839404	-0.359437	1.050099
H	5.145586	0.503062	1.090966
H	4.367838	2.234169	-2.824216
H	2.103427	1.269873	-2.669912
C	6.703232	2.734920	-2.046334
C	7.160448	1.701744	0.208354
H	6.079287	3.624655	-2.178308
H	7.727257	3.057421	-1.870987
H	6.679180	2.145200	-2.968445
H	6.770481	2.131883	1.136581
H	7.319595	0.628508	0.356343
H	8.120672	2.164233	-0.009008
N	6.254908	1.946545	-0.906211
N	2.411196	0.405126	-0.821824
H	0.235705	-0.872882	-2.978980

Vibrational frequencies

-908.1066	11.7879	17.9574
23.8048	31.8677	38.6931
44.5559	51.6893	54.1134
60.6506	66.0775	72.1799
84.1878	87.6482	92.9541
96.3617	110.5502	114.2340
116.5191	121.4064	130.2789
142.6629	150.1770	160.9770
170.5466	178.9615	189.0515
198.1286	199.0826	206.0623
214.4081	221.6551	225.9428
245.5974	246.5782	267.2326
268.7750	281.1960	286.3211
288.3965	295.1787	301.3154
321.0504	327.6363	339.7865
342.5788	365.3271	382.2226
392.4917	412.4101	415.3638

416.9393	440.7721	444.2791
459.4080	478.9016	484.6952
491.1702	497.1711	503.9412
507.9972	523.8007	529.2502
545.0705	548.0301	557.8999
576.3727	581.2184	589.9589
592.7874	622.6124	626.3898
640.8427	655.5629	663.6545
668.9475	679.7820	710.2215
714.9943	726.8183	730.7434
743.9348	749.8093	757.3893
769.0711	782.5657	795.0745
797.2987	816.1734	830.0226
841.1192	844.6246	856.5677
876.4754	878.7264	882.6478
891.1405	903.7453	923.7083
926.5079	946.0852	956.9667
958.4437	970.0319	977.0970
983.4387	984.1245	985.8971
996.1202	1008.0607	1011.6533
1016.2086	1019.6670	1022.7684
1030.4693	1039.1883	1041.2881
1049.6251	1050.3213	1059.1773
1063.5832	1063.9962	1066.7226
1068.7265	1071.2414	1074.9546
1077.4550	1090.8122	1092.2951
1113.7952	1126.1498	1133.5880
1139.0239	1146.4360	1149.0174
1170.5776	1177.7051	1181.3253
1183.3993	1186.4322	1193.4474
1212.1349	1213.3733	1217.2622
1220.5802	1241.2093	1256.0925
1257.8955	1266.1412	1279.0678
1281.7241	1289.1086	1291.0112
1305.7642	1310.2292	1318.1368
1326.6855	1334.0781	1344.5394
1346.6262	1359.6647	1361.7063
1366.1400	1370.3080	1377.9475
1381.3148	1386.4281	1389.4742
1406.4531	1413.8211	1419.9648
1425.8750	1429.6404	1448.0634
1449.4164	1452.9265	1467.0414
1468.6776	1480.6601	1490.1574
1491.5080	1493.5008	1493.6323

1496.6941	1500.7197	1501.4856
1502.6542	1504.1234	1505.0182
1515.7611	1519.3131	1521.4058
1523.7309	1533.8821	1537.3414
1539.4920	1555.1083	1576.9729
1598.8088	1616.8802	1662.0201
1667.6418	1683.6372	1683.8622
1693.1436	1693.7469	1696.4527
1699.0866	1708.1062	1717.8516
2385.0506	3062.6102	3063.5145
3063.9990	3069.0678	3073.2913
3082.7266	3085.3242	3102.3443
3119.9728	3131.2505	3134.7100
3142.6891	3143.4225	3150.5016
3159.7711	3170.3751	3172.0381
3174.8419	3181.7690	3187.4928
3194.0068	3202.9278	3203.3684
3207.7325	3208.1510	3212.5670
3214.9398	3216.3228	3220.5074
3220.9096	3233.3179	3237.2100
3239.7048	3242.7291	3252.0300
3262.1995	3288.0462	3896.1782

***Si*-TS2**

Zero-point correction= 0.705989

Thermal correction to Energy= 0.746981

Thermal correction to Enthalpy= 0.747925

Thermal correction to Gibbs Free Energy= 0.632745

Sum of electronic and zero-point Energies= -1948.822870

Sum of electronic and thermal Energies= -1948.781878

Sum of electronic and thermal Enthalpies= -1948.780934

Sum of electronic and thermal Free Energies= -1948.896114

Cartesian coordinates

H	-0.592990	0.748351	-0.989045
C	-2.676636	1.236441	-1.672783
C	-3.892130	1.812159	-1.408245
C	-3.987581	2.806033	-0.397193
C	-2.766545	3.212210	0.206538
C	-1.599585	2.569920	-0.122780
H	-2.591510	0.454695	-2.420977
H	-4.760365	1.474344	-1.956648
H	-2.737191	3.990612	0.956627
H	-0.669497	2.819137	0.376593
C	-5.229032	4.292683	1.062345

C	-6.403077	2.812914	-0.609250
H	-4.664821	5.196048	0.812544
H	-6.266658	4.572392	1.230898
H	-4.826427	3.867943	1.988614
H	-6.437865	3.006947	-1.685781
H	-6.496512	1.734550	-0.438863
H	-7.249126	3.313626	-0.143581
N	-5.170709	3.323032	-0.023253
N	-1.540140	1.581232	-1.035815
C	0.445742	-0.226027	-1.273669
C	1.663068	0.599614	-1.282710
C	2.166760	1.304570	-0.241746
O	0.041098	-0.603532	-2.597364
C	3.408645	2.109961	-0.261389
C	3.691245	2.992351	0.787771
C	4.324904	2.005957	-1.317246
C	4.844800	3.770723	0.770551
H	3.001647	3.075262	1.623091
C	5.470427	2.792525	-1.337734
H	4.161060	1.289293	-2.115531
C	5.735352	3.681007	-0.295828
H	5.043934	4.450823	1.592202
H	6.168241	2.698843	-2.163565
H	6.634398	4.287978	-0.310439
C	1.420930	1.255275	0.985732
N	0.755265	1.245272	1.936857
H	2.138609	0.707460	-2.257075
C	0.417781	-1.459580	-0.473231
C	-0.295609	-3.374163	0.354277
C	-2.041796	-2.034172	-0.770882
H	-2.004132	-1.560368	-1.755987
N	0.949042	-3.299300	0.718622
N	1.385031	-2.115890	0.191242
N	-0.665270	-2.268321	-0.356589
C	-1.245921	-4.527778	0.499785
H	-1.149379	-4.971807	1.490867
H	-0.978758	-5.283447	-0.252618
C	-2.815928	-3.366810	-0.850533
O	-2.580716	-4.104763	0.341494
C	-4.201821	-1.702236	0.118746
C	-2.882786	-1.254612	0.219438
C	-2.515278	-0.270835	1.123361
C	-3.519167	0.335490	1.880975
C	-4.850790	-0.052225	1.732020

C	-5.200960	-1.088060	0.861429
C	-4.276337	-2.901463	-0.803614
H	-1.476354	0.028450	1.245059
H	-5.620112	0.433320	2.324648
H	-6.230923	-1.425203	0.792547
H	-4.611612	-2.626269	-1.810036
H	-4.926135	-3.696185	-0.431134
C	2.760044	-1.734259	0.340047
C	3.570181	-1.749926	-0.798147
C	3.202555	-1.319032	1.597968
C	4.858344	-1.236186	-0.664966
C	4.498488	-0.809265	1.672739
C	5.323590	-0.729372	0.550407
H	5.508989	-1.218821	-1.535624
H	4.864799	-0.449092	2.630973
C	2.339885	-1.438069	2.826134
H	2.402397	-2.452651	3.231601
H	1.290058	-1.228274	2.612060
H	2.676048	-0.739422	3.594102
C	6.673739	-0.072989	0.648880
H	6.550211	1.014696	0.700066
H	7.291822	-0.300113	-0.222139
H	7.205794	-0.391608	1.548780
C	3.074422	-2.306792	-2.108462
H	2.275439	-1.700315	-2.548491
H	2.673851	-3.316020	-1.969947
H	3.892598	-2.360071	-2.828233
H	-2.553792	-3.961938	-1.733542
H	-3.257509	1.114280	2.590511
H	-0.293343	0.190849	-3.035429

Vibrational frequencies

-1272.8187	19.2684	22.4348
31.0333	34.7149	36.6891
42.1988	61.2374	64.9571
71.0923	77.4618	80.8732
88.5352	93.5941	108.7728
110.8419	116.6277	120.8874
125.2455	130.1822	137.7917
144.4242	150.3946	152.4854
160.6469	166.7220	183.7539
190.8071	200.3810	204.1633
214.5002	227.3790	231.3013
250.2881	260.7272	267.3246
268.5673	289.5107	294.2616

306.3330 308.8606 321.1212
333.2177 336.7103 344.3908
355.1561 375.9080 381.9386
401.9386 405.0135 414.6540
416.5163 428.9982 446.5122
449.8837 475.4102 486.1592
492.7430 500.7885 504.3547
508.7947 516.2905 529.9256
536.7889 549.9122 557.0394
578.7587 583.1976 587.0140
590.6661 628.0932 631.9759
635.3651 650.2756 662.6795
666.2243 685.9869 697.2516
712.1607 725.9533 731.7856
742.8160 747.2808 762.9604
770.2707 774.7255 787.2674
804.6217 807.8469 817.1710
831.8936 836.0768 841.3766
865.5406 878.0988 888.9901
894.6052 908.1222 925.9501
928.8493 944.9731 958.7225
960.8538 966.6268 977.4567
981.8184 986.3570 987.6355
994.5013 997.1394 1011.0850
1014.8514 1017.9605 1020.5797
1024.8265 1036.0969 1038.5081
1044.8280 1046.5272 1060.3744
1062.6335 1063.6347 1064.8091
1068.0826 1070.0485 1075.2955
1078.0886 1095.1896 1095.7573
1112.1917 1113.4985 1132.3152
1140.7923 1151.0679 1158.1778
1160.2321 1174.9420 1177.2188
1185.6273 1188.7210 1196.1827
1205.4534 1216.3441 1218.1384
1223.9233 1236.9027 1250.5392
1252.6396 1269.9716 1284.3088
1286.1462 1288.5260 1299.5885
1305.8763 1310.7681 1317.0615
1325.4337 1330.2338 1342.3319
1347.8255 1355.5102 1361.6144
1368.8502 1372.5920 1373.8078
1378.9874 1380.8683 1383.9559
1410.2461 1413.4202 1419.3533

1424.5921	1433.4760	1448.0134
1454.8035	1461.7971	1464.8179
1472.5712	1486.0462	1490.0191
1491.9849	1493.9170	1494.9220
1495.7002	1496.9943	1503.8995
1504.7596	1505.7223	1507.1342
1514.4804	1521.2668	1524.3697
1526.0578	1533.6823	1537.8984
1548.2466	1557.0802	1571.9628
1593.7597	1614.4122	1664.8424
1674.5154	1678.7341	1682.1776
1688.0337	1695.7636	1696.2800
1703.7579	1706.5534	1712.3638
2384.6238	3058.9343	3066.7850
3066.9666	3068.6854	3070.8041
3078.9243	3083.5358	3103.3438
3127.6317	3135.4189	3138.8817
3140.5170	3144.8231	3150.1908
3154.4396	3169.2356	3169.5528
3179.4259	3180.8619	3188.3625
3194.3336	3195.0506	3201.5978
3201.9358	3207.4448	3208.6699
3209.4640	3209.4931	3212.6694
3218.5117	3221.5175	3226.3426
3231.7748	3236.2189	3241.8405
3257.1782	3269.8656	3843.3643

***Si*-TS2[b]**

Zero-point correction= 0.691407

Thermal correction to Energy= 0.732222

Thermal correction to Enthalpy= 0.733166

Thermal correction to Gibbs Free Energy= 0.617132

Sum of electronic and zero-point Energies= -1948.340665

Sum of electronic and thermal Energies= -1948.299849

Sum of electronic and thermal Enthalpies= -1948.298905

Sum of electronic and thermal Free Energies= -1948.414939

Cartesian coordinates

H	-0.729390	0.550157	-0.504406
C	-2.387281	1.667586	-1.522759
C	-3.414361	2.582819	-1.605074
C	-3.794446	3.316119	-0.452981
C	-3.065788	3.054200	0.735870
C	-2.059337	2.114679	0.722051
H	-2.033460	1.083074	-2.367712

H	-3.909349	2.727679	-2.555622
H	-3.282239	3.575921	1.658221
H	-1.486740	1.887694	1.618844
C	-5.145686	4.969534	0.712622
C	-5.512169	4.469234	-1.728699
H	-4.300028	5.569936	1.065868
H	-5.971142	5.641005	0.484267
H	-5.460325	4.300255	1.520684
H	-4.839543	4.851852	-2.504401
H	-5.988393	3.555409	-2.099724
H	-6.288173	5.211216	-1.551023
N	-4.799810	4.221891	-0.485680
N	-1.724694	1.429127	-0.379216
C	0.240193	-0.212591	-1.160338
C	1.287972	0.780124	-1.007351
C	1.786048	1.316027	0.156924
O	-0.312930	-0.406046	-2.384134
C	2.883038	2.296659	0.235612
C	3.132977	3.001255	1.423250
C	3.716967	2.547076	-0.866290
C	4.159694	3.935552	1.500633
H	2.511307	2.812873	2.294470
C	4.731014	3.495759	-0.791684
H	3.588441	1.975735	-1.779990
C	4.962024	4.196239	0.391678
H	4.330361	4.465303	2.432859
H	5.358012	3.674982	-1.660270
H	5.762232	4.926654	0.451299
C	1.167608	0.902472	1.371445
N	0.589140	0.597172	2.336414
H	1.589638	1.247572	-1.946559
C	0.440554	-1.512498	-0.480387
C	0.031003	-3.624439	0.011330
C	-1.940364	-2.305428	-0.738486
H	-1.966085	-1.624775	-1.600837
N	1.298956	-3.475908	0.255100
N	1.542043	-2.160341	-0.055105
N	-0.531004	-2.457277	-0.413180
C	-0.774391	-4.890883	-0.013103
H	-0.568534	-5.492783	0.873039
H	-0.478746	-5.464934	-0.903201
C	-2.555236	-3.687075	-1.043124
O	-2.154749	-4.608501	-0.030607
C	-4.055564	-2.461599	0.315511

C	-2.809946	-1.835691	0.409225
C	-2.511047	-0.974720	1.452732
C	-3.509862	-0.697493	2.389130
C	-4.769769	-1.284103	2.276808
C	-5.049310	-2.180886	1.242161
C	-4.053665	-3.451322	-0.830185
H	-1.518831	-0.541233	1.555276
H	-5.533709	-1.062580	3.015475
H	-6.018176	-2.667936	1.181174
H	-4.497206	-3.024853	-1.736905
H	-4.568549	-4.387122	-0.601440
C	2.882544	-1.657845	-0.066189
C	3.457976	-1.362210	-1.307061
C	3.529473	-1.439130	1.150270
C	4.709245	-0.750759	-1.294014
C	4.784311	-0.829398	1.105632
C	5.372714	-0.453292	-0.100258
H	5.179093	-0.497209	-2.241749
H	5.303954	-0.630973	2.039902
C	2.916508	-1.869614	2.456211
H	3.044078	-2.947377	2.598733
H	1.846585	-1.653656	2.488007
H	3.397022	-1.354228	3.289939
C	6.680472	0.291802	-0.117397
H	6.490307	1.370924	-0.091218
H	7.249922	0.075482	-1.024536
H	7.294961	0.038155	0.749391
C	2.769602	-1.719589	-2.600606
H	1.798731	-1.224254	-2.732272
H	2.584415	-2.799215	-2.638124
H	3.409377	-1.459981	-3.446401
H	-2.285756	-4.067513	-2.036259
H	-3.297316	-0.026929	3.216120

Vibrational frequencies

-1476.9560	12.7408	21.4244
27.3399	31.7245	38.5639
48.4534	54.3544	61.0659
65.5776	73.1014	74.1227
80.3581	90.4039	101.5383
103.3350	108.4957	111.6646
117.9524	120.0333	130.1215
138.3560	148.8986	155.7367
165.8048	179.9735	193.5042
199.4453	202.9461	211.3630

215.6764	225.3160	228.3930
244.8564	254.9472	261.1273
270.8001	288.1095	289.5758
294.8881	304.6474	326.7410
332.6874	336.7456	349.8067
366.3386	382.3931	403.6320
406.1420	414.9126	417.1127
432.9808	443.1443	448.2239
471.9346	485.9105	489.1306
501.4050	507.6265	513.1637
523.9229	531.9534	549.7010
551.4857	558.3133	577.1055
584.3316	588.1610	591.8151
625.7144	628.0320	636.3578
641.2017	648.4260	669.4479
678.3608	689.1841	708.4653
719.5325	732.8813	746.5368
749.4870	760.4306	766.2944
772.6168	783.0252	802.5623
810.1794	815.7224	840.7876
849.3791	857.2715	863.9784
875.4091	880.1952	885.6348
906.7274	913.1872	922.0572
924.3105	944.0601	961.0071
968.8396	982.7952	985.7714
988.0992	991.4390	993.3329
1009.3574	1014.2566	1016.5683
1019.4322	1025.1693	1031.4908
1041.3419	1043.6813	1046.9363
1053.5697	1058.8131	1062.0648
1064.3374	1069.6162	1070.6201
1070.9966	1073.6709	1077.5934
1092.0052	1111.2461	1113.7770
1116.1268	1119.9925	1141.3183
1144.7622	1145.7349	1154.3758
1169.1114	1175.4110	1183.2829
1190.7819	1200.3682	1207.0718
1211.3512	1212.2483	1223.0493
1237.9176	1251.3913	1254.7165
1279.4772	1281.1003	1282.7193
1288.6153	1298.7734	1307.6761
1312.9947	1319.1726	1327.4986
1336.4502	1341.7853	1348.3987
1355.7024	1358.4313	1361.9040

1364.8477	1376.7475	1380.4105
1381.3809	1402.3735	1407.6698
1418.0974	1425.0495	1435.7730
1444.5798	1451.8441	1459.3728
1467.8627	1473.1489	1475.4246
1486.3610	1489.9321	1491.5875
1493.6785	1494.7091	1495.2616
1497.6741	1498.0927	1501.6482
1502.6279	1510.9403	1516.9229
1517.8797	1524.6013	1530.6918
1536.7619	1539.6864	1547.5849
1559.1906	1559.6455	1595.7366
1633.0464	1638.3370	1663.7000
1678.2799	1682.6654	1688.4620
1689.7076	1697.2732	1705.6581
1710.8827	2328.1496	3048.5945
3053.8944	3054.0883	3060.5297
3062.8496	3078.3153	3080.7236
3084.0138	3100.0516	3113.1391
3119.2539	3120.2443	3137.8534
3145.7847	3152.6817	3157.1436
3158.6232	3167.0909	3167.6144
3179.6529	3184.3164	3188.2103
3192.4118	3193.2402	3197.2002
3199.2414	3200.2895	3206.7858
3208.3602	3210.2921	3212.6133
3217.9357	3223.7885	3224.2707
3233.3718	3260.7666	3266.6524

***Si*-TS2[c]**

Zero-point correction= 0.527205

Thermal correction to Energy= 0.558323

Thermal correction to Enthalpy= 0.559267

Thermal correction to Gibbs Free Energy= 0.465043

Sum of electronic and zero-point Energies= -1566.358425

Sum of electronic and thermal Energies= -1566.327307

Sum of electronic and thermal Enthalpies= -1566.326363

Sum of electronic and thermal Free Energies= -1566.420587

Cartesian coordinates

C	-0.297966	0.333729	-1.413002
C	1.064724	0.830224	-1.371393
C	1.717638	1.367695	-0.306662
O	-0.869584	0.098889	-2.742280
C	3.141291	1.764481	-0.301812

C	3.629094	2.664616	0.654714
C	4.034634	1.243835	-1.249045
C	4.965601	3.049749	0.651842
H	2.952801	3.068943	1.402760
C	5.366852	1.642604	-1.258793
H	3.691890	0.502081	-1.963344
C	5.840300	2.545663	-0.307967
H	5.323179	3.749755	1.400189
H	6.042746	1.231295	-2.002250
H	6.882797	2.846528	-0.310792
C	0.956374	1.591895	0.887020
N	0.308837	1.811264	1.826249
H	1.575752	0.806130	-2.333958
H	-1.114934	1.056693	-1.855467
C	-0.780844	-0.635617	-0.441678
C	-2.147936	-1.973984	0.642348
C	-3.260803	-0.330859	-0.877352
H	-3.022905	-0.227983	-1.941461
N	-0.962205	-2.329694	1.036262
N	-0.118520	-1.499305	0.347443
N	-2.088129	-0.944368	-0.253958
C	-3.468847	-2.598831	0.975912
H	-3.513278	-2.839972	2.038525
H	-3.576992	-3.527660	0.397497
C	-4.496888	-1.233872	-0.656713
O	-4.511754	-1.697454	0.688186
C	-5.101337	1.027992	-0.263188
C	-3.705052	0.986560	-0.271086
C	-2.949532	2.044738	0.216119
C	-3.620455	3.166932	0.705860
C	-5.013450	3.221169	0.699475
C	-5.765373	2.148727	0.216516
C	-5.673188	-0.265593	-0.797760
H	-1.865096	2.001809	0.235160
H	-5.518541	4.100166	1.087064
H	-6.850558	2.183956	0.232806
H	-5.957210	-0.171249	-1.851616
H	-6.539833	-0.627999	-0.240234
C	1.299664	-1.699737	0.386416
C	1.934525	-2.073079	-0.805119
C	1.983413	-1.477166	1.582787
C	3.324971	-2.142423	-0.786281
C	3.376677	-1.561708	1.543080
C	4.062175	-1.863413	0.368196

H	3.848345	-2.422485	-1.697603
H	3.936127	-1.375181	2.456329
C	1.263051	-1.194585	2.874345
H	0.884551	-2.125700	3.306999
H	0.413776	-0.525114	2.727347
H	1.944081	-0.734544	3.592716
C	5.566746	-1.864150	0.331516
H	5.929772	-0.880141	0.013471
H	5.946963	-2.603696	-0.377150
H	5.989291	-2.073924	1.316504
C	1.153356	-2.420272	-2.049094
H	0.657683	-1.559499	-2.515950
H	0.368910	-3.147966	-1.814265
H	1.818696	-2.870102	-2.788192
H	-4.524439	-2.083571	-1.350214
H	-3.049247	4.000751	1.100717

Vibrational frequencies

-1771.5814	17.7368	26.5961
33.9273	40.1003	54.2956
57.1079	75.0529	83.5868
90.0062	102.0964	110.9305
115.7538	118.3606	127.8703
154.4178	156.5856	166.5997
185.5181	192.5984	205.5116
211.3766	215.1996	235.9828
250.9759	256.1233	287.3960
293.1974	300.7689	311.9880
319.3159	335.0667	342.5359
361.0150	377.7988	396.2372
406.5328	419.0725	430.5966
438.4642	459.0883	477.7816
494.5223	497.8516	508.4723
517.0863	529.3097	553.8820
560.7345	582.5321	584.1941
590.5766	616.1956	626.4424
630.3143	644.1791	652.3538
669.8722	684.5862	702.4074
717.1500	729.1358	744.9384
757.1731	759.5981	761.8192
789.4270	797.7545	810.1842
842.1925	868.5580	877.7370
878.7015	883.6790	896.9894
909.7968	917.5036	924.1233
940.6454	951.5717	957.6387

965.3544	981.3655	983.8630
1001.6199	1005.0294	1012.7017
1015.5791	1024.3241	1026.8739
1039.3815	1041.3400	1043.0646
1046.0014	1059.2763	1061.5453
1067.1942	1070.2437	1070.3959
1076.5300	1078.0820	1079.5290
1115.7158	1127.2888	1142.2270
1175.2361	1180.8923	1181.1738
1192.1704	1203.5062	1213.4040
1217.9042	1234.8295	1250.3453
1257.7378	1278.5266	1282.8299
1286.3065	1304.8785	1311.8988
1322.2432	1323.3879	1334.5532
1339.3452	1350.0322	1362.3912
1364.4423	1369.7396	1377.7579
1382.0179	1400.6874	1407.7897
1418.6934	1425.8765	1437.4897
1460.0737	1464.8257	1472.4805
1488.1754	1489.3198	1492.9880
1493.9096	1496.4707	1502.3290
1513.5774	1516.2215	1519.6421
1527.1556	1537.4945	1543.4518
1552.8325	1558.9123	1662.1784
1676.9162	1680.8275	1684.2663
1687.9136	1691.4058	1694.0549
1706.8046	2370.4436	2662.2425
3055.8921	3062.5885	3065.7613
3080.8685	3082.8300	3094.2251
3121.0908	3125.7353	3139.5245
3150.7427	3157.3648	3163.4778
3167.7112	3174.2884	3174.8307
3177.3151	3191.2885	3194.6313
3199.4016	3208.3274	3209.2512
3213.4171	3218.0493	3223.1754
3225.0378	3227.7214	3239.2998

Re-M2

Zero-point correction= 0.530760

Thermal correction to Energy= 0.562670

Thermal correction to Enthalpy= 0.563615

Thermal correction to Gibbs Free Energy= 0.466319

Sum of electronic and zero-point Energies= -1566.433670

Sum of electronic and thermal Energies= -1566.401760

Sum of electronic and thermal Enthalpies= -1566.400816

Sum of electronic and thermal Free Energies= -1566.498111

Cartesian coordinates

C	0.866131	-1.074873	0.982235
C	-0.261961	-1.891776	1.025402
C	-1.251430	-2.023678	0.055224
O	1.961545	-1.381237	1.786276
C	-2.537983	-2.690237	0.301837
C	-3.312049	-3.195196	-0.756295
C	-3.028744	-2.841868	1.608885
C	-4.513303	-3.848792	-0.512629
H	-2.958691	-3.077403	-1.776922
C	-4.224408	-3.510900	1.849533
H	-2.481427	-2.410819	2.442023
C	-4.974849	-4.019492	0.792251
H	-5.091100	-4.232088	-1.348166
H	-4.580507	-3.617305	2.869685
H	-5.913531	-4.529892	0.980394
C	-0.935352	-1.635587	-1.271141
N	-0.656837	-1.369316	-2.371493
H	-0.330849	-2.532110	1.906200
C	0.973512	0.158733	0.297442
C	0.687245	2.261593	-0.315742
C	-1.315375	1.270872	0.630174
H	-1.539213	0.365768	1.201409
N	1.963592	2.075029	-0.421949
N	2.133480	0.752475	-0.081043
N	0.021129	1.123044	0.068398
C	-0.085111	3.535108	-0.257853
H	-0.858997	3.568110	-1.032207
H	0.590075	4.382013	-0.378256
C	-1.353330	2.503371	1.576024
O	-0.643665	3.627628	1.050037
C	-3.336955	2.462327	0.275008
C	-2.438229	1.590433	-0.347389
C	-2.632030	1.178794	-1.658909
C	-3.768363	1.628025	-2.334186
C	-4.684915	2.470543	-1.707147
C	-4.470905	2.899561	-0.396699
C	-2.850015	2.828485	1.657332
H	-1.910042	0.542068	-2.156400
H	-5.561642	2.810809	-2.249079
H	-5.167563	3.581040	0.082379
H	-3.328080	2.208545	2.425359

H	-3.009186	3.877173	1.917194
C	3.432813	0.156003	-0.174303
C	4.375459	0.458057	0.815352
C	3.712811	-0.678053	-1.257379
C	5.640831	-0.106300	0.693533
C	4.996140	-1.226241	-1.331908
C	5.967520	-0.951998	-0.371913
H	6.390245	0.111537	1.450949
H	5.240116	-1.874276	-2.169938
C	2.670437	-0.980135	-2.298327
H	2.138722	-0.074812	-2.605082
H	1.913989	-1.671012	-1.913157
H	3.127376	-1.431945	-3.180371
C	7.343179	-1.560320	-0.461966
H	7.503475	-2.035556	-1.431636
H	7.482120	-2.319838	0.313696
H	8.116854	-0.801690	-0.317215
C	3.999688	1.330606	1.980823
H	3.175958	0.866315	2.532803
H	3.662655	2.315673	1.646149
H	4.846373	1.460726	2.656545
H	-0.904443	2.272231	2.546157
H	-3.934039	1.321381	-3.361898
H	2.465993	-2.096784	1.377888

Vibrational frequencies

16.2566	20.5677	32.7713
39.8864	42.9405	45.0150
58.9932	68.9847	76.1125
94.3874	100.8132	104.3066
109.4584	128.3011	134.0362
141.8154	149.3657	168.9731
171.7088	175.4944	194.5754
208.6657	234.6827	250.1196
261.3216	278.4693	281.8419
299.3035	312.1499	316.0245
332.6181	343.5208	359.1349
375.4820	386.2422	395.8798
417.3545	421.9164	429.0135
435.9018	444.6084	495.2008
498.4012	504.4773	508.6362
522.1083	526.3995	532.2396
559.9413	583.4672	589.0004
595.2467	608.7444	620.8573
624.1789	630.4748	639.9225

666.7393	696.2553	715.1549
716.5068	729.6905	742.5707
761.5327	767.8052	770.7490
784.3833	804.7969	816.5635
839.5773	852.9123	867.3670
878.0016	884.4127	906.0707
915.6797	923.2362	929.0952
946.1320	949.6070	965.6807
981.7413	993.0798	996.1933
1002.6734	1007.0584	1015.9345
1017.4118	1026.2720	1032.2089
1037.6202	1040.6234	1047.0355
1054.4466	1058.0859	1064.3119
1066.7219	1068.4438	1071.5707
1076.3251	1106.7344	1122.6183
1126.0870	1142.6880	1173.1689
1177.5601	1183.2708	1188.5287
1205.2086	1211.6193	1216.8857
1232.9391	1247.1521	1259.0794
1267.9650	1272.4677	1284.1797
1284.9073	1290.1810	1302.3051
1316.2042	1326.3933	1337.2659
1344.0386	1355.2427	1360.1166
1366.2496	1374.0343	1376.7377
1395.5632	1407.8270	1411.7685
1418.1937	1420.9286	1430.9299
1455.6062	1469.2344	1471.5045
1478.1908	1486.5230	1487.8856
1495.0320	1497.0412	1498.8667
1503.1902	1505.6293	1516.2592
1524.5826	1530.4064	1533.2076
1552.2481	1559.2117	1639.6612
1664.9865	1680.7409	1687.2120
1693.6141	1697.5605	1704.2890
1709.1715	2335.4403	3071.7428
3075.0402	3075.1646	3079.3087
3104.8157	3129.5700	3140.5432
3146.1175	3146.9406	3147.2231
3148.1425	3162.5094	3167.8017
3167.9574	3172.5366	3182.9623
3192.5906	3193.8068	3197.8000
3198.4460	3204.5590	3207.7671
3211.4537	3212.1320	3225.4030
3225.7316	3244.0879	3843.6936

***Si*-M2**

Zero-point correction= 0.531832

Thermal correction to Energy= 0.563041

Thermal correction to Enthalpy= 0.563985

Thermal correction to Gibbs Free Energy= 0.470209

Sum of electronic and zero-point Energies= -1566.444987

Sum of electronic and thermal Energies= -1566.413778

Sum of electronic and thermal Enthalpies= -1566.412834

Sum of electronic and thermal Free Energies= -1566.506610

Cartesian coordinates

C	-0.341425	0.517926	-1.382036
C	0.923836	1.128207	-1.317665
C	1.694548	1.332641	-0.190321
O	-1.189341	0.877497	-2.434501
C	3.127719	1.654032	-0.217486
C	3.776637	2.183250	0.909080
C	3.894430	1.413975	-1.369362
C	5.131566	2.492273	0.872667
H	3.208419	2.356928	1.818761
C	5.245283	1.740748	-1.409055
H	3.434239	0.934411	-2.228140
C	5.873489	2.284345	-0.289396
H	5.609207	2.903827	1.756501
H	5.814932	1.547679	-2.313046
H	6.930777	2.527024	-0.316517
C	1.028624	1.316183	1.069356
N	0.453034	1.392515	2.078115
H	1.306340	1.501235	-2.269881
C	-0.804957	-0.550558	-0.600257
C	-2.142686	-2.074245	0.301503
C	-3.334814	-0.286002	-0.951817
H	-3.224686	-0.078510	-2.018057
N	-0.963697	-2.419014	0.698543
N	-0.119890	-1.490194	0.125398
N	-2.119378	-0.961114	-0.498677
C	-3.440615	-2.764131	0.585275
H	-3.416396	-3.201748	1.583652
H	-3.598104	-3.565486	-0.151259
C	-4.573249	-1.186720	-0.726633
O	-4.494731	-1.828667	0.536819
C	-5.086535	1.041312	-0.061024
C	-3.697657	0.977994	-0.197187
C	-2.879980	1.984412	0.302349

C	-3.480720	3.074303	0.935961
C	-4.867528	3.149976	1.057842
C	-5.681562	2.130156	0.562119
C	-5.733007	-0.189863	-0.653849
H	-1.797324	1.915997	0.239920
H	-5.318083	4.002861	1.555265
H	-6.760358	2.180761	0.676508
H	-6.119860	0.009970	-1.659369
H	-6.548897	-0.593914	-0.049964
C	1.290611	-1.665260	0.224119
C	2.045114	-1.841239	-0.944047
C	1.887111	-1.626905	1.493684
C	3.433720	-1.851384	-0.825012
C	3.279800	-1.636675	1.553713
C	4.069521	-1.705643	0.406574
H	4.033319	-1.961039	-1.726440
H	3.758694	-1.568939	2.527777
C	1.077933	-1.606596	2.763033
H	0.781876	-2.624639	3.035101
H	0.171886	-1.009900	2.657981
H	1.671320	-1.190138	3.579714
C	5.567034	-1.586225	0.491400
H	5.855691	-0.530992	0.416272
H	6.057140	-2.123321	-0.324322
H	5.946335	-1.971378	1.440906
C	1.413864	-2.020626	-2.299949
H	1.323262	-1.065642	-2.827737
H	0.411615	-2.450083	-2.225237
H	2.030297	-2.686146	-2.908322
H	-4.683514	-1.938507	-1.519036
H	-2.858920	3.864386	1.343974
H	-1.473732	1.791358	-2.298670

Vibrational frequencies

20.4647	28.5811	32.5417
45.9813	53.3565	64.7035
77.5077	83.7426	91.3018
103.5994	116.5538	116.7893
124.8097	137.6500	140.1709
158.2642	169.4222	184.5738
204.6902	211.6318	213.1244
230.6589	234.0193	247.0212
270.9539	284.8479	293.3673
307.6586	325.6299	328.4817
339.4536	352.1760	361.0916

379.0244 399.1500 413.9588
418.8705 421.7109 429.9815
440.2896 450.4880 477.0936
491.2299 495.9787 507.5402
522.0267 524.8474 551.4720
562.2935 582.4754 584.0256
590.1838 612.1032 628.5322
631.3824 634.1868 643.8180
658.0417 678.5546 699.2694
709.3646 715.0341 727.7525
755.6073 760.5313 768.2890
783.5675 810.5282 817.6734
844.1626 870.2454 873.1196
875.0834 880.5184 900.7608
905.9065 922.2908 925.0156
943.4009 963.2416 968.8070
980.2623 990.5326 997.3527
1003.2777 1014.8659 1016.2368
1022.0376 1025.2528 1041.4325
1045.7484 1049.5759 1053.8939
1061.9799 1062.3532 1064.0146
1067.0937 1070.0467 1076.5306
1082.2965 1110.4052 1116.1567
1124.1701 1172.4431 1177.8290
1178.9293 1189.9825 1196.5910
1210.1148 1213.5624 1218.0040
1230.3034 1250.9717 1267.1746
1269.9963 1281.6923 1287.3734
1299.6530 1307.6034 1319.9796
1321.8543 1336.7516 1339.2734
1349.3784 1352.6871 1362.7839
1366.4858 1375.8419 1385.7219
1388.0511 1402.6694 1415.5758
1418.8386 1420.3064 1429.6910
1445.1840 1464.3023 1470.1644
1477.9530 1482.4124 1490.8777
1495.7747 1497.6170 1499.2436
1508.2217 1510.2205 1517.7543
1519.7958 1531.0406 1536.9317
1551.0646 1563.6137 1656.5148
1668.0477 1677.9076 1680.2453
1691.1550 1698.3016 1706.3211
1713.4178 2346.9022 3051.8771
3065.6108 3072.4225 3075.9738

3077.6309	3086.7513	3139.9762
3144.3919	3145.3905	3147.0215
3149.0464	3159.4879	3167.5059
3170.3440	3172.8469	3179.1072
3183.1925	3192.9855	3194.3499
3200.6724	3204.4670	3209.1149
3211.5818	3215.3761	3221.7846
3228.1500	3229.9009	3831.5216

DQ

Zero-point correction= 0.622022

Thermal correction to Energy= 0.654775

Thermal correction to Enthalpy= 0.655719

Thermal correction to Gibbs Free Energy= 0.559982

Sum of electronic and zero-point Energies= -1240.375040

Sum of electronic and thermal Energies= -1240.342287

Sum of electronic and thermal Enthalpies= -1240.341343

Sum of electronic and thermal Free Energies= -1240.437080

Cartesian coordinates

C	-2.808475	1.282007	-0.003918
C	-1.459368	1.235142	0.033000
C	-0.693431	0.000059	0.012501
C	-1.459306	-1.235063	0.034475
C	-2.808382	-1.281994	-0.002582
C	-3.569664	-0.000038	-0.087733
H	-0.917985	2.167500	0.088036
H	-0.917759	-2.167185	0.091819
C	0.693521	0.000021	-0.011471
C	1.459374	-1.235131	-0.033884
C	1.459591	1.235054	-0.031948
C	2.808472	-1.282090	0.002201
H	0.917938	-2.167298	-0.092025
C	2.808719	1.281885	0.004296
H	0.918214	2.167411	-0.087234
C	3.569910	-0.000232	0.088086
O	4.790490	-0.000581	0.216295
O	-4.790278	-0.000321	-0.216131
C	3.585170	-2.598232	-0.030236
C	4.551552	-2.605940	-1.230311
C	4.374162	-2.775649	1.281067
C	2.646842	-3.801707	-0.178329
H	4.000274	-2.485858	-2.168658
H	5.291160	-1.809373	-1.151089
H	5.075769	-3.566585	-1.266685

H	3.694322	-2.784151	2.139102
H	4.902380	-3.734696	1.257741
H	5.104388	-1.978676	1.417213
H	3.244957	-4.716504	-0.212169
H	1.956807	-3.887927	0.667597
H	2.062096	-3.750129	-1.102706
C	3.585361	2.598194	-0.026617
C	4.375821	2.773678	1.284054
C	4.550753	2.607788	-1.227470
C	2.646724	3.801837	-0.171960
H	3.697090	2.779932	2.142989
H	5.106891	1.977091	1.417756
H	4.903118	3.733258	1.261974
H	3.998670	2.491004	-2.165746
H	5.076440	3.567718	-1.261582
H	5.289264	1.809883	-1.150831
H	3.244757	4.716704	-0.205508
H	2.060770	3.751411	-1.095635
H	1.957821	3.886984	0.674943
C	-3.585185	2.598238	0.026100
C	-4.551654	2.607600	1.226281
C	-2.646869	3.801907	0.173183
C	-4.374298	2.774045	-1.285238
H	-5.290849	1.810532	1.148653
H	-4.000086	2.489538	2.164744
H	-5.076264	3.568091	1.260935
H	-1.957614	3.888171	-0.673339
H	-3.245105	4.716617	0.207364
H	-2.061292	3.750442	1.097072
H	-4.902222	3.733293	-1.263199
H	-3.694909	2.780959	-2.143617
H	-5.104890	1.977089	-1.419798
C	-3.585418	-2.598011	0.029866
C	-4.552201	-2.605394	1.229759
C	-4.373969	-2.775422	-1.281654
C	-2.647650	-3.801836	0.178870
H	-4.000746	-2.487490	2.168306
H	-5.290518	-1.807606	1.151611
H	-5.077964	-3.565237	1.264794
H	-3.694064	-2.782990	-2.139645
H	-4.901629	-3.734799	-1.259002
H	-5.104626	-1.978732	-1.417441
H	-3.246279	-4.716285	0.213208
H	-1.957590	-3.889216	-0.666879

H	-2.063034	-3.749990	1.103286

Vibrational frequencies

14.2571	23.1535	26.9314
45.0192	60.1746	68.7021
71.7073	78.6096	112.5322
127.7313	143.7120	151.0513
160.1680	161.6420	165.0617
183.4848	202.6602	211.7240
221.9422	226.1780	240.6230
240.7371	241.0664	241.2060
266.5640	271.7034	274.0678
289.0996	295.0030	303.1734
314.9161	315.1719	320.3120
335.8343	352.7323	353.1779
359.0662	361.2209	363.1439
367.4347	382.9316	384.3627
385.6257	394.8705	396.6098
406.2502	411.9289	442.5357
444.1891	446.9515	449.4105
468.8731	518.2502	524.5402
529.7427	547.6955	569.3505
578.3699	587.1430	640.8217
675.4508	681.2127	687.6915
764.0060	765.5619	804.7212
818.2532	821.8739	823.4899
835.2622	860.4848	889.5948
905.7906	911.0326	913.5121
915.6245	934.2230	944.1085
947.7880	947.9037	948.0780
948.7422	957.9929	958.3588
958.6305	958.6923	963.7048
963.7482	963.8003	963.8041
1027.1924	1046.0539	1052.0805
1052.6033	1054.8783	1055.3859
1055.8755	1056.2185	1068.0819
1116.7714	1122.3028	1223.5954
1225.4775	1244.5182	1244.6436
1244.7490	1245.2080	1254.1005
1257.1447	1258.9314	1259.0562
1300.4770	1310.5550	1311.6309
1318.7701	1346.2208	1387.4450
1393.9675	1395.2806	1395.4150
1396.9441	1398.2958	1400.3293
1400.9115	1406.5609	1409.7352

1427.3686	1428.3286	1429.2822
1429.5695	1436.1429	1462.1132
1483.3332	1487.1494	1487.1822
1487.3511	1487.3963	1500.8988
1501.5279	1501.6784	1502.0762
1502.2934	1502.7448	1502.9252
1505.2697	1508.1056	1508.5035
1508.6412	1508.8113	1519.0244
1519.1082	1519.4373	1519.5658
1533.9917	1534.0403	1534.2767
1534.7821	1602.8146	1669.1006
1680.4995	1719.7428	1734.4013
1743.4979	1760.7706	3056.7268
3056.7872	3057.0689	3057.1619
3060.2651	3060.3110	3060.3285
3060.3745	3063.7052	3063.7634
3063.7912	3064.1763	3130.8999
3130.9567	3131.0235	3131.0780
3132.0956	3132.1705	3132.2105
3132.3202	3134.7529	3134.8929
3135.1859	3135.3431	3148.8000
3148.8320	3148.8786	3148.9916
3190.4919	3190.7557	3190.9262
3190.9930	3196.2425	3197.2389
3197.4971	3198.0279	3258.6819
3258.9633	3291.9840	3293.8272

TS3

Zero-point correction= 1.150210

Thermal correction to Energy= 1.214117

Thermal correction to Enthalpy= 1.215061

Thermal correction to Gibbs Free Energy= 1.054510

Sum of electronic and zero-point Energies= -2806.834688

Sum of electronic and thermal Energies= -2806.770781

Sum of electronic and thermal Enthalpies= -2806.769837

Sum of electronic and thermal Free Energies= -2806.930388

Cartesian coordinates

C	2.148066	0.053094	-0.884685
C	0.803855	0.137164	-0.571388
C	0.223222	0.796030	0.535103
O	2.667489	-0.812393	-1.721415
C	-1.117335	1.319132	0.591609
C	-1.578391	1.994270	1.748516
C	-1.988023	1.260211	-0.520542

C	-2.832147	2.567359	1.784575
H	-0.922578	2.082394	2.610438
C	-3.246091	1.846042	-0.475297
H	-1.653055	0.788987	-1.440610
C	-3.697169	2.472808	0.682502
H	-3.144335	3.102106	2.675960
H	-3.887943	1.787172	-1.348803
H	-4.687041	2.918178	0.720105
C	1.042823	0.971698	1.688710
N	1.698564	1.073523	2.645949
H	0.148294	-0.409567	-1.245720
C	3.107011	1.123192	-0.525373
C	4.991860	2.244346	-0.452417
C	5.273009	-0.219217	-0.313301
H	4.821080	-0.977357	-0.958557
N	4.064638	3.154579	-0.523917
N	2.899119	2.452098	-0.574231
N	4.453090	0.989247	-0.440416
C	6.476696	2.437541	-0.540615
H	6.786326	3.271694	0.089956
H	6.723837	2.674558	-1.585545
C	6.727880	0.085806	-0.738237
O	7.156253	1.286469	-0.105429
C	6.756433	-1.242371	1.219025
C	5.468686	-0.712433	1.105242
C	4.602141	-0.669375	2.183118
C	5.030930	-1.213980	3.396343
C	6.299204	-1.780866	3.508756
C	7.176887	-1.792120	2.421099
C	7.517494	-1.045968	-0.074183
H	3.620491	-0.212686	2.100518
H	6.618581	-2.198222	4.458402
H	8.176856	-2.202454	2.524175
H	7.490421	-1.942685	-0.702940
H	8.560753	-0.756944	0.070423
C	1.666481	3.151211	-0.828364
C	1.077598	3.007897	-2.090361
C	1.118131	3.938175	0.186807
C	-0.154602	3.626084	-2.288249
C	-0.115522	4.538167	-0.069655
C	-0.774957	4.375804	-1.285800
H	-0.641431	3.520350	-3.254815
H	-0.577611	5.133545	0.714310
C	1.819490	4.176141	1.497957

H	2.393943	5.106777	1.449953
H	2.504608	3.369297	1.757961
H	1.086923	4.270921	2.302915
C	-2.111622	5.027278	-1.523306
H	-2.728655	4.978525	-0.622913
H	-2.650719	4.534657	-2.335517
H	-1.987025	6.081617	-1.791306
C	1.741571	2.238224	-3.203407
H	1.569350	1.160151	-3.119604
H	2.824189	2.397857	-3.206724
H	1.349232	2.567175	-4.167367
H	6.849614	0.157820	-1.825788
H	4.369723	-1.188916	4.256487
H	2.181564	-1.933151	-1.668823
C	-0.604415	-2.570740	-2.206308
C	-1.835634	-2.165074	-1.742994
C	-2.127548	-2.015721	-0.361192
C	-1.158747	-2.520802	0.549515
C	0.072830	-2.989940	0.147860
C	0.427074	-2.852081	-1.234832
H	-2.588404	-1.886750	-2.466599
H	-1.417666	-2.568025	1.598427
C	-3.322964	-1.372074	0.090283
C	-3.498234	-1.005105	1.463823
C	-4.408094	-1.088268	-0.805164
C	-4.656207	-0.484687	1.961807
H	-2.656337	-1.139826	2.130476
C	-5.581424	-0.529018	-0.405895
H	-4.285131	-1.336630	-1.850375
C	-5.796752	-0.270476	1.040232
O	1.678903	-2.992724	-1.612523
O	-6.905232	0.086709	1.461445
C	1.069858	-3.582439	1.149467
C	1.567731	-4.948474	0.643912
C	2.255041	-2.627301	1.352700
C	0.423639	-3.805731	2.523542
H	0.730017	-5.646349	0.542095
H	2.067532	-4.854739	-0.320320
H	2.274546	-5.371180	1.365955
H	1.898579	-1.668451	1.744954
H	2.956371	-3.048538	2.081717
H	2.796751	-2.445426	0.421882
H	1.149139	-4.292006	3.182403
H	0.132388	-2.862187	2.996794

H	-0.458950	-4.450446	2.457924
C	-0.323901	-2.685197	-3.711162
C	0.627054	-1.567243	-4.171948
C	0.287094	-4.061563	-4.029293
C	-1.614061	-2.557694	-4.533936
H	0.191593	-0.585630	-3.947858
H	1.600007	-1.632616	-3.686222
H	0.771758	-1.630885	-5.256312
H	-0.397492	-4.861801	-3.729294
H	0.454392	-4.146536	-5.108286
H	1.237366	-4.201721	-3.515415
H	-1.380891	-2.729189	-5.588820
H	-2.362821	-3.296033	-4.229061
H	-2.057460	-1.559665	-4.455109
C	-6.709622	-0.210547	-1.386898
C	-7.101972	1.274689	-1.267031
C	-6.286496	-0.462165	-2.839300
C	-7.934821	-1.096888	-1.092699
H	-7.441880	1.511271	-0.259168
H	-6.251979	1.920273	-1.514391
H	-7.908645	1.498230	-1.973544
H	-6.058642	-1.517224	-3.022410
H	-7.108203	-0.181344	-3.504671
H	-5.410417	0.134890	-3.116453
H	-8.727061	-0.879175	-1.817494
H	-7.670788	-2.155377	-1.186834
H	-8.316039	-0.916756	-0.087941
C	-4.864647	-0.253747	3.460732
C	-5.436399	1.141027	3.772501
C	-5.851177	-1.322645	3.973808
C	-3.551515	-0.400244	4.239436
H	-4.751519	1.922803	3.438116
H	-6.402310	1.290548	3.294228
H	-5.559973	1.241877	4.856410
H	-5.453747	-2.327649	3.798794
H	-6.001811	-1.197242	5.051894
H	-6.816062	-1.230890	3.472289
H	-3.735794	-0.189205	5.297064
H	-3.143884	-1.414221	4.172376
H	-2.794924	0.304244	3.877004

Vibrational frequencies

-1321.2453	11.5363	13.3279
25.4472	28.8732	31.1608
39.8576	44.4735	45.6665

51.2475	53.7994	55.9492
60.0376	63.7984	67.7665
76.7112	79.4367	81.3412
83.6865	86.8804	90.4311
100.1200	109.6530	112.8044
119.6878	126.0510	130.5440
139.3930	140.6882	155.3029
155.8105	162.8412	164.1636
166.3578	170.6760	173.7299
175.2475	180.0048	187.2388
196.4479	202.1960	205.7078
212.4817	213.3734	221.5141
222.9465	229.6458	236.7926
246.1998	250.9674	253.3368
259.7093	264.4882	269.7206
271.3304	281.0492	283.0476
291.6086	294.3467	295.8407
298.7984	304.8630	308.8539
313.0021	319.0842	322.0637
328.4272	331.4824	332.6782
336.6963	342.6348	349.1215
354.9038	358.2981	361.6106
364.4720	366.7474	368.8365
369.9207	377.7230	387.3012
388.9383	397.3208	400.0173
403.6651	405.4835	409.3597
413.7159	418.6622	425.4807
436.6363	442.8922	444.8780
445.3662	457.8834	469.7245
471.9328	477.9203	489.1087
501.1630	505.9081	509.6465
519.6397	525.1442	527.1199
530.4979	537.1649	552.0286
553.8267	570.2978	575.5678
582.7852	585.4989	589.7345
591.8523	608.5213	614.3745
624.4797	628.1666	628.7258
641.9265	649.2540	667.2377
671.8451	677.8494	685.1646
686.4660	693.2042	698.4186
711.4656	729.9920	749.2415
758.9686	767.0914	775.1145
776.5607	779.6665	787.5231
805.6312	809.6050	812.0338

817.5929 830.6025 833.2392
841.3791 845.8463 849.7658
864.6829 871.1050 874.3223
876.9260 880.3690 881.5943
901.3587 908.0603 908.6285
913.7554 915.3725 916.4250
924.3072 928.5089 931.2024
950.2445 950.9530 952.0612
952.7192 954.2059 955.4452
956.5202 957.9934 959.9924
962.5347 962.6927 963.8624
964.8818 967.5226 970.6736
976.8085 982.9723 994.8219
1000.4654 1007.4304 1012.4696
1013.6685 1026.2778 1038.5343
1040.3489 1041.1707 1045.2028
1049.9169 1052.6145 1053.3227
1053.6337 1055.4657 1056.0222
1056.7041 1058.7183 1060.7453
1062.7208 1065.1700 1065.3027
1066.1786 1067.5726 1077.4980
1099.9838 1114.6187 1122.8392
1123.4340 1130.7202 1141.5840
1147.6121 1178.5166 1180.9191
1181.7606 1189.1916 1207.5152
1215.0763 1217.4926 1224.4446
1235.3473 1236.8279 1241.9171
1243.1037 1250.1522 1251.4212
1253.6210 1253.9237 1255.1640
1258.8825 1260.6256 1263.6477
1275.5355 1284.3244 1286.7984
1292.4296 1298.1710 1298.6297
1305.5201 1313.5324 1318.2354
1319.9602 1322.3130 1337.1012
1343.1631 1349.4677 1356.6436
1358.6904 1362.7722 1366.1189
1377.1001 1378.9429 1379.3583
1380.1825 1389.3297 1392.8816
1393.0172 1394.3815 1395.4169
1397.5018 1398.1916 1399.5522
1403.1932 1408.3191 1409.7032
1417.0764 1420.2164 1426.4900
1427.1413 1427.9978 1429.9776
1430.6759 1437.0464 1457.1126

1459.9959	1464.6692	1467.0572
1473.4306	1478.9732	1484.7650
1485.2341	1487.1889	1487.7778
1490.2900	1492.0647	1493.3298
1493.9396	1495.7839	1497.3773
1498.0920	1500.7538	1501.6542
1502.0222	1504.9277	1505.2747
1505.6203	1506.2642	1507.1617
1507.6706	1508.5393	1511.4419
1514.5345	1514.9365	1516.1622
1518.1909	1518.7374	1519.7276
1520.1465	1522.7650	1523.9870
1531.0649	1534.5018	1535.8382
1536.3841	1536.7199	1539.4193
1548.3963	1554.3393	1582.7859
1591.7610	1613.7839	1621.9260
1635.1483	1665.5777	1672.3841
1682.8538	1686.4195	1687.7393
1690.5206	1696.9299	1703.8376
1709.5705	2328.8592	3050.4965
3053.2749	3055.7390	3056.0180
3057.3055	3057.7186	3059.8592
3060.4047	3061.7342	3061.8554
3063.2384	3066.8639	3067.2942
3069.4741	3075.0270	3077.2562
3090.3271	3111.8852	3120.1848
3127.8921	3128.9065	3129.5321
3132.4504	3133.4272	3133.8289
3136.2895	3136.4174	3137.1048
3137.7094	3139.8156	3140.1720
3142.3001	3143.4327	3144.0185
3144.6358	3146.6613	3148.6854
3150.8493	3160.4837	3167.0592
3169.6828	3170.0011	3170.2824
3172.8772	3181.8937	3183.3596
3185.3352	3187.8814	3188.2304
3189.4718	3194.2786	3195.4779
3197.1856	3200.4325	3201.7783
3204.6867	3210.3793	3214.2432
3220.2302	3221.7540	3225.8222
3230.2939	3233.5473	3238.3607
3240.0650	3266.1456	3268.2529

M3

Zero-point correction= 1.156198
Thermal correction to Energy= 1.220439
Thermal correction to Enthalpy= 1.221383
Thermal correction to Gibbs Free Energy= 1.060273
Sum of electronic and zero-point Energies= -2806.837689
Sum of electronic and thermal Energies= -2806.773448
Sum of electronic and thermal Enthalpies= -2806.772504
Sum of electronic and thermal Free Energies= -2806.933614
Cartesian coordinates

C	-2.309133	-0.055320	0.762014
C	-0.911972	0.072698	0.432972
C	-0.395769	0.824058	-0.592514
O	-2.800243	-1.005190	1.373305
C	0.963752	1.319512	-0.708227
C	1.359899	2.034193	-1.857703
C	1.859098	1.225165	0.374524
C	2.602959	2.635248	-1.913551
H	0.677150	2.129537	-2.697440
C	3.102071	1.837450	0.312365
H	1.565154	0.699818	1.278332
C	3.489247	2.523331	-0.834790
H	2.889696	3.190041	-2.800685
H	3.788797	1.741318	1.145978
H	4.472392	2.981520	-0.887285
C	-1.305705	1.162593	-1.661632
N	-2.045676	1.361234	-2.531818
H	-0.244790	-0.468867	1.099659
C	-3.256752	1.123659	0.582342
C	-5.108145	2.277757	0.627891
C	-5.460032	-0.182646	0.449436
H	-5.058696	-0.917438	1.149070
N	-4.152089	3.160293	0.724545
N	-3.008441	2.435066	0.697088
N	-4.601530	1.013690	0.546469
C	-6.586924	2.515573	0.690755
H	-6.847076	3.386544	0.088466
H	-6.862471	2.712340	1.736551
C	-6.919250	0.184186	0.812515
O	-7.274169	1.403881	0.176625
C	-6.910629	-1.205614	-1.112380
C	-5.602625	-0.746230	-0.946325
C	-4.662089	-0.847879	-1.956620
C	-5.045104	-1.443449	-3.159849
C	-6.342724	-1.924900	-3.327027

C	-7.287461	-1.807169	-2.304792
C	-7.730907	-0.917168	0.124851
H	-3.655875	-0.459064	-1.836000
H	-6.626812	-2.384222	-4.268246
H	-8.302324	-2.164929	-2.448214
H	-7.797593	-1.796448	0.774587
H	-8.743950	-0.568949	-0.087569
C	-1.747151	3.119292	0.875962
C	-1.053774	2.908182	2.074281
C	-1.295869	3.971215	-0.134141
C	0.186197	3.524705	2.204849
C	-0.040701	4.557212	0.051487
C	0.717453	4.336577	1.197331
H	0.752780	3.368008	3.119317
H	0.348629	5.204026	-0.730962
C	-2.106504	4.313202	-1.357234
H	-2.574040	5.293326	-1.222314
H	-2.894585	3.589832	-1.561842
H	-1.457587	4.366157	-2.234503
C	2.060777	4.993243	1.369626
H	2.541607	5.153790	0.402301
H	2.721896	4.378269	1.984203
H	1.951741	5.965886	1.860474
C	-1.620989	2.068040	3.188479
H	-1.508372	0.996012	2.995845
H	-2.685698	2.268650	3.339830
H	-1.099529	2.285088	4.121754
H	-7.076934	0.257426	1.895427
H	-4.325971	-1.525551	-3.968243
H	-2.105797	-2.771167	1.413018
C	0.612026	-2.688226	2.016952
C	1.829527	-2.127082	1.635772
C	2.228665	-1.997372	0.293962
C	1.359946	-2.525034	-0.674483
C	0.117568	-3.072332	-0.362644
C	-0.274043	-3.089607	0.991705
H	2.488838	-1.753132	2.406962
H	1.680852	-2.520737	-1.706719
C	3.489237	-1.338878	-0.080009
C	3.754113	-0.942530	-1.407348
C	4.495418	-1.071094	0.873494
C	4.931245	-0.338312	-1.802574
H	2.978803	-1.095283	-2.149676
C	5.681489	-0.437268	0.570605

H	4.333117	-1.394634	1.895194
C	5.972536	-0.069231	-0.814200
O	-1.533797	-3.554261	1.325360
O	7.083378	0.439352	-1.140765
C	-0.792883	-3.628622	-1.468741
C	-1.173085	-5.090334	-1.171024
C	-2.054758	-2.761445	-1.590639
C	-0.103753	-3.610635	-2.840881
H	-0.272383	-5.709672	-1.108587
H	-1.723239	-5.178797	-0.234917
H	-1.795813	-5.480414	-1.983696
H	-1.774404	-1.733204	-1.851017
H	-2.703177	-3.143484	-2.387157
H	-2.637844	-2.740250	-0.667161
H	-0.784842	-4.035290	-3.584459
H	0.145396	-2.593917	-3.161373
H	0.812265	-4.209383	-2.842926
C	0.263161	-2.870703	3.504955
C	-0.950248	-2.014755	3.905909
C	-0.028752	-4.356505	3.785406
C	1.426390	-2.452828	4.415770
H	-0.768452	-0.961208	3.663554
H	-1.866052	-2.334592	3.409997
H	-1.110713	-2.085262	4.987296
H	0.848407	-4.966449	3.546846
H	-0.258442	-4.493935	4.847859
H	-0.873779	-4.711544	3.194949
H	1.153891	-2.656229	5.455527
H	2.339010	-3.013037	4.191038
H	1.647159	-1.383307	4.334055
C	6.729873	-0.145674	1.649445
C	7.016561	1.366795	1.695800
C	6.262882	-0.567606	3.047877
C	8.033466	-0.906327	1.344641
H	7.334555	1.720980	0.715324
H	6.118413	1.917358	2.000246
H	7.803460	1.580176	2.429350
H	6.093504	-1.647527	3.114301
H	7.034225	-0.306057	3.779823
H	5.337820	-0.056487	3.338069
H	8.784373	-0.692799	2.114958
H	7.849181	-1.986220	1.341410
H	8.422826	-0.610980	0.370590
C	5.219865	-0.041030	-3.279995

C	5.635721	1.423510	-3.505590
C	6.365011	-0.960692	-3.745821
C	4.002880	-0.310109	-4.173207
H	4.799748	2.094585	-3.291376
H	6.476871	1.684440	-2.865360
H	5.920326	1.568959	-4.554825
H	6.076981	-2.012120	-3.639083
H	6.596030	-0.774819	-4.801739
H	7.258831	-0.777231	-3.147725
H	4.251993	-0.059018	-5.209743
H	3.699763	-1.362402	-4.150122
H	3.145747	0.302995	-3.871584

Vibrational frequencies

9.7007	17.4549	24.9219
29.5032	32.9904	36.1043
38.1430	43.6898	47.4436
52.0993	55.1139	59.0170
68.4137	72.3129	75.1213
77.0779	85.1969	89.6210
93.3251	95.5245	102.4230
107.1538	115.7326	120.7306
129.8045	130.9856	133.3296
141.4764	144.7448	149.9964
160.5537	164.0799	164.9889
168.6036	175.4656	176.0837
179.7272	192.7030	194.7900
197.7345	207.5762	212.4167
220.5173	223.6899	228.8791
233.7392	237.7097	243.3385
251.4892	254.5570	261.9652
264.4876	267.8923	270.2820
273.7537	283.3442	285.0488
292.0932	295.3459	298.4069
301.1101	309.3359	315.7680
322.2726	325.2481	330.1283
332.1546	334.6381	339.3855
340.7220	344.4906	347.0271
353.3091	359.2531	362.8276
367.8528	373.6898	380.1463
385.5997	386.8355	389.9302
393.8470	399.3755	400.9567
402.3162	404.9846	407.8835
409.9839	413.8005	414.7960
438.1196	440.9529	444.2737

447.2379	455.2973	465.0357
471.8691	475.8201	481.9672
492.8209	497.2825	505.4515
521.9945	524.8528	525.2898
531.6858	540.1042	551.4956
554.6679	556.0970	575.4377
583.4156	583.7961	586.9337
595.5680	607.8494	623.7573
629.1912	641.2298	641.5677
643.2021	648.3207	655.2860
663.0718	673.8956	681.6666
685.5812	692.9145	699.8400
716.0670	728.0037	752.1037
755.0891	767.9216	773.7804
775.6299	779.6516	783.1112
787.8129	791.3407	806.3062
806.9333	821.0738	837.1743
842.0790	842.6204	844.3606
856.9813	870.6377	874.8234
879.4192	883.4278	899.5556
902.6878	905.5519	919.1112
920.0775	922.4695	922.7583
929.0209	943.4890	945.3627
948.0268	949.1961	950.8379
951.0356	953.9377	955.4414
955.9182	957.5629	958.6529
958.8615	960.3634	964.3711
966.0839	969.7186	974.3552
975.9983	988.4689	990.4681
997.1153	1013.8128	1019.4526
1020.7986	1022.3581	1039.2750
1042.0411	1042.9716	1047.1909
1049.3452	1049.5651	1053.8632
1054.8534	1054.9650	1057.2001
1057.6368	1058.1083	1060.6495
1063.7933	1064.5735	1066.8947
1070.6884	1071.1645	1081.5788
1118.7938	1126.7386	1131.8370
1135.7378	1142.1784	1152.3353
1179.6941	1187.0481	1188.2508
1194.7854	1205.2045	1211.1685
1218.8566	1222.0990	1229.2681
1237.6878	1242.5820	1243.1398
1246.8640	1248.8115	1251.7285

1252.3305 1253.6680 1254.5801
1255.9469 1261.1017 1265.7805
1273.8649 1284.1194 1284.8365
1288.6217 1298.5001 1300.2471
1311.1987 1317.4696 1321.4642
1321.7507 1325.0348 1327.9030
1329.6818 1334.0250 1341.7041
1350.6101 1358.7304 1360.9126
1364.9747 1368.5744 1374.0672
1381.1552 1381.4102 1382.2881
1385.2624 1385.9333 1390.7036
1393.9893 1397.3631 1398.0546
1401.3333 1403.8662 1412.7711
1416.5349 1418.2240 1419.5949
1422.1808 1429.0696 1430.2481
1431.5954 1440.9943 1454.0489
1456.9468 1463.5087 1472.5974
1476.0877 1481.5085 1483.8848
1485.0853 1486.6188 1489.9707
1491.8124 1494.6636 1495.1806
1495.6084 1497.6481 1499.1628
1499.2551 1500.6218 1501.2573
1502.2983 1503.7939 1504.1972
1504.9911 1506.2775 1508.8092
1509.2486 1510.3315 1516.7135
1517.8274 1517.8800 1518.5012
1519.5993 1520.0720 1520.7940
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1540.1349 1541.2069 1542.3161
1557.8445 1565.2039 1584.9546
1608.6818 1638.6088 1649.8845
1655.6457 1661.5385 1677.8897
1685.8713 1686.5633 1688.1701
1693.0442 1703.7820 1710.4587
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3048.1579 3050.2009 3052.7698
3053.6055 3056.6312 3057.2618
3058.4218 3059.5949 3063.0864
3064.0071 3068.5247 3076.3101
3078.0971 3087.2385 3092.0896
3106.6604 3112.0134 3117.0058
3119.1380 3123.0816 3124.0545
3126.5061 3128.4715 3130.4864

3133.7024	3134.9660	3135.3698
3137.1140	3139.3437	3142.3447
3144.9785	3147.4064	3148.7406
3153.4050	3155.9706	3156.8079
3167.9186	3170.9280	3171.0756
3176.3194	3179.1884	3179.3311
3181.8283	3183.5606	3188.2810
3190.5354	3192.9888	3193.2126
3194.8613	3196.9978	3199.5180
3201.0496	3203.0360	3205.9553
3211.8405	3216.0089	3216.5128
3216.7872	3225.5580	3230.7785
3236.9761	3237.2073	3240.1206
3257.0292	3272.0755	3685.2674

R2

Zero-point correction= 0.157609

Thermal correction to Energy= 0.168158

Thermal correction to Enthalpy= 0.169102

Thermal correction to Gibbs Free Energy= 0.120174

Sum of electronic and zero-point Energies= -460.001241

Sum of electronic and thermal Energies= -459.990692

Sum of electronic and thermal Enthalpies= -459.989748

Sum of electronic and thermal Free Energies= -460.038676

Cartesian coordinates

C	-2.823960	0.919313	0.622341
C	-2.240420	-0.327615	0.012729
H	-3.761826	1.170914	0.128317
H	-3.000256	0.753332	1.689988
H	-2.109722	1.740816	0.526096
C	-0.871419	-0.763166	0.516971
C	0.222224	0.123546	-0.041824
H	-0.820753	-0.709855	1.610163
H	-0.681015	-1.795006	0.214802
O	1.428547	-0.365264	0.245855
O	-2.815505	-0.976870	-0.833005
O	0.037542	1.142298	-0.667706
C	2.549208	0.400923	-0.240316
C	3.804560	-0.337357	0.164716
H	2.459265	0.498757	-1.325489
H	2.500702	1.402932	0.194930
H	4.682278	0.211917	-0.182608
H	3.862482	-0.432615	1.251214
H	3.823029	-1.336364	-0.276267

Vibrational frequencies

33.4988	55.8522	82.4971
104.2796	126.5427	149.7192
218.7625	265.7657	333.8085
379.2504	417.6896	503.5438
557.5953	595.7209	736.7014
816.1093	830.8834	899.8187
907.2519	979.7794	1039.7136
1049.9590	1090.5886	1150.7093
1182.7081	1188.5497	1231.2114
1292.1723	1309.6150	1370.1088
1399.4754	1411.2880	1443.9330
1448.9219	1470.0450	1482.3471
1492.0097	1504.8200	1531.9985
1845.5354	1872.6421	3075.2784
3082.4567	3096.8664	3106.9576
3153.0104	3158.1338	3165.6488
3170.5116	3175.2718	3194.7231

LiCl

Zero-point correction= 0.001002
Thermal correction to Energy= 0.003635
Thermal correction to Enthalpy= 0.004579
Thermal correction to Gibbs Free Energy= -0.019946
Sum of electronic and zero-point Energies= -467.812045
Sum of electronic and thermal Energies= -467.809412
Sum of electronic and thermal Enthalpies= -467.808468
Sum of electronic and thermal Free Energies= -467.832993
Cartesian coordinates

Cl	0.000000	0.000000	0.333819
Li	0.000000	0.000000	-1.891641

Vibrational frequencies
439.8802

THF

Zero-point correction= 0.118363
Thermal correction to Energy= 0.123201
Thermal correction to Enthalpy= 0.124145
Thermal correction to Gibbs Free Energy= 0.090046
Sum of electronic and zero-point Energies= -232.229403
Sum of electronic and thermal Energies= -232.224565
Sum of electronic and thermal Enthalpies= -232.223620
Sum of electronic and thermal Free Energies= -232.257720
Cartesian coordinates

C	-1.135731	-0.455614	0.145980
O	-0.012055	-1.195285	-0.304751
C	1.114542	-0.483782	0.177974
C	0.790901	0.996369	-0.072361
C	-0.756381	1.027125	-0.030928
H	-2.004196	-0.763219	-0.439741
H	-1.328312	-0.678415	1.207023
H	1.246793	-0.673172	1.254256
H	1.999461	-0.842083	-0.353187
H	1.249240	1.646814	0.675442
H	1.156544	1.304436	-1.055406
H	-1.140903	1.638011	0.789057
H	-1.162177	1.425326	-0.963426

Vibrational frequencies

51.9169	298.7829	637.6275
660.0439	807.2230	877.0046
926.4658	955.3435	964.0938
999.2622	1063.5367	1149.2475
1166.7577	1223.5908	1242.7908
1268.4023	1287.8325	1323.1391
1329.6303	1377.7100	1415.9037
1495.5611	1513.9793	1520.1224
1539.6308	3026.5468	3030.6084
3094.6094	3105.7109	3139.4961
3146.3546	3152.5164	3163.7425

LiCl·3THF

Zero-point correction= 0.362187

Thermal correction to Energy= 0.382634

Thermal correction to Enthalpy= 0.383578

Thermal correction to Gibbs Free Energy= 0.309706

Sum of electronic and zero-point Energies= -1164.560209

Sum of electronic and thermal Energies= -1164.539762

Sum of electronic and thermal Enthalpies= -1164.538818

Sum of electronic and thermal Free Energies= -1164.612689

Cartesian coordinates

Li	-0.028984	-0.585927	0.835196
Cl	0.825770	-1.129874	2.838378
C	-2.938830	-0.172164	0.884810
C	-2.182638	-1.292214	-1.054972
C	-3.900044	0.135157	-0.257717
H	-2.538944	0.714876	1.384688
H	-3.399908	-0.825155	1.633819
C	-3.687920	-1.075771	-1.170111

H	-1.869503	-2.330462	-1.181879
H	-1.632701	-0.669340	-1.773163
H	-4.929621	0.246864	0.085659
H	-3.602993	1.056010	-0.770769
H	-4.226397	-1.943683	-0.777767
H	-4.005086	-0.905828	-2.200281
C	1.276397	-0.615883	-1.808184
C	2.062950	-2.242155	-0.361608
C	2.817979	-0.584826	-1.895415
H	0.830642	0.373373	-1.675964
H	0.830837	-1.090748	-2.689631
C	3.269976	-1.361045	-0.646005
H	2.031376	-3.111417	-1.032293
H	1.969398	-2.561955	0.676781
H	3.155488	-1.087626	-2.804563
H	3.206172	0.435753	-1.914993
H	4.184721	-1.933000	-0.810138
H	3.428538	-0.685899	0.200777
O	-1.840709	-0.873655	0.276313
O	0.949824	-1.384719	-0.643260
C	1.390743	1.905425	0.795148
C	-0.670641	2.170390	-0.327629
C	1.266164	3.356383	0.347331
H	2.149700	1.369499	0.207651
H	1.606227	1.769780	1.856244
C	0.303284	3.229832	-0.836047
H	-1.477378	2.620789	0.263503
H	-1.114780	1.558099	-1.119963
H	0.816774	3.960894	1.140939
H	2.229380	3.792962	0.078748
H	-0.198651	4.163355	-1.094790
H	0.837889	2.866439	-1.720583
O	0.106281	1.316286	0.524740

Vibrational frequencies

25.5298	37.8371	48.7386
51.9923	59.6129	68.8939
76.9808	85.8252	89.2272
102.0091	107.8783	117.0169
127.2952	133.8125	148.9329
167.1335	169.9727	183.5487
272.0027	279.7653	298.5028
433.0078	484.0958	526.8005
576.1615	577.1776	597.9325
697.3368	703.3754	707.3053

811.1100	862.1491	866.3581
889.2093	889.5080	892.0057
930.2464	933.0070	936.5723
943.3838	945.5700	947.5440
949.3928	953.9405	968.0255
971.8670	975.7552	978.0243
1050.8957	1054.6152	1059.3924
1129.2464	1134.2339	1134.8504
1160.2859	1172.4318	1174.0234
1201.3198	1201.7949	1205.9798
1209.8393	1216.3079	1244.7807
1255.9088	1267.0814	1270.6717
1272.0175	1275.1640	1296.9549
1318.2542	1320.5300	1323.1520
1338.4515	1353.7963	1354.5955
1378.9709	1381.4076	1383.8679
1411.8232	1414.3875	1417.5460
1490.1168	1490.5116	1490.6634
1501.5102	1502.7065	1506.9514
1513.0721	1527.1810	1533.7214
1539.2972	1544.1845	1548.1531
3054.3860	3054.9779	3064.3699
3069.7466	3077.7908	3082.9032
3083.2941	3086.9338	3092.0961
3094.6649	3096.7203	3101.8835
3121.8293	3138.8257	3145.3057
3146.3648	3156.4156	3157.3462
3157.4231	3159.1587	3164.0172
3165.3194	3165.9612	3171.8928

R2[l]

Zero-point correction= 0.282008

Thermal correction to Energy= 0.301808

Thermal correction to Enthalpy= 0.302752

Thermal correction to Gibbs Free Energy= 0.229467

Sum of electronic and zero-point Energies= -1160.086608

Sum of electronic and thermal Energies= -1160.066808

Sum of electronic and thermal Enthalpies= -1160.065864

Sum of electronic and thermal Free Energies= -1160.139148

Cartesian coordinates

C	-0.934570	3.699457	0.608595
C	-0.761283	2.236708	0.330255
H	-0.023616	4.109096	1.041951
H	-1.200479	4.231657	-0.308802

H	-1.767061	3.826121	1.308742
C	-1.844818	1.591734	-0.518632
C	-2.038693	0.110416	-0.300787
O	-3.311064	-0.228542	-0.378518
O	0.202513	1.615263	0.738722
O	-1.144606	-0.693076	-0.106672
C	-3.614851	-1.637815	-0.235881
C	-5.115793	-1.779013	-0.330312
H	-3.094615	-2.179444	-1.029690
H	-3.223404	-1.976271	0.726132
H	-5.387053	-2.832170	-0.232470
H	-5.607159	-1.218945	0.467894
H	-5.479414	-1.414697	-1.293320
Li	0.665146	-0.267592	0.467988
Cl	1.581880	-1.393160	2.160794
H	-2.794551	2.114572	-0.399156
O	1.816584	-0.145253	-1.097647
C	2.811839	0.883810	-1.085170
C	2.516574	-1.379867	-1.329609
C	3.960504	0.276005	-0.288915
H	3.109364	1.108251	-2.118455
H	2.363973	1.771129	-0.634149
C	3.912060	-1.210896	-0.697056
H	1.927804	-2.178389	-0.873055
H	2.579580	-1.546743	-2.411074
H	3.753375	0.375799	0.779217
H	4.918287	0.750091	-0.510835
H	4.027812	-1.858022	0.172992
H	4.692712	-1.455654	-1.420631
H	-1.536181	1.729745	-1.564760

Vibrational frequencies

16.4430	18.3146	30.9992
48.5879	60.0535	79.6675
85.7032	89.3075	97.0723
112.6070	117.5262	133.8019
143.9335	159.5156	172.6574
180.7054	257.7684	277.1351
314.6510	324.6070	364.4970
401.8097	433.9477	459.7607
477.8971	526.3058	590.0343
606.9276	612.5736	693.3572
782.3957	796.2994	824.3654
851.4165	871.7697	882.3964
929.1484	933.5006	958.8777

963.1348	978.4967	990.5233
1023.6554	1058.9228	1067.6023
1084.6193	1126.9414	1152.2755
1158.4981	1186.7749	1198.3705
1217.4507	1226.8315	1250.5160
1262.2266	1309.5884	1315.7534
1321.6016	1332.2565	1338.8901
1383.6025	1392.2028	1408.2769
1414.7325	1425.0109	1436.1824
1460.8496	1470.3153	1478.1875
1488.1633	1493.7354	1504.1041
1505.1680	1520.9329	1528.6399
1537.4966	1799.5480	1854.3180
3063.0231	3071.7040	3074.3430
3076.5285	3088.1066	3104.6256
3108.5476	3115.4300	3147.7659
3154.3047	3158.9731	3164.0153
3165.5300	3170.0070	3172.6746
3174.3928	3185.4779	3206.9696

R2^{I-}

Zero-point correction= 0.269359
Thermal correction to Energy= 0.288663
Thermal correction to Enthalpy= 0.289607
Thermal correction to Gibbs Free Energy= 0.218463
Sum of electronic and zero-point Energies= -1159.628974
Sum of electronic and thermal Energies= -1159.609670
Sum of electronic and thermal Enthalpies= -1159.608726
Sum of electronic and thermal Free Energies= -1159.679870
Cartesian coordinates

C	-0.738541	3.816222	0.059880
C	-0.736373	2.307326	0.229942
H	0.060941	4.096416	-0.632749
H	-1.688565	4.203863	-0.311324
H	-0.510038	4.283644	1.022149
C	-1.909754	1.614529	-0.081977
C	-2.045342	0.209075	0.071682
O	-3.288979	-0.236987	-0.254703
O	0.345908	1.797867	0.648353
O	-1.192047	-0.607761	0.457700
C	-3.508529	-1.642881	-0.134880
C	-4.921998	-1.915946	-0.604481
H	-2.772144	-2.181247	-0.739791
H	-3.363923	-1.948661	0.906511

H	-5.143024	-2.983283	-0.529191
H	-5.643163	-1.368029	0.006712
H	-5.046501	-1.608198	-1.645568
Li	0.616045	-0.050518	0.676487
Cl	1.891434	-1.093131	2.270128
H	-2.778212	2.159348	-0.426556
O	1.499243	-0.364542	-1.085907
C	2.446656	0.649482	-1.423919
C	2.187029	-1.617118	-1.177941
C	3.727067	0.205796	-0.723922
H	2.576655	0.677930	-2.515644
H	2.039147	1.597706	-1.070538
C	3.664500	-1.330581	-0.840001
H	1.710307	-2.300450	-0.472839
H	2.077396	-2.007763	-2.197588
H	3.685823	0.501991	0.327128
H	4.623128	0.633787	-1.178402
H	3.948730	-1.806458	0.099190
H	4.319636	-1.699853	-1.632978

Vibrational frequencies

17.1611	35.6356	46.7146
49.8488	58.3546	68.4367
90.0774	95.9766	119.9237
128.4328	138.0728	145.7290
163.2181	166.3015	178.9276
182.7722	257.7209	268.5581
312.8521	331.6724	392.2271
423.8731	426.0411	465.6542
537.3167	603.4927	608.2448
617.9735	700.2134	735.0798
781.7716	791.1722	809.2890
809.4279	889.4549	898.9322
935.6737	958.9652	970.8418
983.7284	989.3169	1001.4182
1048.4926	1053.6197	1069.7949
1130.7349	1138.6991	1153.6702
1160.6741	1185.0016	1195.1539
1226.2965	1247.9672	1262.6282
1296.9606	1298.0407	1303.5113
1320.4616	1341.9957	1381.5694
1389.3134	1399.6530	1413.0631
1434.2114	1477.1901	1481.6803
1491.5932	1494.5113	1503.6954
1508.8135	1512.2468	1528.7791

1531.1263	1556.8418	1581.6350
1733.4968	3040.9926	3055.9330
3065.8718	3072.0907	3082.5225
3097.2210	3105.6877	3124.7956
3136.7519	3153.9750	3158.4195
3160.7883	3162.6983	3170.7284
3179.4431	3181.5936	3245.7241

TS3'

Zero-point correction= 0.817256

Thermal correction to Energy= 0.867265

Thermal correction to Enthalpy= 0.868210

Thermal correction to Gibbs Free Energy= 0.734370

Sum of electronic and zero-point Energies= -2726.533239

Sum of electronic and thermal Energies= -2726.483229

Sum of electronic and thermal Enthalpies= -2726.482285

Sum of electronic and thermal Free Energies= -2726.616125

Cartesian coordinates

C	1.530195	-0.459141	-1.228304
C	0.297695	-0.591510	-0.719606
C	-0.295200	-0.023248	0.500707
O	2.013606	-1.198649	-2.282384
C	-1.450282	0.901782	0.327674
C	-1.785185	1.834045	1.319340
C	-2.286069	0.796438	-0.792636
C	-2.918922	2.629902	1.196270
H	-1.147741	1.940355	2.194487
C	-3.426100	1.584529	-0.906929
H	-2.065985	0.076782	-1.572744
C	-3.750111	2.507685	0.084432
H	-3.151009	3.351911	1.975111
H	-4.064532	1.467582	-1.777864
H	-4.635983	3.128903	-0.008132
C	0.647383	0.338636	1.513414
N	1.392756	0.530807	2.387857
H	-0.362269	-1.303817	-1.225305
C	2.549280	0.531828	-0.853571
C	4.492482	1.483671	-0.551856
C	4.606950	-0.989496	-0.865297
H	4.221034	-1.508323	-1.745689
N	3.628685	2.454942	-0.517252
N	2.423275	1.856436	-0.712527
N	3.875768	0.284541	-0.766184
C	5.985986	1.569875	-0.460717

H	6.268602	2.282441	0.314968
H	6.381230	1.919080	-1.425076
C	6.123453	-0.714911	-1.014497
O	6.512896	0.312794	-0.115292
C	5.785461	-2.480180	0.542828
C	4.546097	-1.862875	0.367917
C	3.485175	-2.105665	1.226510
C	3.678269	-3.003437	2.277252
C	4.908429	-3.638227	2.449075
C	5.973467	-3.378466	1.584631
C	6.765200	-2.009467	-0.507961
H	2.534238	-1.597011	1.106388
H	5.043027	-4.332849	3.271795
H	6.935375	-3.859384	1.733749
H	6.850624	-2.732820	-1.326040
H	7.766950	-1.811747	-0.120246
C	1.250935	2.688871	-0.810105
C	0.467702	2.645721	-1.969239
C	0.999594	3.576004	0.249382
C	-0.643195	3.489644	-2.014951
C	-0.111851	4.403223	0.131774
C	-0.953880	4.366347	-0.981034
H	-1.277609	3.459224	-2.897598
H	-0.338192	5.085334	0.947826
C	1.882410	3.681937	1.465993
H	2.747934	4.317096	1.257268
H	2.249095	2.708144	1.793097
H	1.319136	4.128901	2.287701
C	-2.145971	5.280434	-1.072744
H	-1.852666	6.259391	-1.466459
H	-2.593969	5.434912	-0.088279
H	-2.908407	4.862848	-1.734042
C	0.760219	1.776506	-3.165004
H	0.132669	0.879527	-3.155562
H	1.801404	1.449740	-3.213748
H	0.537935	2.330581	-4.079294
H	6.399531	-0.445913	-2.041594
H	2.865541	-3.203910	2.968170
C	-1.962187	-1.237186	2.413082
C	-1.229333	-1.732527	1.155362
C	-3.313030	-0.584924	2.251635
H	-2.160163	-2.137668	3.013802
C	-0.029791	-2.592146	1.537696
O	-1.905078	-2.117861	0.149065

O	-3.586321	0.198876	3.292254
O	-4.121374	-0.787535	1.363515
H	0.592213	-2.128530	2.308109
H	-0.415916	-3.540993	1.926187
H	0.571268	-2.813104	0.652158
Li	-3.746843	-2.028902	-0.099177
C	-4.886285	0.818501	3.304619
O	-3.957762	-1.543119	-1.995520
Cl	-4.918108	-3.993392	0.101241
C	-4.910075	1.770643	4.478813
H	-5.030742	1.335477	2.352736
H	-5.644647	0.035074	3.392135
C	-5.297947	-1.607493	-2.514470
C	-3.087233	-2.390709	-2.765734
H	-4.139300	2.536851	4.364152
H	-5.883687	2.262369	4.536256
H	-4.734558	1.237161	5.415608
C	-5.309110	-2.793111	-3.470879
H	-5.984250	-1.727735	-1.672582
H	-5.515540	-0.665372	-3.033026
C	-3.879013	-2.764113	-4.014932
H	-2.167078	-1.835578	-2.975921
H	-2.840541	-3.275367	-2.167891
H	-6.073052	-2.699262	-4.244956
H	-5.478525	-3.712503	-2.903764
H	-3.555407	-3.716678	-4.438293
H	-3.775948	-1.988565	-4.780701
H	1.469252	-1.989737	-2.392853
H	-1.325791	-0.595902	3.028362

Vibrational frequencies

-254.3344	20.0334	23.9564
26.8600	37.7429	40.1538
43.8155	46.0723	55.6942
60.2496	66.9974	68.9309
69.4814	78.3236	82.6851
86.2552	93.5662	98.0405
102.6213	111.3852	115.4847
117.8085	123.0293	129.0431
130.6346	135.6526	138.2942
144.9687	149.3145	157.2806
161.2165	172.2134	173.8843
184.0325	194.0366	199.0618
211.4929	214.9481	219.8392
226.1577	241.1253	246.3156

250.4341 261.5536 268.6645
275.1972 279.6110 283.0428
286.5738 295.6453 298.7271
309.5243 316.8946 321.0614
328.8690 334.6227 343.0763
350.3759 359.8618 367.6679
385.7971 391.5698 403.0195
409.9536 423.4506 429.1877
434.5143 442.3715 453.4449
478.2674 479.4549 485.4774
495.4315 504.3772 509.2347
525.2844 529.8656 540.2003
551.2072 554.5445 575.2330
578.5355 580.3653 586.1296
589.9615 593.4133 609.9546
624.3097 629.9743 630.6167
646.3660 654.9070 669.3896
686.2787 686.6816 706.7390
708.4697 726.4601 750.4435
754.8164 764.2296 773.8535
778.6048 785.0480 809.8542
817.5478 819.6837 843.6783
849.7397 857.6595 860.8526
874.3295 879.0066 882.4664
891.9043 900.4658 901.5533
915.7326 921.2217 922.2587
928.3865 936.8242 941.0377
946.9244 951.8536 958.5101
971.0508 975.8433 978.8087
981.8851 984.5477 987.6739
1001.5785 1007.2891 1017.4105
1018.0433 1020.1330 1024.8028
1042.5901 1047.2532 1048.6995
1053.1772 1054.8877 1055.3139
1059.9180 1063.8414 1065.9091
1068.0879 1071.5847 1076.1304
1082.1716 1096.5577 1117.5016
1121.0452 1128.8343 1132.1343
1152.3862 1169.4036 1174.1115
1176.5389 1179.1375 1184.2364
1187.9661 1188.9278 1196.9439
1208.5885 1212.5077 1213.2525
1216.0036 1222.2241 1227.5984
1238.6078 1252.3337 1256.1224

1265.4244	1274.1124	1276.2910
1280.6484	1286.8545	1292.4862
1295.0032	1307.0011	1311.9848
1317.7545	1319.0300	1325.3628
1329.0362	1340.8939	1342.4153
1346.9039	1359.3983	1364.8972
1366.7559	1372.0253	1378.6099
1382.0431	1387.8465	1391.3513
1398.5932	1409.1759	1414.2413
1418.5006	1419.2892	1420.2743
1420.6441	1430.2972	1440.1929
1460.4686	1462.8805	1464.7706
1472.3490	1478.5755	1487.9233
1488.4727	1489.7090	1490.3694
1492.9493	1493.5686	1494.2171
1496.6251	1497.9419	1502.5141
1506.2361	1507.8219	1518.2447
1519.5244	1520.9184	1522.1251
1533.0559	1535.6954	1540.6096
1541.9307	1545.0663	1559.3933
1596.4722	1664.0355	1675.5309
1683.8781	1689.8808	1691.7004
1700.8639	1710.1700	1749.8163
1818.0002	2334.9915	3053.2239
3059.5044	3060.7896	3067.7107
3068.6942	3079.4917	3080.7554
3080.9054	3083.6018	3087.4344
3092.2630	3095.8242	3103.7554
3105.8523	3124.8665	3129.2372
3139.9798	3143.6208	3147.0609
3152.2244	3153.0888	3153.7739
3154.0424	3154.7702	3157.0358
3158.9874	3167.6015	3168.3734
3168.8060	3169.0439	3170.6687
3174.2125	3176.3514	3179.8193
3188.9558	3190.4679	3191.1190
3196.9582	3205.8627	3206.2215
3212.2777	3218.1048	3228.9229
3235.0015	3242.8047	3858.4526

M3'

Zero-point correction= 0.818579

Thermal correction to Energy= 0.868824

Thermal correction to Enthalpy= 0.869769

Thermal correction to Gibbs Free Energy= 0.735337
Sum of electronic and zero-point Energies= -2726.534930
Sum of electronic and thermal Energies= -2726.484684
Sum of electronic and thermal Enthalpies= -2726.483740
Sum of electronic and thermal Free Energies= -2726.618171
Cartesian coordinates

C	1.568914	-0.398518	-1.317992
C	0.370124	-0.679819	-0.802412
C	-0.297053	-0.276733	0.479977
O	2.050554	-0.960108	-2.472881
C	-1.384675	0.768089	0.287505
C	-1.673377	1.697393	1.289822
C	-2.207341	0.714145	-0.841997
C	-2.772920	2.543885	1.174648
H	-1.045104	1.755204	2.175798
C	-3.304510	1.561331	-0.955391
H	-2.028448	-0.026849	-1.611773
C	-3.596499	2.475570	0.053888
H	-2.981249	3.260212	1.965002
H	-3.943006	1.485168	-1.830136
H	-4.456691	3.133014	-0.031411
C	0.689589	0.135361	1.472503
N	1.483614	0.379007	2.281904
H	-0.249546	-1.394003	-1.348895
C	2.585232	0.565812	-0.847685
C	4.530886	1.476601	-0.467060
C	4.635076	-0.962592	-0.988297
H	4.240201	-1.399907	-1.908321
N	3.671567	2.447925	-0.363487
N	2.464472	1.873683	-0.607158
N	3.907998	0.301557	-0.773502
C	6.024772	1.548533	-0.364116
H	6.307105	2.184658	0.475275
H	6.423324	1.984058	-1.291078
C	6.151080	-0.676696	-1.123953
O	6.545404	0.262996	-0.135078
C	5.825375	-2.570671	0.274413
C	4.585573	-1.939369	0.164882
C	3.532445	-2.255119	1.007861
C	3.731752	-3.239713	1.976383
C	4.962950	-3.886118	2.083550
C	6.020685	-3.554641	1.234675
C	6.794814	-2.012349	-0.742916
H	2.580335	-1.741179	0.936537

H	5.104017	-4.647810	2.843315
H	6.983020	-4.047270	1.334281
H	6.865749	-2.659837	-1.623537
H	7.802317	-1.852855	-0.352694
C	1.297040	2.719070	-0.638012
C	0.502522	2.755077	-1.789778
C	1.076845	3.557816	0.468409
C	-0.592648	3.620396	-1.777434
C	-0.014012	4.417261	0.403214
C	-0.868120	4.454409	-0.700225
H	-1.238516	3.645391	-2.651628
H	-0.216113	5.063624	1.254025
C	1.966916	3.580797	1.684431
H	2.826069	4.236618	1.518003
H	2.345029	2.589988	1.937747
H	1.405224	3.962280	2.539584
C	-2.041908	5.395595	-0.731297
H	-1.726781	6.394815	-1.049445
H	-2.493949	5.488238	0.259400
H	-2.806743	5.043267	-1.426749
C	0.759600	1.951014	-3.037374
H	0.120247	1.062538	-3.059701
H	1.795006	1.617479	-3.132030
H	0.519636	2.557139	-3.913056
H	6.421546	-0.313277	-2.123025
H	2.922207	-3.499785	2.650850
C	-1.836787	-1.394111	2.303500
C	-1.060586	-1.715638	0.992993
C	-3.175882	-0.707736	2.195682
H	-2.064174	-2.367031	2.760401
C	0.056773	-2.706449	1.371473
O	-1.801983	-2.161221	-0.010513
O	-3.409369	0.065107	3.258106
O	-4.011541	-0.872380	1.324804
H	0.683027	-2.363897	2.202564
H	-0.423589	-3.645204	1.660352
H	0.686661	-2.912431	0.501052
Li	-3.618443	-2.110510	-0.130535
C	-4.697216	0.704457	3.312087
O	-4.215360	-1.367390	-1.867909
Cl	-4.939437	-4.001545	0.068053
C	-4.683872	1.624373	4.512214
H	-4.853054	1.249852	2.377534
H	-5.467437	-0.068165	3.392780

C	-5.641581	-1.191800	-1.939758
C	-3.768240	-2.215649	-2.937608
H	-3.904610	2.382956	4.403386
H	-5.648997	2.127408	4.604151
H	-4.496367	1.062134	5.429752
C	-6.125700	-2.170149	-3.004796
H	-6.062660	-1.391604	-0.950904
H	-5.846006	-0.150708	-2.219579
C	-4.915919	-2.239722	-3.939892
H	-2.837529	-1.800355	-3.335090
H	-3.576299	-3.217974	-2.535363
H	-7.040803	-1.834192	-3.496252
H	-6.298527	-3.147827	-2.546802
H	-4.901918	-3.133191	-4.566675
H	-4.878138	-1.356944	-4.586661
H	1.486896	-1.702613	-2.732238
H	-1.221505	-0.844944	3.022721

Vibrational frequencies

22.3257	25.0075	27.0042
31.0189	38.1609	44.6548
50.0901	58.0652	59.7948
63.1162	64.6425	68.2670
75.2659	80.3414	81.5704
89.9361	95.2994	96.9654
105.9347	113.0089	115.9398
120.9766	126.4742	130.9070
134.1896	139.1219	143.5941
153.0848	160.0563	162.9540
173.1088	176.2502	187.1306
192.2856	198.9649	213.4232
214.8728	221.1132	226.0736
242.8219	249.3247	253.6371
268.4723	277.2296	281.3630
286.0231	286.4256	289.8915
290.5177	300.6905	309.8596
311.5142	319.5638	326.6410
329.9075	347.1102	351.0955
355.2086	364.7935	380.4766
386.3444	397.2240	403.3353
414.4088	427.8031	429.7908
433.0460	443.1315	465.8125
478.8466	480.5396	492.6734
495.5895	506.9662	510.7893
524.7310	529.9334	547.3205

551.8089 556.7603 573.4025
581.4284 582.1099 588.9985
597.5884 612.1953 624.4796
631.7890 632.7819 650.8128
656.7175 669.3247 672.9000
686.3075 709.1854 710.2149
725.6614 730.0567 746.9078
752.3652 765.5790 777.4397
785.9544 802.5417 811.6862
816.3997 821.0227 842.2879
856.6894 863.6788 864.3292
874.8686 876.3003 882.7511
894.9075 897.8653 907.9298
919.2689 926.9589 928.0957
929.9330 933.0053 941.7508
948.5596 952.4279 958.4137
968.3820 971.7818 979.7108
980.5518 982.3215 983.4458
1004.4006 1009.4855 1015.4077
1021.3792 1025.5412 1026.9512
1043.1007 1046.0505 1049.2650
1054.2330 1055.0156 1058.0216
1062.0739 1064.4134 1068.2188
1071.2751 1076.7027 1082.7788
1086.7759 1097.4971 1119.2044
1121.5012 1128.0271 1133.9253
1153.1055 1153.8660 1174.9209
1178.5126 1180.8537 1183.3216
1185.8674 1188.5279 1195.0818
1207.1267 1211.6487 1212.9890
1214.7289 1221.4370 1223.3597
1238.0834 1240.8193 1253.9138
1256.0395 1267.9809 1276.2322
1277.8799 1283.7612 1289.9118
1290.6617 1293.8850 1310.5240
1315.4854 1318.7861 1325.9467
1327.8653 1338.0066 1339.9551
1344.2553 1347.8612 1362.3525
1366.5363 1366.9542 1373.2846
1380.3842 1388.5114 1389.5018
1390.8658 1393.2648 1410.8711
1415.6197 1416.9398 1420.1774
1421.4740 1423.5131 1428.6750
1447.1486 1462.1552 1462.9750

1463.4002	1471.9796	1476.2113
1486.7082	1488.6891	1492.6555
1492.8385	1493.4089	1495.3232
1499.2489	1499.4455	1501.3934
1501.8476	1507.6085	1510.1008
1517.9718	1518.3227	1518.7999
1522.4275	1531.7984	1535.1871
1538.6037	1540.6571	1547.4962
1603.9109	1671.2759	1673.0913
1683.6970	1688.3882	1695.8715
1699.4895	1709.5794	1775.3385
1819.4655	2383.2512	3057.8014
3066.3915	3066.4670	3068.3931
3068.7609	3078.4629	3079.5495
3081.0927	3081.1840	3090.3342
3091.5524	3101.4021	3103.3218
3107.8501	3133.0936	3133.1763
3141.3081	3142.6530	3145.4634
3149.0265	3150.4104	3150.8783
3151.2883	3154.5284	3155.2000
3156.5693	3163.7352	3167.2735
3169.8777	3171.3859	3171.4091
3172.0103	3178.9431	3185.0110
3189.7817	3194.5844	3201.1247
3207.2654	3208.7234	3210.8929
3218.0917	3219.5211	3241.5911
3245.1372	3255.2595	3853.1672

TS4

Zero-point correction= 1.436552

Thermal correction to Energy= 1.521258

Thermal correction to Enthalpy= 1.522202

Thermal correction to Gibbs Free Energy= 1.313436

Sum of electronic and zero-point Energies= -3966.940032

Sum of electronic and thermal Energies= -3966.855327

Sum of electronic and thermal Enthalpies= -3966.854383

Sum of electronic and thermal Free Energies= -3967.063149

Cartesian coordinates

C	4.493624	-0.010451	0.018116
C	3.036251	-0.073528	0.081561
C	2.320868	-1.150656	0.499015
O	5.119307	0.751555	-0.696115
C	0.928940	-1.129222	0.951539
C	0.248561	-2.331117	1.208715

C	0.317150	0.093510	1.269152
C	-1.015517	-2.304994	1.778908
H	0.715541	-3.282708	0.972057
C	-0.954771	0.114331	1.821912
H	0.836481	1.031259	1.097297
C	-1.615818	-1.082912	2.089185
H	-1.535798	-3.235382	1.978748
H	-1.435040	1.067841	2.022282
H	-2.607996	-1.063206	2.529697
C	2.986758	-2.435398	0.508989
N	3.527518	-3.456702	0.436054
H	2.537863	0.863138	-0.161537
C	5.348010	-0.794312	1.004422
C	7.114523	-1.681021	1.911535
C	7.408123	-1.047894	-0.493348
H	7.329034	-0.009195	-0.820321
N	6.228824	-1.621347	2.868336
N	5.133618	-1.070123	2.295768
N	6.617478	-1.162555	0.751540
C	8.519144	-2.199062	1.975846
H	8.547863	-3.103496	2.584133
H	9.164051	-1.437487	2.435835
C	8.887362	-1.417089	-0.208000
O	8.946056	-2.524659	0.677106
C	8.168218	-2.479503	-2.216848
C	7.012577	-2.015035	-1.587030
C	5.752148	-2.410190	-2.010469
C	5.656197	-3.290997	-3.087551
C	6.807246	-3.753536	-3.724559
C	8.072011	-3.351322	-3.293691
C	9.402302	-1.899574	-1.566478
H	4.846620	-2.070539	-1.517926
H	6.718020	-4.440891	-4.559254
H	8.966040	-3.722199	-3.785201
H	9.792036	-1.053895	-2.142816
H	10.210332	-2.621379	-1.429335
C	3.941826	-0.875873	3.091457
C	3.420683	0.414105	3.239316
C	3.358333	-2.011078	3.675943
C	2.221281	0.538756	3.939440
C	2.156271	-1.820372	4.354507
C	1.562498	-0.563678	4.480685
H	1.785514	1.528987	4.048269
H	1.666502	-2.686646	4.791759

C	3.982745	-3.381457	3.631312
H	4.727850	-3.477958	4.426316
H	4.482625	-3.588460	2.684800
H	3.215426	-4.141761	3.785453
C	0.253197	-0.403282	5.204808
H	-0.272121	0.494575	4.872086
H	0.417504	-0.320572	6.283961
H	-0.393687	-1.265879	5.028643
C	4.063578	1.648434	2.662265
H	3.554687	1.958503	1.740337
H	5.126335	1.517153	2.443684
H	3.972006	2.477481	3.367283
H	9.448079	-0.571736	0.208590
H	4.678768	-3.617292	-3.426475
H	5.023725	2.161647	-2.123027
C	2.789936	3.389828	-1.108053
C	1.482594	3.230602	-0.632451
C	0.540320	2.406233	-1.264886
C	0.967345	1.698311	-2.394141
C	2.275152	1.754629	-2.876447
C	3.178277	2.608063	-2.214417
H	1.176981	3.777902	0.250285
H	0.243588	1.095751	-2.924530
C	-0.856534	2.288959	-0.775676
C	-1.678580	1.227188	-1.169281
C	-1.413479	3.223952	0.105660
C	-2.995177	1.081270	-0.751183
H	-1.260927	0.458161	-1.808058
C	-2.714259	3.128125	0.589779
H	-0.812941	4.076057	0.401964
C	-3.552899	2.049899	0.144883
O	4.472152	2.714352	-2.695805
O	-4.787562	2.005858	0.584217
C	2.702275	0.905848	-4.085512
C	3.244136	1.794452	-5.219190
C	3.767015	-0.112673	-3.642471
C	1.527680	0.102956	-4.663016
H	2.473064	2.498662	-5.547961
H	4.121370	2.358564	-4.905701
H	3.516012	1.168808	-6.076335
H	3.366995	-0.743365	-2.838800
H	4.037354	-0.766181	-4.479486
H	4.678501	0.369389	-3.284720
H	1.884034	-0.477466	-5.519084

H	1.111591	-0.600437	-3.934573
H	0.722439	0.755185	-5.014896
C	3.719242	4.468824	-0.518180
C	5.105411	3.937498	-0.105216
C	3.908258	5.559239	-1.589974
C	3.101166	5.130079	0.722301
H	5.027089	3.038493	0.511907
H	5.731094	3.712209	-0.968734
H	5.622880	4.702642	0.482617
H	2.945808	6.007252	-1.855404
H	4.561550	6.350505	-1.205731
H	4.360848	5.138691	-2.490283
H	3.784779	5.898767	1.093646
H	2.148601	5.617410	0.495947
H	2.936710	4.409070	1.531218
C	-3.261324	4.166089	1.582299
C	-3.664282	3.467418	2.894519
C	-2.218234	5.234034	1.938340
C	-4.476146	4.900028	0.986670
H	-4.406682	2.691253	2.707511
H	-2.785029	3.012162	3.365927
H	-4.079352	4.198866	3.598114
H	-1.914684	5.816330	1.061922
H	-2.650833	5.928704	2.665390
H	-1.320649	4.795811	2.388237
H	-4.842743	5.653117	1.694273
H	-4.192995	5.414225	0.061803
H	-5.278185	4.195956	0.767822
C	-3.854401	-0.077225	-1.266417
C	-4.360033	-0.941034	-0.093281
C	-5.012619	0.501861	-2.102024
C	-3.083140	-1.030260	-2.189807
H	-3.540554	-1.567844	0.272774
H	-4.713260	-0.339005	0.746070
H	-5.167780	-1.601923	-0.427967
H	-4.618556	0.897277	-3.044778
H	-5.750447	-0.274911	-2.334645
H	-5.510595	1.324322	-1.588742
H	-3.760069	-1.826940	-2.516355
H	-2.708246	-0.522223	-3.084458
H	-2.236306	-1.496264	-1.672827
H	-5.919377	1.326934	0.425203
C	-7.971761	2.842958	-0.922966
C	-7.872030	1.366217	-0.628831

H	-8.346495	3.000741	-1.933794
H	-8.642520	3.318630	-0.200804
H	-6.984538	3.301974	-0.805037
C	-7.169740	1.026069	0.612028
C	-7.243041	-0.345777	1.125699
O	-6.804706	-0.421782	2.388380
O	-8.306091	0.548232	-1.442788
O	-7.592193	-1.353059	0.519242
C	-6.693621	-1.742476	2.944034
C	-6.126588	-1.591085	4.337947
H	-7.681899	-2.211224	2.950966
H	-6.041731	-2.338450	2.297742
H	-6.015926	-2.573771	4.801638
H	-5.146272	-1.109782	4.302149
H	-6.788525	-0.984931	4.960314
Li	-8.232192	-1.354333	-1.286219
Cl	-7.274693	-2.770231	-2.770598
H	-7.322465	1.764272	1.401306
O	-10.045798	-2.032874	-0.998844
C	-10.784577	-2.242573	-2.217591
C	-9.960274	-3.264909	-0.256006
C	-10.912615	-3.753520	-2.363994
H	-11.764013	-1.760517	-2.116210
H	-10.232984	-1.774951	-3.037528
C	-10.976080	-4.200117	-0.901634
H	-8.941253	-3.658798	-0.353085
H	-10.162239	-3.043270	0.794501
H	-10.011055	-4.149666	-2.839571
H	-11.787574	-4.043132	-2.948886
H	-10.719886	-5.251203	-0.756828
H	-11.975147	-4.024080	-0.489982

Vibrational frequencies

-1125.4762	10.7517	12.7292
16.7195	20.0651	23.8749
25.2338	27.7789	30.5827
33.8303	35.6664	39.3867
41.8067	45.6251	49.9424
50.2883	54.2680	55.1540
59.0301	61.8224	63.5445
68.4322	70.3921	73.7006
77.6076	77.7264	81.3810
83.3018	85.2454	90.2517
94.9494	97.5669	101.3901
102.4946	114.8757	118.8034

120.5774 121.8881 123.7040
127.6928 131.4103 134.4675
135.8100 140.3093 140.9628
143.6642 149.3447 149.9043
154.6422 159.3307 161.7717
163.4963 164.8114 168.8249
176.1374 177.9290 184.9365
189.7707 197.2634 201.7564
202.8229 208.1264 213.6766
214.8704 220.1871 227.0184
231.2002 234.2908 236.3137
242.7763 249.7094 256.1272
261.7893 265.3835 266.2496
269.2441 271.6294 275.2669
276.4145 281.8303 288.0068
296.4497 299.1456 300.7965
304.9814 309.3169 309.7618
314.7058 325.2507 326.6812
328.7886 329.6154 330.8978
335.7097 338.1370 339.8083
350.3931 353.1879 354.4617
358.5708 359.2821 379.5287
382.0682 382.9847 384.0292
386.1826 386.9157 390.3829
396.7436 397.6282 400.2518
405.1233 408.1990 410.2591
413.1501 413.9148 420.7484
427.5772 434.4602 436.6336
440.7750 443.4036 447.6748
455.0044 458.5472 468.5021
469.9257 470.4630 474.8456
479.8644 482.7579 489.1035
494.6244 506.9789 527.9581
538.3868 541.5499 546.3966
549.6578 551.0535 557.6154
565.2211 569.3113 574.6589
582.8500 590.6154 591.5315
600.1329 600.4815 616.5787
624.8107 629.6415 629.8823
641.2732 645.7483 650.4646
652.3543 658.3349 662.7719
680.6763 682.2182 682.5578
694.4455 697.2938 703.3458
713.8645 724.8060 742.3066

747.2129	753.8240	762.1489
776.0895	781.2590	782.1010
784.2259	787.9930	797.8666
799.0819	801.0039	808.0298
816.1021	823.3629	839.6990
843.8879	850.3622	859.7414
868.7294	869.9006	871.9938
877.2037	886.1445	890.6251
891.7652	893.7658	900.2246
908.9121	913.9734	918.5802
921.0408	923.7795	928.5870
929.2571	932.4991	933.5297
934.8508	938.0785	948.4184
949.8992	951.0372	953.4289
953.8924	956.3772	956.5722
958.7129	959.2326	959.9972
961.0105	961.7687	962.1965
966.7794	967.1727	970.5473
975.3315	976.7795	978.4813
979.4065	984.6483	996.8606
999.9328	1010.9757	1018.7606
1022.4531	1030.2652	1041.0666
1041.7253	1043.6978	1044.9143
1046.7181	1048.1157	1050.9817
1051.7930	1054.3965	1054.7089
1055.5459	1056.4063	1057.8445
1058.0317	1058.7414	1059.4976
1063.4928	1068.3719	1070.5477
1070.8341	1072.9126	1077.2024
1084.6716	1108.7032	1123.3467
1125.8850	1128.2652	1143.5482
1147.7529	1150.3413	1155.3852
1160.3894	1175.3908	1179.4164
1180.8266	1184.4361	1187.1515
1194.3818	1194.6262	1207.7025
1210.3667	1210.5741	1213.1858
1215.0394	1228.6935	1229.9141
1233.1849	1237.0116	1244.1831
1245.2895	1246.7402	1249.8215
1250.5980	1252.2130	1253.0815
1254.5378	1256.3530	1263.8541
1269.1870	1281.4218	1282.6695
1284.5330	1287.7289	1288.1077
1290.8452	1296.7266	1301.7998

1306.5474 1312.4016 1313.9682
1316.2502 1321.2271 1326.6987
1327.3556 1327.5257 1328.7291
1333.3319 1335.4442 1342.7853
1345.8012 1353.4820 1355.8215
1358.3804 1365.4188 1366.3240
1372.0304 1379.4562 1380.1881
1383.0520 1384.5529 1386.3397
1392.5070 1392.6716 1394.8950
1397.3537 1399.9665 1402.0502
1405.3392 1405.5399 1406.8222
1411.4376 1411.4549 1419.1939
1422.3284 1422.7824 1424.4363
1428.7531 1430.7411 1431.4553
1433.6617 1441.3740 1451.5192
1457.9384 1465.1572 1466.2445
1470.3856 1471.7716 1472.9751
1478.6161 1481.3123 1485.3002
1485.5286 1486.4338 1490.0037
1490.2062 1492.5046 1495.4539
1495.6955 1496.3422 1496.6972
1497.7565 1498.4885 1500.3219
1500.8975 1502.5333 1503.4006
1503.5560 1504.6286 1504.9254
1505.5820 1506.7408 1509.2293
1511.3939 1512.6879 1512.9643
1514.0408 1517.5004 1517.6353
1519.2036 1519.8447 1521.2952
1521.6139 1525.7533 1526.3248
1531.6763 1532.3234 1533.9709
1534.4036 1534.7120 1536.8363
1536.9874 1540.0889 1540.5703
1542.2409 1553.1198 1563.8024
1567.2032 1621.6425 1637.8822
1650.0890 1664.4848 1668.1562
1677.0759 1684.1182 1686.5053
1688.5358 1690.4275 1692.3314
1707.5938 1733.5067 1787.3151
1814.8800 2404.9386 3044.8200
3046.7971 3050.6876 3052.1225
3055.2702 3056.0695 3056.2439
3058.6158 3060.1784 3065.7606
3066.6395 3068.2801 3069.0920
3069.6513 3073.1571 3073.6046

3075.6890	3077.8580	3084.2317
3089.3330	3089.6184	3091.5278
3093.5070	3102.5536	3110.4830
3114.7143	3119.9374	3122.6504
3124.1867	3131.5595	3131.6923
3132.5642	3133.1816	3133.5551
3136.2760	3137.8746	3139.7394
3140.2804	3140.8298	3142.3317
3144.3385	3144.4781	3144.4853
3145.2257	3146.8757	3149.5279
3151.8339	3155.2267	3155.6199
3155.8635	3164.0520	3164.7347
3164.8071	3165.4493	3168.4044
3169.6623	3170.3097	3172.3428
3176.9304	3177.9236	3179.8771
3182.1261	3182.8480	3184.6787
3191.2705	3193.6777	3195.6855
3198.4950	3204.4310	3206.3210
3206.7020	3206.9567	3210.5835
3211.8573	3217.1034	3217.4506
3223.0721	3224.3568	3225.5469
3230.7495	3235.2483	3238.1874
3256.7317	3262.4197	3840.9771

TS4'

Zero-point correction= 1.310835

Thermal correction to Energy= 1.386373

Thermal correction to Enthalpy= 1.387317

Thermal correction to Gibbs Free Energy= 1.199910

Sum of electronic and zero-point Energies= -3266.839306

Sum of electronic and thermal Energies= -3266.763768

Sum of electronic and thermal Enthalpies= -3266.762824

Sum of electronic and thermal Free Energies= -3266.950231

Cartesian coordinates

C	-3.603182	0.075203	0.589954
C	-2.163027	0.176204	0.370463
C	-1.564771	0.862124	-0.636719
O	-4.142874	-0.885738	1.109686
C	-0.157679	1.258068	-0.683973
C	0.388458	1.788717	-1.863668
C	0.618970	1.238194	0.486504
C	1.687295	2.274675	-1.871824
H	-0.207072	1.822689	-2.771578
C	1.916103	1.726818	0.471896

H	0.202713	0.852346	1.412774
C	2.457429	2.234430	-0.707402
H	2.103190	2.677550	-2.789199
H	2.518982	1.682129	1.372339
H	3.481540	2.595261	-0.718298
C	-2.389963	1.225731	-1.768336
N	-3.062389	1.431348	-2.688605
H	-1.560869	-0.336937	1.118472
C	-4.518542	1.270789	0.351990
C	-6.355267	2.437096	0.238996
C	-6.723385	-0.028311	0.137217
H	-6.423897	-0.709466	0.935195
N	-5.395948	3.314099	0.361943
N	-4.261639	2.582851	0.430374
N	-5.859630	1.167235	0.243655
C	-7.829715	2.690461	0.149489
H	-8.014837	3.553787	-0.490560
H	-8.215977	2.903933	1.155937
C	-8.210541	0.375547	0.297253
O	-8.461362	1.573145	-0.421415
C	-7.987552	-1.133374	-1.527911
C	-6.699066	-0.693595	-1.220527
C	-5.636654	-0.902835	-2.084772
C	-5.876555	-1.580428	-3.280732
C	-7.157734	-2.037565	-3.586949
C	-8.224022	-1.815413	-2.713519
C	-8.955594	-0.744411	-0.434972
H	-4.639238	-0.534927	-1.864521
H	-7.330413	-2.560170	-4.521964
H	-9.223266	-2.156970	-2.964993
H	-9.143636	-1.579930	0.247568
H	-9.916781	-0.380986	-0.804540
C	-3.000746	3.279264	0.568083
C	-2.248120	3.105014	1.731376
C	-2.606587	4.115235	-0.487841
C	-1.007439	3.741615	1.784169
C	-1.351690	4.709743	-0.381598
C	-0.530645	4.520078	0.731995
H	-0.392053	3.604172	2.670171
H	-1.005194	5.337885	-1.198505
C	-3.484961	4.415592	-1.674458
H	-4.144494	5.257472	-1.443395
H	-4.112319	3.572091	-1.963918
H	-2.868372	4.689018	-2.532280

C	0.831138	5.157311	0.789937
H	1.373733	4.982415	-0.142940
H	1.423310	4.749714	1.611423
H	0.746388	6.239395	0.930067
C	-2.688569	2.255846	2.894519
H	-2.134751	1.310212	2.909171
H	-3.757660	2.030995	2.887843
H	-2.464925	2.768726	3.832232
H	-8.498266	0.494772	1.348789
H	-5.059592	-1.746362	-3.975078
H	-3.645858	-2.745024	1.630244
C	-1.020932	-2.429552	2.461790
C	0.241887	-1.936638	2.118612
C	0.794740	-2.092989	0.840047
C	0.031139	-2.780252	-0.108213
C	-1.253280	-3.257374	0.154071
C	-1.776116	-3.049937	1.445283
H	0.819297	-1.404726	2.864074
H	0.470262	-2.964179	-1.079178
C	2.140142	-1.568494	0.500835
C	2.509993	-1.323512	-0.826936
C	3.084485	-1.284033	1.493489
C	3.762023	-0.836104	-1.189133
H	1.771479	-1.488822	-1.602481
C	4.336235	-0.749256	1.208478
H	2.832215	-1.509077	2.523391
C	4.698489	-0.519595	-0.156262
O	-3.052462	-3.504363	1.735196
O	5.865345	0.029130	-0.427786
C	-2.059940	-3.972766	-0.941865
C	-2.490367	-5.376555	-0.480745
C	-3.287989	-3.122795	-1.306694
C	-1.240554	-4.153050	-2.228324
H	-1.609345	-5.982181	-0.245249
H	-3.129278	-5.333502	0.399810
H	-3.036708	-5.875443	-1.288532
H	-2.963751	-2.132580	-1.650601
H	-3.848735	-3.593343	-2.121937
H	-3.969657	-2.991524	-0.463809
H	-1.853993	-4.676124	-2.967856
H	-0.940109	-3.194419	-2.663482
H	-0.341514	-4.752615	-2.055081
C	-1.536830	-2.340902	3.909772
C	-2.887497	-1.608193	4.012734

C	-1.691204	-3.768423	4.465025
C	-0.550806	-1.587855	4.813636
H	-2.856787	-0.644836	3.493185
H	-3.709377	-2.195599	3.604067
H	-3.114411	-1.409949	5.065393
H	-0.726138	-4.284419	4.464388
H	-2.057336	-3.728502	5.496895
H	-2.397675	-4.344202	3.864831
H	-0.945256	-1.568142	5.833506
H	0.429028	-2.073215	4.845195
H	-0.412835	-0.550576	4.487763
C	5.333513	-0.432531	2.333443
C	5.716945	1.058832	2.308290
C	4.749592	-0.729762	3.721194
C	6.600140	-1.291292	2.174337
H	6.160305	1.325782	1.348699
H	4.833205	1.685412	2.480690
H	6.436776	1.271040	3.109132
H	4.512934	-1.791504	3.847369
H	5.487149	-0.461391	4.484456
H	3.841018	-0.148873	3.915868
H	7.283724	-1.106955	3.012299
H	6.340811	-2.355709	2.176645
H	7.122968	-1.048941	1.249415
C	4.162149	-0.725049	-2.669689
C	4.780638	0.636291	-3.038190
C	5.180497	-1.842683	-2.957696
C	2.964039	-0.936018	-3.607078
H	4.082410	1.445447	-2.805221
H	5.718220	0.823599	-2.519789
H	4.974853	0.659147	-4.116633
H	4.706998	-2.825867	-2.861493
H	5.584970	-1.746762	-3.972485
H	6.012554	-1.797641	-2.253413
H	3.300890	-0.844187	-4.644568
H	2.517444	-1.929062	-3.493380
H	2.185594	-0.184053	-3.434955
H	6.903079	-0.424265	-0.937925
C	8.617043	-2.054892	-3.253835
C	8.299420	-0.651979	-2.753580
H	8.337528	-2.145756	-4.304328
H	9.694411	-2.228291	-3.155734
H	8.107728	-2.819897	-2.662054
C	8.225842	-0.509978	-1.294699

C	8.587618	0.777562	-0.692049
O	9.020817	0.605109	0.589168
O	8.117200	0.251484	-3.560429
O	8.483024	1.887862	-1.174947
C	9.267177	1.805940	1.321222
C	9.680344	1.404527	2.720995
H	10.050607	2.383577	0.819579
H	8.359832	2.418478	1.327741
H	9.885905	2.293794	3.322022
H	8.883679	0.833197	3.204514
H	10.581692	0.787174	2.695295
H	8.636879	-1.356193	-0.745259

Vibrational frequencies

-1230.8101	5.5082	14.0542
16.0951	20.9162	25.8314
28.6122	33.1281	38.6221
40.5938	42.5669	46.2829
49.2950	54.7364	61.7362
63.1400	66.2716	71.3142
77.1463	79.4614	82.8688
83.9805	84.6138	89.0918
93.6615	100.6220	103.0336
105.2103	107.1522	112.1362
116.3528	119.7403	121.4330
128.0462	131.7765	138.6728
139.7868	140.8306	145.8710
151.4828	153.4355	156.3481
159.9017	166.8950	168.2763
172.4378	176.5410	179.1435
183.7610	200.5249	204.6551
208.4683	210.7487	213.4987
221.8670	222.3328	227.7408
232.7709	236.5833	241.7293
242.9984	251.9922	253.4488
262.9450	264.8096	265.6727
268.0215	271.6966	281.2650
287.5185	288.3102	288.9713
296.5828	304.2901	305.4977
310.4581	320.7592	322.7894
326.6081	327.2146	328.7126
329.2125	333.3312	341.7343
342.7563	345.0021	345.9744
352.5281	355.4099	359.7156
361.4267	363.4411	365.2396

366.2072 379.0111 386.4641
389.3882 394.6285 398.9067
401.7669 405.0518 408.4803
409.3840 410.1193 420.6092
423.5647 426.6598 433.2277
434.7370 443.3440 445.7885
456.4502 466.3637 467.6415
477.8815 480.4055 486.3081
497.5885 498.0895 505.9637
512.5207 525.8074 532.9256
543.0547 543.3676 552.1523
557.2066 557.7430 572.3256
578.4082 581.6806 588.7115
592.1104 596.0521 597.3450
623.9104 627.9564 633.5109
640.4216 643.9266 646.6586
651.5936 659.1300 660.8332
673.2519 683.2713 692.1268
699.0038 703.2400 714.3292
716.5509 726.0578 751.4661
751.9538 763.9570 777.7584
778.3824 779.5481 783.3409
785.2953 790.2697 790.3991
806.4894 810.4537 817.3162
825.9630 837.8090 842.0092
844.9796 864.7329 870.3508
871.7992 876.9751 883.7547
886.1065 890.2310 896.7135
898.0091 910.4334 916.6948
921.4603 925.6596 926.4229
927.0057 934.4590 941.8959
945.8549 946.9077 947.4847
948.8196 953.8522 954.1940
954.7048 955.5565 956.8770
957.5792 958.8130 962.4108
963.0261 963.8858 966.3498
967.5269 974.7090 977.7767
980.6885 985.5436 997.3672
1008.6611 1019.1424 1021.8764
1023.9901 1031.9999 1036.5590
1039.1619 1042.5470 1042.7372
1043.8057 1047.0665 1048.2903
1049.4997 1050.8584 1053.3990
1055.3884 1055.9613 1056.0500

1057.4098 1057.8824 1060.8087
1064.7966 1067.7351 1068.0472
1073.0809 1084.0287 1119.1008
1122.5571 1137.0691 1143.2263
1146.9061 1150.0691 1155.3496
1157.6999 1175.5424 1177.0059
1183.6615 1188.9230 1189.9829
1191.2331 1203.6745 1209.3914
1226.4743 1227.3496 1228.7799
1232.9672 1238.8495 1244.2742
1245.0612 1246.2046 1246.5490
1249.8292 1250.0461 1250.5881
1252.9098 1253.7700 1263.3460
1265.5770 1266.6617 1283.6630
1284.5845 1286.5545 1287.1365
1295.2272 1301.3625 1307.3943
1309.2564 1310.4534 1313.8664
1317.1446 1321.2774 1327.1431
1330.6595 1334.4900 1338.3278
1339.6627 1343.0278 1358.2675
1361.3920 1365.0078 1370.5301
1378.6986 1380.6082 1381.6376
1385.0910 1385.6509 1388.4037
1389.5525 1393.3775 1397.9186
1399.3824 1400.9086 1402.0242
1403.2930 1410.2756 1412.2042
1418.8201 1420.6880 1421.8228
1428.7484 1429.1077 1429.4869
1430.8799 1433.0779 1449.1413
1452.0453 1453.0418 1464.7539
1473.7862 1474.3872 1475.0918
1479.7157 1481.0301 1481.5059
1485.2712 1486.7157 1488.0794
1491.5707 1492.1223 1492.9649
1493.3953 1494.2060 1495.1018
1495.8095 1496.2018 1498.1909
1499.9263 1500.5446 1501.3331
1501.6494 1503.5346 1505.3358
1505.4457 1506.9086 1507.6418
1509.1247 1510.4687 1511.5606
1514.2307 1515.4614 1516.9265
1517.6744 1518.5884 1520.7329
1522.2697 1527.0506 1530.9112
1531.4078 1533.1473 1536.2793

1536.8975	1537.1366	1538.1091
1547.8841	1557.2740	1557.4563
1619.2960	1637.3558	1650.6160
1660.1327	1667.3129	1677.0122
1684.3514	1685.4968	1687.5041
1688.7439	1691.4681	1708.6504
1773.1854	1781.1034	1851.9211
2404.5564	3040.3375	3044.8616
3048.9766	3050.3408	3051.8943
3052.3898	3054.9620	3055.9036
3058.5342	3064.5873	3065.2971
3069.2903	3071.0949	3072.3548
3073.3648	3073.8801	3078.9087
3086.5020	3086.5487	3091.0657
3102.6707	3106.6192	3120.5269
3123.9199	3124.0779	3126.0032
3128.6860	3128.9452	3129.5748
3131.4108	3131.6552	3136.2330
3137.4012	3137.5715	3138.2460
3141.0373	3142.3572	3142.6058
3142.6982	3145.7089	3146.7814
3156.4863	3162.2244	3162.3336
3163.6374	3164.1605	3166.9057
3167.5116	3168.0327	3168.4554
3177.3513	3177.9199	3180.8050
3181.3952	3181.4731	3185.2674
3189.9919	3192.5684	3192.8250
3194.2758	3198.7293	3207.0421
3207.3814	3207.9017	3214.3728
3217.1459	3222.0238	3223.0022
3226.8352	3230.7802	3233.9257
3238.3861	3245.0772	3245.9273
3248.7237	3270.4638	3790.9431

DQH_2

Zero-point correction= 0.646981

Thermal correction to Energy= 0.679993

Thermal correction to Enthalpy= 0.680937

Thermal correction to Gibbs Free Energy= 0.585465

Sum of electronic and zero-point Energies= -1241.597174

Sum of electronic and thermal Energies= -1241.564162

Sum of electronic and thermal Enthalpies= -1241.563218

Sum of electronic and thermal Free Energies= -1241.658691

Cartesian coordinates

H	-5.281344	-0.771836	-0.225091
C	-2.857439	-1.169112	-0.375144
C	-1.461742	-1.134339	-0.370267
C	-0.742148	0.000341	0.001355
C	-1.457959	1.139877	0.374243
C	-2.850704	1.181615	0.385419
C	-3.535791	0.006855	0.008975
H	-0.905071	-2.008182	-0.686431
H	-0.896610	2.012756	0.684953
C	0.742148	0.000334	-0.001485
C	1.457988	1.139864	-0.374345
C	1.461716	-1.134362	0.370146
C	2.850734	1.181573	-0.385460
H	0.896670	2.012752	-0.685090
C	2.857410	-1.169140	0.375117
H	0.905021	-2.008213	0.686250
C	3.535797	0.006817	-0.008960
O	-4.903176	0.072188	0.036095
O	4.903185	0.072145	-0.036004
C	-3.603879	2.455958	0.800666
C	-4.481398	2.960278	-0.360190
C	-4.470074	2.188609	2.045189
C	-2.634258	3.590835	1.160086
H	-3.861859	3.183887	-1.234778
H	-5.235802	2.227473	-0.645846
H	-4.989529	3.883553	-0.060975
H	-3.844707	1.851147	2.878117
H	-4.967909	3.115546	2.350375
H	-5.232709	1.434074	1.854452
H	-3.213333	4.476021	1.439141
H	-1.996184	3.328676	2.009839
H	-1.993919	3.863430	0.315075
C	-3.612607	-2.442826	-0.798006
C	-4.462245	-2.986565	0.371508
C	-4.472790	-2.178602	-2.052833
C	-2.646309	-3.574367	-1.179161
H	-3.807848	-3.266974	1.201810
H	-5.194361	-2.282266	0.775875
H	-5.008472	-3.878584	0.049455
H	-3.826798	-1.890773	-2.887128
H	-5.007925	-3.091214	-2.332929
H	-5.215654	-1.384239	-1.942866
H	-3.226781	-4.456042	-1.465788
H	-2.015162	-3.298126	-2.028646

H	-2.001911	-3.855131	-0.340954
C	3.612539	-2.442857	0.798031
C	4.472589	-2.178587	2.052930
C	2.646187	-3.574392	1.179065
C	4.462319	-2.986621	-0.371374
H	5.215475	-1.384242	1.942951
H	3.826524	-1.890694	2.887148
H	5.007697	-3.091184	2.333135
H	2.001884	-3.855118	0.340772
H	3.226617	-4.456077	1.465745
H	2.014940	-3.298165	2.028481
H	5.008490	-3.878633	-0.049223
H	3.808019	-3.267040	-1.201752
H	5.194499	-2.282341	-0.775661
C	3.603954	2.455899	-0.800666
C	4.481426	2.960160	0.360247
C	4.470181	2.188580	-2.045172
C	2.634362	3.590804	-1.160092
H	3.861836	3.183812	1.234788
H	5.235766	2.227311	0.645964
H	4.989641	3.883402	0.061071
H	3.844832	1.851125	-2.878120
H	4.968004	3.115530	-2.350333
H	5.232818	1.434044	-1.854447
H	3.213461	4.475993	-1.439085
H	1.996323	3.328679	-2.009883
H	1.993984	3.863378	-0.315103
H	5.281276	-0.771946	0.225079

Vibrational frequencies

16.9163	29.5876	38.5974
46.0050	52.4790	71.3535
71.9997	83.5034	107.2819
125.7435	148.7919	161.1577
162.0057	170.4790	173.3716
177.5548	185.8048	196.4260
206.0054	211.8600	222.8387
228.2938	242.4463	244.1465
273.2945	275.8510	277.4404
286.1329	303.1615	312.3747
314.0049	326.4670	328.3796
334.6060	354.7135	357.2040
371.8227	380.2618	382.5420
382.6269	392.1901	393.2872
403.2591	404.2211	408.5152

409.4411	416.0255	447.1822
448.8217	449.2936	452.8312
458.9840	477.0470	479.9790
531.7227	533.5850	545.2492
555.3523	593.8378	628.4049
639.0531	641.7664	642.1024
673.4905	684.6513	771.8649
775.8646	777.4791	788.5008
789.5848	832.7361	838.5144
866.1387	911.4081	918.0662
924.1255	939.0269	942.9955
947.0472	948.1655	949.9856
953.7437	954.3845	954.7823
955.7735	961.9632	962.1529
964.6367	964.6392	978.3605
978.3996	980.5681	1047.7246
1049.8360	1052.6655	1053.0799
1057.4551	1057.5497	1059.2022
1059.2744	1153.0143	1159.1797
1160.4181	1186.7573	1188.9429
1233.1372	1234.0354	1242.2081
1242.2911	1248.3508	1248.5751
1249.1163	1251.5396	1285.9221
1291.3366	1294.1198	1300.0031
1311.0990	1315.3463	1321.5005
1328.0334	1359.1887	1364.0726
1391.5320	1397.7382	1397.7666
1405.4293	1405.6129	1414.5972
1414.8568	1421.3224	1421.3352
1431.8002	1431.9962	1447.4724
1447.5299	1461.6191	1484.4547
1486.5735	1486.6532	1487.7765
1487.7814	1492.9017	1495.4102
1499.3552	1502.3631	1502.9998
1503.1685	1505.4220	1507.0274
1507.1191	1509.6354	1511.8506
1515.2815	1519.7028	1519.7191
1519.7809	1519.8094	1530.2106
1533.6578	1535.7574	1537.4523
1537.7840	1546.7180	1665.5105
1679.1604	1691.7466	1694.8875
3057.9734	3057.9819	3059.9494
3059.9941	3065.4248	3065.5965
3066.8798	3066.9195	3068.2607

3068.3620	3072.9059	3072.9679
3129.0384	3129.0463	3131.4483
3131.4536	3142.8228	3143.2463
3144.8833	3144.9000	3146.1142
3146.1538	3149.5713	3149.6421
3150.4780	3150.5029	3151.6569
3151.8116	3152.6462	3152.8019
3156.0953	3156.1639	3183.9553
3183.9703	3185.3148	3185.3233
3244.7136	3247.0245	3250.6118
3253.4213	3936.7070	3937.1739

M4

Zero-point correction= 0.793931

Thermal correction to Energy= 0.844729

Thermal correction to Enthalpy= 0.845673

Thermal correction to Gibbs Free Energy= 0.708805

Sum of electronic and zero-point Energies= -2725.353471

Sum of electronic and thermal Energies= -2725.302674

Sum of electronic and thermal Enthalpies= -2725.301729

Sum of electronic and thermal Free Energies= -2725.438598

Cartesian coordinates

C	0.803170	-0.526444	1.275248
C	-0.582984	-0.194571	0.940359
C	-1.210061	-0.493914	-0.222640
O	1.426801	-0.049200	2.200056
C	-2.667050	-0.599681	-0.398230
C	-3.206980	-0.836151	-1.669884
C	-3.517198	-0.576160	0.714987
C	-4.570489	-1.041429	-1.824453
H	-2.555528	-0.844272	-2.538626
C	-4.883067	-0.771497	0.555290
H	-3.115481	-0.434153	1.712836
C	-5.411728	-1.006445	-0.713143
H	-4.979533	-1.221431	-2.812616
H	-5.533896	-0.750544	1.423410
H	-6.478538	-1.166829	-0.834517
C	-0.390449	-0.790798	-1.375623
N	0.294740	-0.998705	-2.285904
H	-1.143770	0.229965	1.766196
C	1.482126	-1.712664	0.598708
C	3.053169	-3.060424	-0.062549
C	3.846788	-0.762310	0.563924
H	3.710770	-0.385655	1.581425

N	1.964025	-3.779080	-0.063605
N	0.992338	-2.931209	0.353459
N	2.800610	-1.785781	0.359524
C	4.448450	-3.481596	-0.409761
H	4.434171	-4.103004	-1.305625
H	4.865309	-4.065517	0.422759
C	5.241983	-1.421927	0.405852
O	5.220192	-2.338690	-0.678300
C	5.198511	0.653524	-0.761889
C	3.868644	0.357160	-0.453957
C	2.820287	1.090564	-0.994415
C	3.124919	2.131962	-1.872727
C	4.451216	2.426905	-2.189012
C	5.499024	1.691815	-1.633677
C	6.141933	-0.258745	-0.013707
H	1.771379	0.907748	-0.769187
H	4.670742	3.239586	-2.874144
H	6.530767	1.923714	-1.880317
H	6.551056	0.238499	0.872335
H	6.977620	-0.624817	-0.614426
C	-0.369816	-3.386106	0.496386
C	-0.973932	-3.300622	1.756135
C	-1.039474	-3.849362	-0.645281
C	-2.332396	-3.606191	1.831506
C	-2.397029	-4.133992	-0.505329
C	-3.065077	-3.997390	0.711321
H	-2.828163	-3.530545	2.796333
H	-2.949084	-4.463503	-1.382060
C	-0.361876	-4.090851	-1.969194
H	0.008348	-5.119949	-2.008448
H	0.482956	-3.427087	-2.145049
H	-1.078531	-3.955419	-2.781670
C	-4.535375	-4.300928	0.815933
H	-4.698206	-5.375363	0.948284
H	-5.059971	-3.990500	-0.090748
H	-4.983415	-3.784024	1.667226
C	-0.234196	-2.905724	3.010503
H	-0.428257	-1.863101	3.283579
H	0.846156	-3.042276	2.924936
H	-0.581256	-3.521839	3.842168
H	5.563558	-1.930764	1.322835
H	2.299737	2.700574	-2.286889
C	-2.179623	2.198586	-2.175336
C	-0.802554	2.191750	-2.409835

C	-2.753746	2.431822	-0.894647
H	-2.863640	1.993930	-2.988091
C	-0.316878	1.919467	-3.819759
O	0.097171	2.398424	-1.539920
O	-4.107262	2.334510	-0.899782
O	-2.167487	2.690032	0.171975
H	-1.115255	1.600670	-4.492568
H	0.138401	2.832455	-4.216963
H	0.461746	1.152729	-3.781177
Li	-0.354883	3.260175	0.043367
C	-4.770814	2.696881	0.312093
O	0.549818	2.514396	1.590271
Cl	-0.049897	5.534818	0.206492
C	-6.258481	2.585879	0.057335
H	-4.450380	2.029119	1.118309
H	-4.484282	3.716201	0.590675
C	-0.211383	2.695914	2.790592
C	1.908273	2.941250	1.801465
H	-6.520454	1.562504	-0.223049
H	-6.815264	2.855779	0.957949
H	-6.560788	3.255063	-0.751734
C	0.558412	3.736408	3.590269
H	-1.221035	2.997556	2.500557
H	-0.253296	1.738843	3.331334
C	2.001006	3.333372	3.276147
H	2.577233	2.117967	1.533669
H	2.090924	3.792897	1.137563
H	0.319555	3.712749	4.655350
H	0.348880	4.732343	3.190023
H	2.723825	4.133549	3.444527
H	2.290419	2.467340	3.880436

Vibrational frequencies

13.9154	25.7312	28.3328
30.5119	41.5480	43.9993
47.7124	48.7237	50.4694
58.5982	66.3423	69.7654
75.3770	79.7000	85.3223
86.7337	91.8963	100.5570
104.6413	111.1251	112.2931
116.8219	117.3166	125.0560
128.0926	130.5565	137.8970
145.6406	146.4320	147.4413
150.8386	167.2906	168.7104
173.4755	175.0702	180.3820

188.6584	197.9553	207.3438
213.9873	214.2503	216.4929
237.5966	249.9198	259.7012
265.9613	269.8682	282.4869
286.7828	287.4353	297.4951
302.3934	307.1181	326.9487
329.8235	335.8597	338.8834
349.5742	353.1502	380.3941
389.3347	394.1537	406.8062
410.8471	424.9519	438.3563
441.7577	449.9130	470.7388
478.4973	486.2582	493.6766
495.6033	503.6514	521.8828
535.8897	547.1394	557.6070
575.6910	581.7740	583.3619
585.9200	598.3498	605.5043
625.4702	630.8277	633.6729
638.8992	649.9583	659.1623
687.8570	690.5295	692.4133
704.6500	710.9452	725.7449
749.4230	752.5313	754.1203
776.9481	780.8818	784.8274
790.5923	802.2150	810.8797
818.2648	820.8862	842.6205
861.0107	863.9010	868.5409
878.1662	884.9148	887.0374
898.4142	900.5241	905.2953
924.3466	928.6289	937.6587
947.8478	952.0149	954.4999
962.9701	968.7527	976.7232
981.9440	990.3743	995.9790
996.7508	1000.2688	1002.3052
1019.4606	1025.7631	1027.9182
1041.4927	1042.7468	1047.1017
1048.5441	1050.7276	1054.0384
1055.2929	1056.0510	1056.7346
1060.2491	1062.0539	1063.9116
1065.9828	1074.0093	1082.3422
1120.0214	1130.4949	1130.7749
1135.1959	1141.9251	1156.5961
1173.7553	1176.9474	1180.7528
1185.3241	1185.5092	1189.4093
1196.9614	1205.3288	1207.3491
1212.9513	1219.1218	1220.3115

1227.9228	1248.4790	1253.5795
1267.9027	1275.5382	1282.0833
1286.6982	1288.7126	1290.3248
1297.0939	1304.7861	1309.4417
1316.2589	1326.2274	1329.1100
1333.3964	1342.1878	1346.2665
1361.6067	1362.6114	1363.6930
1372.2673	1373.0613	1378.0090
1386.0345	1387.6398	1391.7770
1400.0253	1410.8421	1419.7835
1422.4906	1423.2142	1431.6847
1436.4950	1457.2485	1464.5881
1471.5174	1475.7444	1476.6027
1481.0442	1489.5898	1492.7935
1492.9042	1495.1553	1497.8871
1501.6805	1503.9000	1504.9603
1510.5374	1511.1634	1511.6237
1517.2719	1523.2330	1527.1417
1527.9016	1534.9476	1535.5884
1538.8418	1549.9572	1559.4343
1569.3809	1577.6259	1656.0288
1663.5582	1676.4538	1678.2902
1684.3917	1693.2832	1693.7058
1700.8104	1724.7357	1801.7103
2405.0733	3041.4026	3066.7828
3070.4172	3071.7366	3077.6001
3079.2378	3080.7903	3084.6996
3086.5049	3089.8187	3092.8879
3101.2295	3104.4269	3133.4752
3135.1895	3140.0437	3142.8420
3145.4237	3145.6684	3148.3095
3150.5126	3154.7561	3158.3620
3162.6572	3166.2270	3167.6568
3168.9901	3169.5806	3170.3688
3181.8839	3196.9232	3199.3735
3203.6838	3205.0272	3209.7811
3213.7811	3223.6382	3226.1323
3229.2752	3235.8346	3240.0633
3240.9999	3242.9594	3244.5410

M4'

Zero-point correction= 0.667966

Thermal correction to Energy= 0.710238

Thermal correction to Enthalpy= 0.711183

Thermal correction to Gibbs Free Energy= 0.592994
Sum of electronic and zero-point Energies= -2025.235692
Sum of electronic and thermal Energies= -2025.193419
Sum of electronic and thermal Enthalpies= -2025.192475
Sum of electronic and thermal Free Energies= -2025.310663
Cartesian coordinates

C	0.341344	-0.917721	1.670457
C	-0.952191	-0.265899	1.598156
C	-1.488083	0.353998	0.510061
O	0.989495	-1.047994	2.694241
C	-2.910790	0.702318	0.379646
C	-3.330953	1.663722	-0.547669
C	-3.860425	0.017088	1.153675
C	-4.687610	1.918892	-0.707883
H	-2.596561	2.243140	-1.102845
C	-5.212517	0.287761	0.994872
H	-3.542132	-0.752031	1.850540
C	-5.628238	1.233790	0.056201
H	-5.008785	2.671567	-1.419662
H	-5.943268	-0.249837	1.590360
H	-6.686168	1.438927	-0.072750
C	-0.656513	0.554667	-0.655075
N	0.038033	0.662782	-1.576886
H	-1.499824	-0.262430	2.535033
C	0.890409	-1.666597	0.462286
C	2.285092	-2.739482	-0.818045
C	3.375633	-1.339971	0.946691
H	3.162763	-1.474789	2.009442
N	1.100000	-3.120594	-1.208274
N	0.240429	-2.448531	-0.403636
N	2.199329	-1.855430	0.219567
C	3.619241	-3.211558	-1.313654
H	3.626146	-3.223686	-2.404160
H	3.789355	-4.232889	-0.944979
C	4.626021	-2.151446	0.531340
O	4.623828	-2.331299	-0.877781
C	5.171666	0.159622	0.637833
C	3.776114	0.086852	0.638330
C	2.992598	1.214614	0.436634
C	3.637569	2.439439	0.248704
C	5.029384	2.519964	0.263435
C	5.808900	1.378660	0.453168
C	5.781452	-1.205256	0.859299
H	1.905879	1.177671	0.393378

H	5.511294	3.480878	0.114040
H	6.892904	1.439993	0.446704
H	6.091161	-1.339005	1.901417
H	6.640132	-1.415983	0.217991
C	-1.180787	-2.670591	-0.520343
C	-1.867986	-3.198243	0.578441
C	-1.804029	-2.353705	-1.735267
C	-3.252662	-3.319558	0.462853
C	-3.190635	-2.485047	-1.783246
C	-3.932885	-2.941651	-0.693856
H	-3.810133	-3.722530	1.305051
H	-3.702827	-2.225920	-2.706246
C	-1.049492	-1.954944	-2.976527
H	-0.789863	-2.850122	-3.550028
H	-0.127773	-1.417581	-2.759851
H	-1.676957	-1.318612	-3.603121
C	-5.433838	-3.010781	-0.767854
H	-5.766846	-3.322210	-1.760532
H	-5.859281	-2.020754	-0.570168
H	-5.837772	-3.705055	-0.028369
C	-1.189309	-3.646315	1.848809
H	-1.257374	-2.884117	2.632092
H	-0.134402	-3.889922	1.701934
H	-1.686275	-4.540900	2.228854
H	4.680632	-3.122957	1.037632
H	3.032506	3.323838	0.085054
C	-1.905466	2.812383	2.996307
C	-1.832646	3.398810	1.586523
H	-2.656238	2.011949	2.993894
H	-0.955919	2.406200	3.352423
H	-2.256930	3.579214	3.691707
C	-0.628829	3.155464	0.873572
C	-0.384768	3.580881	-0.465673
H	0.208344	2.706048	1.395533
O	0.930727	3.349094	-0.810940
O	-2.834821	3.996928	1.162086
O	-1.163210	4.047917	-1.293905
C	1.284296	3.588022	-2.169830
C	1.615940	5.051826	-2.401685
H	2.153896	2.949751	-2.353283
H	0.465793	3.265520	-2.817648
H	1.929011	5.215012	-3.436825
H	0.735267	5.665050	-2.200154
H	2.427510	5.371762	-1.741583

Vibrational frequencies

20.1297	26.1587	30.0477
42.7487	48.2151	53.9820
55.0774	60.5107	62.2906
65.1926	73.0893	81.0693
89.8630	92.9524	98.4818
103.1988	105.8352	107.8520
121.8508	127.5303	131.5324
135.4818	143.9910	147.4491
156.7093	166.8027	176.2254
180.1213	193.2467	197.6420
205.0329	211.0993	212.2201
218.4611	233.9617	240.2079
254.1582	277.1194	283.0287
291.9458	295.9631	318.3692
324.9100	327.8105	335.4711
346.3348	362.3652	364.2404
385.5145	395.9340	398.2829
408.1399	418.5434	437.1840
444.8793	463.6350	466.9518
481.8716	493.5979	496.8005
505.4514	519.8008	536.9929
557.2674	568.6466	573.8466
582.7667	584.6840	596.8326
608.6903	624.5278	631.3862
640.5563	643.8342	652.4532
686.4141	697.2201	705.1940
709.6241	725.7591	729.8474
737.7170	746.6169	753.8310
772.9050	777.4972	793.0598
794.2192	809.6887	816.7833
824.6506	841.8270	857.9501
868.3509	872.6911	879.8967
882.4390	889.3310	900.1043
921.5386	923.5217	958.4131
961.5683	963.3145	969.2583
978.0690	978.4979	992.0899
995.8926	1000.9050	1020.1386
1022.9865	1027.5515	1029.0537
1038.8463	1039.6500	1041.9441
1043.4306	1046.7212	1053.3775
1054.5426	1061.3245	1065.2316
1065.4473	1066.9929	1074.7194
1079.9249	1113.9279	1118.3207

1137.7630	1141.6782	1152.5230
1177.9051	1180.9931	1181.1512
1185.2105	1190.8137	1200.4193
1207.4762	1212.5673	1222.3686
1228.4964	1244.2186	1253.2792
1257.5017	1271.3794	1285.6187
1287.1855	1290.9353	1310.3022
1316.6816	1333.9053	1335.8310
1338.5809	1341.6513	1343.0393
1361.8164	1362.5610	1373.3967
1375.2700	1379.4162	1382.6315
1383.1073	1395.5838	1407.8296
1417.5427	1423.1539	1426.5025
1432.3513	1459.6226	1465.8363
1471.0642	1472.2363	1480.6215
1482.7070	1486.9898	1489.1071
1491.1457	1494.4166	1495.4060
1501.8790	1508.4888	1511.6965
1513.0634	1515.6176	1517.5918
1523.9510	1529.9396	1533.6945
1534.4589	1548.1624	1569.2733
1629.2006	1663.6067	1669.6739
1670.0245	1683.6638	1686.1546
1689.7221	1690.8720	1703.2947
1754.8502	1781.9849	2390.7575
3053.5257	3062.7765	3067.3986
3070.7714	3073.4263	3086.8077
3089.3055	3096.7515	3101.6599
3131.7644	3141.6011	3143.6673
3146.5917	3153.3847	3154.3577
3156.6613	3165.5022	3165.6593
3166.5081	3167.8196	3172.9407
3173.5322	3190.7917	3198.4781
3201.9080	3203.4158	3204.1432
3208.4985	3212.3935	3216.5096
3220.4352	3221.4243	3224.7482
3227.4441	3231.3872	3239.7546

TS5R

Zero-point correction= 0.793055

Thermal correction to Energy= 0.843017

Thermal correction to Enthalpy= 0.843961

Thermal correction to Gibbs Free Energy= 0.709501

Sum of electronic and zero-point Energies= -2725.344528

Sum of electronic and thermal Energies= -2725.294566
Sum of electronic and thermal Enthalpies= -2725.293621
Sum of electronic and thermal Free Energies= -2725.428081
Cartesian coordinates

C	0.585342	-0.464946	0.991527
C	-0.542335	0.261346	0.539972
C	-1.319188	0.020662	-0.611803
O	1.332309	-0.164030	1.929840
C	-2.810423	-0.047641	-0.569904
C	-3.541396	-0.445761	-1.695659
C	-3.489675	0.276870	0.605864
C	-4.926746	-0.515528	-1.646032
H	-3.019723	-0.702557	-2.615730
C	-4.880825	0.230571	0.646223
H	-2.934047	0.546544	1.498689
C	-5.602524	-0.171178	-0.474036
H	-5.481697	-0.833701	-2.522139
H	-5.398758	0.489719	1.564855
H	-6.686179	-0.220048	-0.435217
C	-0.682389	-0.781106	-1.643092
N	-0.120608	-1.379051	-2.461734
H	-0.859970	1.047723	1.217608
C	0.841590	-1.887331	0.496519
C	1.896834	-3.741570	0.046272
C	3.391123	-1.790458	0.528649
H	3.329844	-1.330727	1.518867
N	0.641601	-4.077152	0.121619
N	-0.006012	-2.916028	0.411559
N	2.068204	-2.407602	0.296592
C	3.074269	-4.624521	-0.230930
H	2.863127	-5.261418	-1.091145
H	3.266322	-5.260375	0.644184
C	4.481347	-2.893795	0.490234
O	4.186477	-3.823282	-0.541061
C	5.228632	-0.981914	-0.728050
C	3.865244	-0.789417	-0.499137
C	3.178183	0.265588	-1.081592
C	3.880510	1.134942	-1.916936
C	5.239853	0.938436	-2.162132
C	5.924218	-0.122261	-1.568958
C	5.751430	-2.147463	0.077347
H	2.124792	0.447104	-0.891470
H	5.772254	1.623102	-2.815544
H	6.983507	-0.270462	-1.755767

H	6.288503	-1.797304	0.965184
H	6.414997	-2.812646	-0.480217
C	-1.422370	-2.953923	0.690017
C	-1.856948	-2.606536	1.980037
C	-2.294285	-3.397276	-0.308818
C	-3.224998	-2.649193	2.223498
C	-3.658282	-3.408191	-0.003935
C	-4.143633	-3.029965	1.242267
H	-3.584379	-2.375638	3.213035
H	-4.355573	-3.723185	-0.776692
C	-1.857062	-3.892760	-1.663627
H	-1.976314	-4.981066	-1.708582
H	-0.822425	-3.653903	-1.898061
H	-2.495092	-3.454525	-2.438258
C	-5.617203	-3.063139	1.544783
H	-5.875480	-3.962838	2.112417
H	-6.205926	-3.060499	0.624762
H	-5.911376	-2.197182	2.144254
C	-0.920057	-2.212680	3.094432
H	-0.778146	-1.128727	3.135775
H	0.067681	-2.671136	2.991670
H	-1.340116	-2.529285	4.050766
H	4.567893	-3.416889	1.450778
H	3.355572	1.976580	-2.357812
C	-1.294853	1.871381	-1.882022
C	0.118540	1.998168	-2.111268
C	-1.974816	2.712313	-0.908282
H	-1.908292	1.566857	-2.722110
C	0.669929	1.533468	-3.437952
O	0.905003	2.421539	-1.246633
O	-3.271914	2.857434	-1.189159
O	-1.470948	3.215834	0.095059
H	-0.101867	1.139601	-4.098979
H	1.158953	2.385123	-3.921024
H	1.425721	0.761056	-3.270875
Li	0.425686	3.554211	0.212630
C	-4.045800	3.623993	-0.248379
O	1.307058	2.944732	1.807462
Cl	1.006702	5.730986	-0.054833
C	-5.457476	3.689701	-0.784486
H	-4.001081	3.126053	0.725280
H	-3.593654	4.613921	-0.146168
C	1.245322	3.839849	2.933148
C	2.679907	2.662082	1.470881

H	-5.874500	2.684515	-0.882281
H	-6.085060	4.265165	-0.100337
H	-5.475181	4.174190	-1.762885
C	2.659048	4.381916	3.099263
H	0.511389	4.618507	2.709853
H	0.923687	3.270551	3.812591
C	3.500963	3.187628	2.643505
H	2.769166	1.585712	1.311076
H	2.926406	3.192247	0.541800
H	2.867517	4.699497	4.122465
H	2.803738	5.227214	2.420128
H	4.516391	3.458712	2.348821
H	3.556216	2.433869	3.435915

Vibrational frequencies

-275.0641	15.9847	22.7441
27.2188	38.5315	41.9949
44.0153	50.8249	54.6861
58.4760	62.5624	66.4569
72.4409	74.4898	78.6690
87.0760	92.3678	95.6103
102.4083	106.3188	110.9099
118.4761	121.3434	125.9963
133.6085	136.0048	140.5871
143.6704	151.1597	151.2935
159.9787	161.0187	164.7551
169.7492	173.9086	181.1562
192.0302	200.9094	209.3812
213.8788	216.1596	222.9140
238.5675	239.2674	249.9079
269.4252	276.5110	280.0094
281.6460	285.1097	286.3094
300.2686	307.1145	322.4735
331.8854	335.7867	350.4566
351.3327	362.9363	391.2976
392.8302	402.0003	416.6412
418.1328	425.1500	435.6012
446.5815	448.4352	468.5667
477.8685	483.3115	494.0927
501.5914	514.9426	526.8293
531.4417	537.1667	561.4492
572.7138	576.6727	583.2466
585.7507	592.3378	599.9813
605.5130	625.6846	629.2299
631.8150	641.5906	650.8538

673.8650 684.8442 693.5758
707.1025 713.8576 722.6469
751.1069 755.3924 760.2181
772.1916 778.8530 792.1381
796.0160 807.0662 808.5556
811.8141 818.5259 846.0022
857.6446 866.5482 875.3620
881.0475 883.5933 889.9746
900.5266 901.5237 902.1433
917.5965 922.3779 924.5380
937.8960 950.4108 956.4903
958.0827 973.2309 977.3532
978.6565 981.5145 992.6708
997.9886 1005.6659 1013.4980
1022.0247 1024.5339 1029.7661
1032.7732 1040.0313 1045.4907
1047.8010 1051.9739 1055.5876
1056.3922 1057.2011 1058.8327
1062.5186 1064.5476 1067.3095
1072.2076 1072.3753 1082.4648
1113.7954 1119.0281 1124.1877
1124.8847 1138.4542 1154.1977
1169.8919 1173.5620 1179.5712
1181.3182 1184.7790 1191.6087
1205.2671 1208.2106 1209.2114
1212.2265 1212.7036 1217.3794
1234.3570 1250.5941 1257.2213
1266.7934 1276.1141 1278.2120
1286.3155 1287.4094 1288.1116
1290.7496 1306.6689 1308.5583
1311.7373 1324.3137 1327.3412
1331.0683 1340.4633 1349.5661
1354.8657 1357.1377 1366.8446
1369.0826 1375.8883 1380.1819
1388.8672 1390.9493 1395.5438
1401.6411 1416.5632 1420.1331
1421.4588 1424.0607 1430.3229
1436.9177 1455.3126 1465.3950
1470.4091 1471.0040 1475.9180
1481.9622 1485.7385 1486.5132
1491.9830 1492.7709 1494.9547
1496.7939 1498.0382 1501.6585
1504.4435 1506.5559 1506.9812
1511.2465 1512.5958 1514.4552

1516.7608	1524.9381	1526.2782
1532.9232	1536.3394	1537.6621
1550.2290	1567.1788	1664.1940
1673.1524	1675.0750	1681.9066
1686.6118	1691.0438	1696.9556
1697.3438	1705.6276	1761.3405
2395.3363	3066.7868	3069.4667
3072.9194	3074.1597	3078.7464
3078.9510	3079.5595	3080.7461
3085.8282	3087.6643	3096.5327
3098.9061	3102.9273	3128.9354
3134.4925	3146.2684	3149.4568
3150.5000	3150.7677	3151.7595
3155.0155	3159.1143	3165.4237
3166.9975	3168.3689	3168.6042
3171.3716	3173.2431	3174.6364
3185.5683	3187.3756	3187.7156
3191.0821	3201.7611	3204.0834
3212.4219	3216.6538	3218.9594
3222.2087	3225.5923	3232.3887
3234.6210	3235.7660	3240.5048

TS5R[b]

Zero-point correction= 0.793611

Thermal correction to Energy= 0.843178

Thermal correction to Enthalpy= 0.844122

Thermal correction to Gibbs Free Energy= 0.712833

Sum of electronic and zero-point Energies= -2725.341130

Sum of electronic and thermal Energies= -2725.291563

Sum of electronic and thermal Enthalpies= -2725.290619

Sum of electronic and thermal Free Energies= -2725.421908

Cartesian coordinates

C	0.693481	-0.299100	0.860639
C	-0.494812	0.335105	0.438351
C	-1.360324	0.001577	-0.624442
O	1.503711	0.147537	1.684442
C	-2.840079	-0.044725	-0.415332
C	-3.669125	-0.702854	-1.327051
C	-3.406829	0.577659	0.703484
C	-5.042984	-0.753485	-1.118833
H	-3.237087	-1.189233	-2.198430
C	-4.783146	0.534553	0.901164
H	-2.780478	1.102295	1.420337
C	-5.604919	-0.134633	-0.004279

H	-5.674512	-1.280274	-1.827370
H	-5.212499	1.020265	1.771739
H	-6.677281	-0.176395	0.159627
C	-0.821613	-0.915040	-1.617046
N	-0.328099	-1.569902	-2.435552
H	-0.787002	1.143643	1.105562
C	0.998015	-1.758448	0.516508
C	2.150450	-3.596100	0.281544
C	3.550344	-1.546777	0.600103
H	3.459044	-1.031091	1.558146
N	0.912213	-3.983147	0.367238
N	0.201890	-2.833684	0.521620
N	2.254796	-2.237566	0.397339
C	3.368495	-4.448224	0.098775
H	3.187996	-5.183982	-0.686011
H	3.592079	-4.975790	1.036520
C	4.689845	-2.600857	0.644256
O	4.438956	-3.630063	-0.300358
C	5.358986	-0.749423	-0.707498
C	3.990911	-0.586547	-0.480626
C	3.273948	0.418578	-1.116140
C	3.946620	1.249386	-2.012685
C	5.308577	1.076588	-2.259580
C	6.026028	0.076221	-1.603731
C	5.927229	-1.837720	0.169910
H	2.219917	0.592186	-0.923506
H	5.815912	1.731507	-2.960683
H	7.088600	-0.052790	-1.786181
H	6.455474	-1.406839	1.027023
H	6.613070	-2.514335	-0.345416
C	-1.224735	-2.937021	0.725305
C	-1.793630	-2.393106	1.883916
C	-1.971849	-3.663849	-0.218739
C	-3.176297	-2.519213	2.034539
C	-3.343340	-3.759066	-0.003690
C	-3.967933	-3.182809	1.103736
H	-3.638617	-2.083311	2.916923
H	-3.943948	-4.298323	-0.732514
C	-1.365221	-4.372331	-1.403003
H	-1.014947	-5.365447	-1.107383
H	-0.519579	-3.833515	-1.828270
H	-2.121108	-4.493933	-2.181674
C	-5.453899	-3.317466	1.301490
H	-5.698291	-4.291878	1.737265

H	-5.981157	-3.235350	0.347715
H	-5.831730	-2.541414	1.970405
C	-1.015103	-1.703217	2.974713
H	-1.108680	-0.614771	2.892873
H	0.049240	-1.945956	2.963670
H	-1.417118	-1.999085	3.945916
H	4.799902	-3.037209	1.644780
H	3.397281	2.046468	-2.503576
C	-1.388364	1.634426	-2.065883
C	0.030698	1.843891	-2.201899
C	-2.176752	2.604473	-1.314964
H	-1.911757	1.189828	-2.905791
C	0.716486	1.310674	-3.437820
O	0.705972	2.372415	-1.303763
O	-3.451204	2.632528	-1.710494
O	-1.765174	3.317220	-0.404894
H	1.439166	0.539975	-3.153935
H	0.011852	0.886836	-4.152814
H	1.267423	2.128062	-3.911697
Li	0.020312	3.283255	0.371533
C	-4.327767	3.513392	-0.984649
O	1.725219	4.276137	0.504252
Cl	-0.571973	3.111810	2.653420
C	-5.717650	3.311467	-1.543880
H	-4.273678	3.260935	0.078300
H	-3.975697	4.541365	-1.110853
C	2.696265	3.272291	0.861996
C	1.838843	5.409854	1.385081
H	-6.029548	2.272658	-1.410129
H	-6.423453	3.959992	-1.020007
H	-5.745960	3.554872	-2.608535
C	3.176806	3.658611	2.253518
H	2.216041	2.288462	0.830373
H	3.509974	3.292031	0.125849
C	3.117418	5.186264	2.188077
H	1.860878	6.316895	0.775438
H	0.958436	5.422823	2.035586
H	4.172734	3.268910	2.473524
H	2.467873	3.284434	2.997635
H	3.074975	5.663059	3.169177
H	3.984997	5.578797	1.647644

Vibrational frequencies

-311.8047	25.7487	34.3614
40.3052	43.1378	43.8023

45.9926 53.7924 67.5221
71.0670 72.4957 77.4059
80.3467 84.2583 89.5544
93.8476 100.1737 107.2642
111.3005 111.7136 120.7014
123.0868 125.1431 127.7909
138.9890 139.6162 142.2234
145.1237 151.4452 162.7591
164.3458 167.1077 170.8564
180.1262 188.4658 193.1906
196.5114 204.6585 208.6824
211.3906 214.9428 221.2920
225.3790 232.3421 240.1040
260.3761 269.4552 275.8317
285.6509 287.2050 289.5377
299.0408 300.8462 308.5528
330.0750 335.8481 351.3386
352.0532 365.4195 375.1281
391.4439 400.2547 408.2190
410.6526 428.1967 431.7967
438.5223 445.1027 449.7404
470.1894 480.7787 494.6931
505.9860 514.7458 523.3674
531.7935 554.5435 562.3386
574.0393 580.4002 582.8545
583.3380 587.9299 598.4557
605.6807 626.2889 632.2827
636.9789 643.2903 653.5356
678.4052 691.0909 695.4027
705.7193 706.8119 723.3926
747.5891 756.5340 771.4182
775.3474 786.9783 791.1020
796.6641 808.7582 812.3620
818.3572 846.0893 861.1838
863.0378 868.1580 879.4212
879.7503 882.5571 894.4507
900.3891 901.3455 914.1820
919.7395 923.3908 930.3022
937.0522 946.4411 952.5331
962.3796 969.6427 978.0718
979.7344 980.9322 994.4493
995.5864 999.6439 1013.4639
1018.5084 1021.5440 1032.1626
1033.9119 1039.7943 1045.4056

1046.0837	1048.0270	1051.6240
1054.8874	1060.4122	1061.2316
1061.9928	1064.3185	1066.8175
1073.3952	1076.4285	1084.5482
1113.8339	1121.7388	1123.7103
1130.6654	1141.1123	1152.5335
1173.8935	1177.4652	1180.0134
1182.0557	1183.5938	1195.0579
1204.9543	1205.1310	1210.6581
1212.8598	1216.8492	1221.8199
1234.2307	1253.8300	1266.5329
1273.9934	1276.4611	1278.3972
1281.6073	1287.0723	1290.2771
1293.0719	1306.2651	1310.9954
1318.1668	1322.6545	1324.6360
1334.3485	1337.9834	1342.8650
1357.5307	1358.5752	1366.7642
1374.1848	1376.5871	1380.0586
1385.6976	1393.3005	1394.0163
1402.3674	1414.7597	1418.1036
1419.8493	1422.1390	1427.0974
1433.0777	1453.0243	1465.0514
1469.9185	1470.8859	1472.1650
1487.8830	1488.6929	1489.9647
1492.5533	1493.0764	1496.4670
1497.1588	1501.7888	1502.3988
1504.6694	1504.8259	1505.8464
1509.4883	1513.5036	1516.2822
1524.5122	1525.5586	1528.1185
1531.4132	1537.0039	1537.7762
1556.8418	1559.0349	1664.0360
1675.7077	1676.0232	1681.9583
1686.1170	1693.3584	1695.2739
1700.2651	1705.2335	1774.0503
2396.3406	3065.8548	3066.1806
3068.0646	3076.3033	3077.1384
3081.6677	3083.7156	3083.8053
3085.6395	3092.2160	3094.4904
3097.7533	3105.8606	3141.7724
3142.4151	3142.5684	3146.4176
3147.9481	3150.2539	3153.8772
3157.0707	3158.4615	3161.7260
3163.8547	3167.6042	3168.4231
3170.6309	3173.6385	3174.0502

3179.9955	3187.4840	3190.7319
3191.6127	3194.0837	3197.7349
3200.7092	3204.5435	3206.2010
3213.6539	3218.3819	3223.0886
3224.2512	3229.0866	3239.2652

TS5R[c]

Zero-point correction= 0.792112
Thermal correction to Energy= 0.842420
Thermal correction to Enthalpy= 0.843364
Thermal correction to Gibbs Free Energy= 0.709735
Sum of electronic and zero-point Energies= -2725.341439
Sum of electronic and thermal Energies= -2725.291131
Sum of electronic and thermal Enthalpies= -2725.290187
Sum of electronic and thermal Free Energies= -2725.423817
Cartesian coordinates

C	0.217168	-0.157151	0.948372
C	-1.040136	0.401562	0.629423
C	-1.768794	0.251427	-0.545055
O	1.022115	0.312488	1.771157
C	-3.251913	0.278953	-0.593419
C	-3.929569	-0.004700	-1.784754
C	-3.987439	0.554073	0.564031
C	-5.317654	-0.027379	-1.815033
H	-3.366678	-0.215739	-2.690214
C	-5.378007	0.550719	0.525142
H	-3.479181	0.754048	1.501638
C	-6.047154	0.251293	-0.659524
H	-5.831711	-0.258762	-2.741967
H	-5.938743	0.770407	1.428449
H	-7.132153	0.234870	-0.682629
C	-1.112333	-0.417816	-1.648140
N	-0.557217	-0.925800	-2.530268
H	-1.398601	1.124446	1.356060
C	0.557384	-1.575063	0.513672
C	1.710329	-3.412701	0.289877
C	3.092774	-1.338842	0.404847
H	3.005025	-0.560264	1.164188
N	0.465021	-3.797208	0.347652
N	-0.242592	-2.646372	0.485467
N	1.808468	-2.055379	0.388858
C	2.942505	-4.268657	0.260050
H	2.832253	-5.056999	-0.485509
H	3.061384	-4.731409	1.249752

C	4.231670	-2.333773	0.717275
O	4.065597	-3.497470	-0.085266
C	4.918102	-0.871798	-1.017350
C	3.529620	-0.755798	-0.919481
C	2.776084	-0.176252	-1.926257
C	3.443393	0.290183	-3.061873
C	4.832028	0.205226	-3.155554
C	5.582438	-0.373325	-2.129588
C	5.471364	-1.614256	0.179181
H	1.696434	-0.089572	-1.843930
H	5.333117	0.578760	-4.042661
H	6.661653	-0.458136	-2.214842
H	5.869077	-0.927373	0.935407
H	6.253953	-2.333162	-0.073317
C	-1.675225	-2.716863	0.669708
C	-2.198884	-2.382446	1.926929
C	-2.465236	-3.149726	-0.397240
C	-3.581678	-2.428727	2.069272
C	-3.848656	-3.159179	-0.197936
C	-4.423657	-2.796762	1.015478
H	-4.014705	-2.166160	3.031730
H	-4.486865	-3.465302	-1.023209
C	-1.904204	-3.651867	-1.702554
H	-1.928109	-4.746010	-1.712393
H	-0.877795	-3.334676	-1.878618
H	-2.515895	-3.294074	-2.534443
C	-5.915823	-2.834903	1.211407
H	-6.209459	-3.738192	1.755863
H	-6.438712	-2.830086	0.252720
H	-6.253502	-1.971924	1.790886
C	-1.328609	-1.984714	3.090882
H	-1.147080	-0.905121	3.103680
H	-0.358421	-2.488621	3.071572
H	-1.823535	-2.244782	4.027938
H	4.283363	-2.602249	1.779505
H	2.876953	0.724689	-3.878849
C	-1.470317	2.394078	-1.531261
C	-0.042227	2.363837	-1.550616
C	-2.226494	3.023546	-0.461423
H	-1.977123	2.356198	-2.490533
C	0.617489	2.293673	-2.911063
O	0.664619	2.322158	-0.527087
O	-3.475457	3.338003	-0.877923
O	-1.853485	3.236266	0.680604

H	0.454307	1.303789	-3.355216
H	0.185613	3.033255	-3.589272
H	1.688034	2.468379	-2.801603
Li	1.423146	2.272703	1.216308
C	-4.318823	3.955991	0.101260
O	3.312993	1.760931	0.920228
Cl	1.503764	3.913168	2.776748
C	-5.683713	4.127831	-0.527701
H	-4.359502	3.320205	0.990914
H	-3.879638	4.914356	0.396923
C	4.089444	1.656642	2.127866
C	4.017183	2.553590	-0.054338
H	-6.092692	3.155455	-0.814392
H	-6.365891	4.597623	0.184770
H	-5.623431	4.758223	-1.418029
C	5.243205	2.639090	1.963033
H	3.437801	1.885833	2.973724
H	4.458969	0.624961	2.218239
C	5.453255	2.617834	0.447467
H	3.907433	2.069840	-1.027591
H	3.561911	3.551619	-0.089817
H	6.125796	2.344404	2.533653
H	4.928856	3.635438	2.288517
H	5.989482	3.489403	0.067851
H	5.994414	1.713647	0.145677

Vibrational frequencies

-234.0918	23.5092	35.0283
40.2642	42.2981	47.6944
52.7946	58.8254	62.5569
64.1269	66.6751	70.8021
76.5495	78.1896	81.3733
88.5557	91.5959	94.7697
102.1449	104.6384	109.3507
114.5835	120.5713	123.6052
126.8555	128.9422	134.4423
137.2011	146.1536	148.7293
153.3257	160.2276	164.3616
166.8304	169.8177	177.4162
180.5853	187.6147	192.8047
203.1907	208.8586	211.3176
226.2767	244.2887	247.9764
253.0382	253.4752	271.0347
283.1650	284.0280	292.3060
296.1285	304.6750	307.4751

328.2900	334.1493	340.2082
345.3530	353.9014	361.8168
381.1823	393.4798	404.4848
411.3392	412.7138	423.5854
428.5346	430.5372	447.7230
476.0872	485.1314	500.9555
503.5815	505.0387	506.0224
523.6315	537.1841	554.0874
576.4902	579.7736	581.4727
582.4456	586.9691	592.2731
600.1414	625.1634	629.3327
633.9577	639.8956	654.5871
683.8411	690.2212	690.8612
705.7932	714.2735	725.3434
750.9350	751.3305	758.6294
764.0324	778.2004	782.2366
791.7019	807.5359	812.0776
821.6135	829.0301	839.9977
858.8470	866.2126	869.3748
876.0021	880.5543	884.6691
893.2302	898.9302	903.5241
922.7313	922.8977	932.0379
939.6705	946.8181	951.9837
958.6795	966.3447	970.4048
976.0900	981.3194	983.0497
997.4766	998.8321	999.7367
1016.0659	1018.0181	1022.7138
1023.1655	1039.5513	1041.3368
1044.3619	1047.5392	1050.1816
1055.2020	1055.6870	1058.6051
1059.4540	1060.0080	1065.0623
1067.4079	1075.4440	1078.5757
1114.8608	1123.4333	1127.7938
1130.7516	1141.8251	1155.1326
1175.1289	1175.6286	1180.2004
1182.3015	1183.5877	1189.3196
1195.0952	1207.5599	1208.5803
1213.7752	1214.9829	1221.7934
1234.5664	1256.1171	1258.8559
1268.5625	1279.5967	1280.6260
1282.8335	1286.4734	1289.7429
1293.7108	1307.5328	1310.9609
1316.5820	1320.0650	1325.3135
1333.6626	1339.7331	1350.4102

1358.6207	1363.6972	1365.4790
1374.3745	1377.5150	1380.5711
1383.6004	1388.5829	1390.8234
1399.9525	1409.2287	1417.2073
1419.0386	1422.4640	1428.0824
1437.8989	1463.3591	1466.4721
1473.6322	1475.4033	1476.5920
1480.5616	1487.3855	1491.6464
1492.1056	1492.3556	1495.6225
1496.5557	1496.9145	1498.3560
1502.9356	1504.3060	1505.0935
1516.0994	1516.7276	1526.0346
1529.5563	1530.4823	1533.2730
1535.4797	1540.9051	1547.8781
1563.8077	1575.0945	1639.7641
1663.8335	1673.6794	1681.6456
1688.4180	1693.4354	1696.1497
1702.9527	1708.4864	1790.6805
2397.7753	3036.1532	3067.3996
3069.7282	3070.5005	3071.5549
3072.1313	3075.3526	3075.4522
3081.1496	3083.5530	3092.8694
3096.0743	3107.0115	3137.7351
3143.4387	3144.7303	3144.8941
3147.9769	3149.9428	3153.1649
3154.3673	3162.2554	3164.1531
3164.9179	3165.4908	3167.0314
3167.6922	3177.0829	3188.5662
3190.5126	3190.8564	3196.3302
3198.8554	3202.7663	3206.9514
3208.3132	3210.2068	3214.7810
3219.5814	3220.9779	3226.1304
3226.4923	3231.2480	3234.9258

TS5R[d]

Zero-point correction= 0.792687

Thermal correction to Energy= 0.842684

Thermal correction to Enthalpy= 0.843628

Thermal correction to Gibbs Free Energy= 0.710353

Sum of electronic and zero-point Energies= -2725.338869

Sum of electronic and thermal Energies= -2725.288872

Sum of electronic and thermal Enthalpies= -2725.287928

Sum of electronic and thermal Free Energies= -2725.421203

Cartesian coordinates

C	-0.464583	-0.141044	-0.878328
C	0.819097	0.312553	-0.499213
C	1.538248	-0.031057	0.642033
O	-1.249975	0.458228	-1.634013
C	3.017262	-0.139356	0.673882
C	3.669995	-0.638583	1.807956
C	3.770263	0.205083	-0.453352
C	5.047711	-0.810737	1.806446
H	3.094120	-0.902031	2.691063
C	5.153094	0.053739	-0.442376
H	3.278334	0.571594	-1.348049
C	5.794863	-0.463219	0.680612
H	5.540165	-1.212014	2.685969
H	5.727732	0.324740	-1.322626
H	6.872108	-0.596320	0.679157
C	0.837054	-0.767478	1.672851
N	0.259579	-1.326329	2.508511
H	1.224920	1.098508	-1.130747
C	-0.877218	-1.580470	-0.622013
C	-2.115836	-3.372128	-0.651242
C	-3.408953	-1.245457	-0.443878
H	-3.326031	-0.364323	-1.088550
N	-0.890301	-3.804309	-0.767820
N	-0.128722	-2.681277	-0.747371
N	-2.152016	-2.011078	-0.559382
C	-3.380844	-4.172485	-0.732332
H	-3.291269	-5.075114	-0.126469
H	-3.532745	-4.465491	-1.781246
C	-4.596509	-2.144560	-0.857581
O	-4.462110	-3.423066	-0.244070
C	-5.170210	-0.957095	1.106752
C	-3.785922	-0.845497	0.964854
C	-2.986190	-0.389454	1.997748
C	-3.596744	-0.059909	3.210023
C	-4.978098	-0.168049	3.359832
C	-5.777799	-0.612402	2.304909
C	-5.786894	-1.471305	-0.173494
H	-1.910148	-0.299721	1.878773
H	-5.436520	0.091192	4.308760
H	-6.853384	-0.698796	2.425794
H	-6.150124	-0.642143	-0.790433
H	-6.601723	-2.182955	-0.024638
C	1.296194	-2.802900	-0.961556
C	1.820665	-2.364153	-2.186156

C	2.072807	-3.401173	0.032127
C	3.193008	-2.493702	-2.369949
C	3.447408	-3.489703	-0.204252
C	4.024040	-3.042570	-1.388168
H	3.626788	-2.154119	-3.307509
H	4.077233	-3.927179	0.566759
C	1.503217	-3.989420	1.296983
H	1.520837	-5.081549	1.231426
H	0.478164	-3.678122	1.491122
H	2.113944	-3.694326	2.154273
C	5.504178	-3.177133	-1.627515
H	5.720225	-4.085643	-2.199132
H	6.049275	-3.233093	-0.682871
H	5.887606	-2.326920	-2.197074
C	0.959011	-1.769678	-3.269925
H	0.825665	-0.691676	-3.128233
H	-0.033356	-2.227923	-3.304917
H	1.431337	-1.917114	-4.242401
H	-4.691588	-2.249809	-1.944969
H	-2.990083	0.280956	4.042917
C	1.420818	2.022562	1.864209
C	0.005230	2.169793	1.751000
C	2.344626	2.665659	0.944005
H	1.822734	1.811377	2.850329
C	-0.802163	2.005664	3.019372
O	-0.571750	2.363251	0.664330
O	3.571518	2.783725	1.501770
O	2.114858	3.043176	-0.194493
H	-0.640600	1.007905	3.444621
H	-0.473689	2.733428	3.766766
H	-1.861171	2.148711	2.803736
Li	-1.700779	2.260198	-0.873134
C	4.575763	3.392118	0.681967
O	-0.982764	3.619792	-2.067179
Cl	-3.975305	2.252494	-0.877356
C	5.886377	3.280024	1.428475
H	4.612858	2.875280	-0.281227
H	4.298565	4.434579	0.492684
C	-0.451561	4.774335	-1.406539
C	-1.921962	4.116756	-3.029379
H	6.126564	2.228715	1.606508
H	6.691223	3.729478	0.842121
H	5.828858	3.793860	2.391078
C	-1.681174	5.641463	-1.151819

H	0.076585	4.424079	-0.519954
H	0.256720	5.274525	-2.082249
C	-2.567361	5.360242	-2.385836
H	-1.378231	4.376241	-3.946219
H	-2.634182	3.316245	-3.233753
H	-1.430039	6.697835	-1.037619
H	-2.182816	5.305834	-0.239451
H	-3.596782	5.152352	-2.090444
H	-2.569001	6.200413	-3.083757

Vibrational frequencies

-220.5920	22.8175	31.2934
37.2352	40.6874	45.3296
47.0562	53.3437	55.4575
61.8849	66.5806	71.9485
73.7000	78.1326	79.3617
85.3812	93.8189	97.4216
101.0273	107.8657	116.9807
121.7186	126.7830	128.4867
134.2944	138.4781	138.8728
143.2338	152.0713	155.4925
158.8352	162.1758	165.4197
171.2806	174.0933	181.2674
186.7284	192.5678	199.4278
206.1620	214.5331	218.9968
221.9099	241.7436	248.4645
250.9797	257.7297	270.0550
278.6582	287.0091	296.4485
307.9996	321.2670	323.0451
330.7807	346.8937	347.7100
354.7268	363.2609	368.1559
384.5550	400.6211	409.1401
410.3145	424.3678	426.1972
433.8560	448.7705	464.4350
477.5204	485.9924	498.5331
500.2132	503.5364	509.8096
523.7669	538.4747	554.7956
574.9245	581.5072	583.2050
587.1039	592.5176	599.5362
618.5582	626.2754	629.2999
635.5075	638.8295	654.5467
684.0238	685.0794	696.3061
702.0462	715.3696	725.7800
752.3576	753.0364	758.5208
763.6511	779.5885	784.4696

793.4788 804.3877 807.5166
817.5179 822.6090 830.4077
840.9470 853.2017 861.7006
871.8373 877.5878 880.1105
881.8202 894.1935 905.3907
915.2797 922.3851 930.6341
940.4567 956.8482 958.2035
967.8340 971.5360 972.0824
976.6140 979.8659 981.2452
996.0672 997.5244 998.3477
1015.5425 1018.9413 1022.3276
1023.7206 1039.8684 1042.4464
1043.0501 1050.9095 1053.2458
1053.7121 1060.3127 1060.6827
1063.0055 1065.1644 1066.1081
1066.8728 1074.3544 1078.5027
1115.6354 1125.4277 1128.3160
1129.4066 1140.3729 1155.1725
1156.7577 1178.3682 1181.3162
1183.7286 1186.4664 1192.1375
1198.7229 1205.2418 1212.4393
1218.7574 1224.6490 1233.5059
1253.2535 1254.9101 1260.7200
1262.7034 1270.5706 1278.9437
1283.7740 1285.3982 1292.9512
1303.2249 1307.3404 1310.4644
1315.7485 1318.2995 1320.8784
1331.7579 1334.9054 1339.3570
1348.8044 1362.1709 1363.3091
1372.9133 1374.6129 1380.2983
1380.3544 1382.5929 1391.7812
1402.1756 1408.0886 1411.9981
1420.6394 1422.8629 1431.8768
1438.2256 1460.0022 1465.3591
1467.1327 1476.6195 1479.3604
1483.6162 1490.6599 1491.8650
1492.2672 1494.9143 1495.6533
1497.3916 1501.9441 1503.6369
1505.7052 1506.4587 1510.9092
1515.8448 1518.2620 1519.0775
1521.8787 1529.0975 1532.3654
1534.4839 1536.7510 1545.3852
1561.8502 1568.6362 1632.0746
1664.4543 1671.4513 1684.2120

1687.2115	1691.6822	1693.2349
1697.1730	1713.4086	1787.0098
2398.8844	3054.6205	3063.7375
3064.6855	3068.4598	3068.8769
3073.7206	3076.2840	3080.2498
3088.8024	3089.7273	3092.7239
3105.6459	3114.8302	3137.0028
3140.9213	3141.7762	3142.2465
3143.2777	3147.5857	3150.3476
3154.2842	3161.1433	3163.3812
3165.8108	3167.1499	3172.2352
3174.6403	3175.2947	3190.7586
3191.5626	3196.0312	3196.2631
3200.3364	3202.5398	3203.2997
3206.6865	3212.9362	3216.6095
3217.7230	3223.1262	3223.5699
3228.3461	3230.7970	3238.5768

TS5R[e]

Zero-point correction= 0.790961

Thermal correction to Energy= 0.842110

Thermal correction to Enthalpy= 0.843054

Thermal correction to Gibbs Free Energy= 0.704093

Sum of electronic and zero-point Energies= -2725.330570

Sum of electronic and thermal Energies= -2725.279421

Sum of electronic and thermal Enthalpies= -2725.278477

Sum of electronic and thermal Free Energies= -2725.417438

Cartesian coordinates

C	-0.265983	0.059189	-0.690037
C	0.961565	0.544266	-0.181068
C	1.759591	-0.006367	0.815752
O	-1.145907	0.768770	-1.203042
C	3.228507	0.196682	0.879249
C	4.021649	-0.644087	1.669693
C	3.845854	1.180084	0.097768
C	5.404615	-0.505313	1.677443
H	3.555627	-1.426980	2.262473
C	5.228016	1.324432	0.118328
H	3.252508	1.829876	-0.535579
C	6.012191	0.481858	0.904766
H	6.007638	-1.170534	2.286476
H	5.695130	2.092032	-0.490200
H	7.091784	0.590910	0.909753
C	1.242485	-1.182679	1.480531

N	0.786193	-2.098233	2.025355
H	1.223073	1.526498	-0.563359
C	-0.496703	-1.422354	-0.912775
C	-1.515658	-3.259129	-1.480718
C	-3.043764	-1.450371	-0.666821
H	-3.091696	-0.436257	-1.077365
N	-0.253532	-3.480086	-1.729482
N	0.370404	-2.329303	-1.375392
N	-1.709111	-2.001564	-0.986029
C	-2.681078	-4.158370	-1.764086
H	-2.446523	-5.178573	-1.457584
H	-2.871909	-4.149403	-2.846921
C	-4.133026	-2.363072	-1.276379
O	-3.802985	-3.727700	-1.039237
C	-4.749230	-1.772453	0.936775
C	-3.399753	-1.442749	0.801600
C	-2.621914	-1.101575	1.894771
C	-3.217045	-1.114086	3.157941
C	-4.561913	-1.451190	3.302622
C	-5.341535	-1.778699	2.191083
C	-5.359693	-2.057791	-0.415737
H	-1.576103	-0.824498	1.802365
H	-5.010080	-1.457321	4.291414
H	-6.389893	-2.037078	2.307368
H	-5.873050	-1.171024	-0.803723
H	-6.057484	-2.898095	-0.427359
C	1.791998	-2.187132	-1.583494
C	2.243418	-1.233106	-2.505164
C	2.653524	-3.013111	-0.853525
C	3.620963	-1.057322	-2.611549
C	4.022711	-2.787482	-1.002524
C	4.524183	-1.806806	-1.855840
H	3.997631	-0.311363	-3.307503
H	4.712998	-3.395647	-0.423108
C	2.169612	-4.138895	0.022465
H	2.103204	-5.060466	-0.564328
H	1.188599	-3.946540	0.455111
H	2.876152	-4.305677	0.838131
C	6.006995	-1.585056	-1.993409
H	6.538333	-1.929244	-1.103425
H	6.229771	-0.524977	-2.136811
H	6.400109	-2.131345	-2.857111
C	1.318377	-0.409837	-3.365977
H	1.149441	0.581498	-2.932596

H	0.344631	-0.883586	-3.511861
H	1.769061	-0.264685	-4.349660
H	-4.276809	-2.190466	-2.350092
H	-2.612600	-0.844531	4.015747
C	1.321143	1.412672	2.725281
C	0.572657	0.567507	3.631692
C	0.713567	2.384543	1.864270
H	2.360471	1.599573	2.968732
C	1.404553	-0.184103	4.656064
O	-0.647471	0.423847	3.607738
O	1.624880	3.275801	1.415012
O	-0.445403	2.398076	1.443477
H	2.381833	-0.465495	4.253961
H	1.576926	0.461725	5.523677
H	0.862445	-1.073404	4.979110
Li	-1.780749	2.288352	-0.012206
C	1.145723	4.316226	0.550338
O	-1.377643	3.703926	-1.317201
Cl	-4.047384	1.996583	-0.267509
C	2.322138	5.218664	0.248680
H	0.718438	3.878003	-0.356564
H	0.341122	4.856510	1.061269
C	-1.936005	4.990389	-0.994966
C	-1.713526	3.345376	-2.673165
H	3.119457	4.659930	-0.248295
H	2.006399	6.031673	-0.409566
H	2.723986	5.650715	1.167859
C	-2.907781	5.308933	-2.124355
H	-2.416066	4.925565	-0.014253
H	-1.119224	5.722603	-0.947489
C	-2.226132	4.629392	-3.313955
H	-0.816435	2.937583	-3.145912
H	-2.490512	2.574489	-2.638082
H	-3.055697	6.382169	-2.256953
H	-3.873158	4.835472	-1.924783
H	-2.902633	4.433494	-4.147720
H	-1.392346	5.239978	-3.675518

Vibrational frequencies

-188.9633	11.9499	22.4359
27.7517	33.0084	34.5513
39.8478	44.6373	47.5238
52.2868	56.6983	61.5580
62.1432	72.9457	74.2354
77.5844	82.5990	83.5707

92.0215 94.9399 96.5891
97.9053 104.4223 116.4523
117.7403 122.7628 125.3935
131.0494 139.2981 141.5521
148.0747 150.4834 153.8503
162.7189 174.0675 180.4673
186.2623 189.7482 193.3404
200.8643 210.3427 216.3768
226.4666 228.7707 238.9155
242.8136 245.4325 261.5113
273.3568 280.9121 282.0577
292.9507 299.1229 316.1701
325.7950 332.2662 336.0667
341.2215 349.9983 357.4926
376.0003 395.8492 399.6380
405.6302 409.4322 419.2306
421.1694 427.4694 449.5643
472.7564 476.2233 479.6173
495.9053 499.8637 504.8466
523.1677 539.2445 556.3847
570.9275 575.7618 576.9142
582.9586 588.3630 590.5330
599.0085 614.0782 626.6918
632.6589 638.9717 654.0173
683.3925 687.5597 691.6056
705.1673 713.4384 722.5889
752.1163 753.0003 762.2188
765.7184 779.2757 780.6926
786.5342 807.8073 821.0607
822.7264 825.6705 841.9694
862.5660 865.6552 866.5360
869.3166 875.5701 888.3798
889.9356 894.0737 897.2682
917.8074 923.6665 933.7496
938.4693 944.0250 952.0230
960.6686 964.0457 968.5150
976.8990 983.6990 984.3333
990.2181 996.6568 998.5572
1020.4246 1022.4583 1026.5258
1032.3778 1038.2999 1040.7434
1041.6916 1048.1848 1052.9226
1054.7692 1055.6856 1058.4963
1060.7877 1063.0492 1065.2385
1066.2611 1073.6984 1078.1289

1117.6729	1125.8922	1126.6954
1129.9110	1144.8112	1152.5292
1175.1728	1176.8315	1181.0934
1182.4597	1184.1320	1192.3726
1203.1177	1207.9889	1209.2314
1214.1649	1215.0191	1217.2971
1232.8534	1251.7874	1255.6805
1266.6646	1277.1166	1277.7932
1285.0052	1285.2916	1286.6703
1296.8539	1311.2314	1312.1145
1313.2441	1319.8588	1325.9705
1334.2406	1342.8652	1346.6303
1358.8695	1361.4284	1363.0333
1368.7446	1376.8823	1382.8657
1383.4163	1386.5435	1389.2628
1402.1663	1410.6923	1418.6514
1418.9461	1420.4025	1429.3995
1437.6345	1458.0609	1465.2713
1466.2942	1472.9983	1473.7889
1479.6928	1488.2976	1490.4088
1490.8409	1491.2408	1493.3966
1498.5584	1501.7115	1502.9345
1504.7850	1506.0002	1506.8360
1516.7991	1517.8879	1523.2821
1527.4461	1532.8705	1534.9755
1540.4602	1544.7740	1546.4288
1563.2509	1570.3127	1648.1934
1665.7027	1671.7988	1686.2906
1687.1626	1692.0119	1693.0002
1702.5296	1709.5035	1781.1726
2392.4402	3055.4913	3060.2293
3066.8290	3068.5388	3077.6517
3081.6074	3083.4171	3085.3077
3086.0695	3089.5867	3094.0457
3098.5468	3103.2219	3130.5445
3138.0657	3139.9931	3142.3517
3143.1061	3146.5835	3148.2015
3153.6118	3157.4032	3157.9726
3159.8730	3168.0235	3168.1195
3170.4395	3171.5921	3176.6270
3183.8574	3194.4079	3196.9345
3200.6350	3202.1634	3204.0997
3204.1634	3209.2461	3209.4343
3214.8066	3222.8948	3238.3343

3239.9748 3246.3247 3263.4615

TS5R[f]

Zero-point correction= 0.792568

Thermal correction to Energy= 0.842889

Thermal correction to Enthalpy= 0.843833

Thermal correction to Gibbs Free Energy= 0.709144

Sum of electronic and zero-point Energies= -2725.337135

Sum of electronic and thermal Energies= -2725.286814

Sum of electronic and thermal Enthalpies= -2725.285870

Sum of electronic and thermal Free Energies= -2725.420559

Cartesian coordinates

C	-0.073597	-0.148251	-0.970034
C	1.065303	0.547338	-0.503909
C	1.700850	0.416859	0.732117
O	-0.895786	0.287909	-1.792942
C	3.159113	0.635108	0.912793
C	3.791552	0.237020	2.097492
C	3.927342	1.181307	-0.119946
C	5.166543	0.371226	2.240796
H	3.205909	-0.196285	2.904775
C	5.301348	1.330859	0.033962
H	3.463014	1.468954	-1.056785
C	5.926383	0.921317	1.209300
H	5.645051	0.046610	3.158872
H	5.886252	1.756608	-0.775167
H	7.000605	1.027938	1.320668
C	1.061355	-0.462079	1.689058
N	0.509758	-1.147722	2.443465
H	1.393998	1.343350	-1.165362
C	-0.211100	-1.629832	-0.682712
C	-1.037959	-3.641470	-0.604393
C	-2.758739	-1.829101	-0.780050
H	-2.761176	-1.104300	-1.599154
N	0.255883	-3.805359	-0.600112
N	0.760588	-2.547652	-0.652630
N	-1.367823	-2.317501	-0.666879
C	-2.097470	-4.699196	-0.633330
H	-1.858025	-5.484279	0.084998
H	-2.130403	-5.137492	-1.640859
C	-3.697041	-3.026235	-1.082523
O	-3.332798	-4.136873	-0.273620
C	-4.678025	-1.667676	0.598020
C	-3.349417	-1.250349	0.486942

C	-2.778754	-0.395154	1.416581
C	-3.554669	0.009906	2.504240
C	-4.876128	-0.419003	2.632232
C	-5.453878	-1.251991	1.671823
C	-5.056550	-2.552061	-0.567131
H	-1.760794	-0.028154	1.328474
H	-5.464502	-0.097994	3.486300
H	-6.484324	-1.580141	1.769329
H	-5.577059	-1.982728	-1.345701
H	-5.679325	-3.406950	-0.295138
C	2.189810	-2.367012	-0.782106
C	2.680869	-1.852451	-1.992526
C	3.017000	-2.743585	0.277293
C	4.052947	-1.649879	-2.085494
C	4.387299	-2.509365	0.126001
C	4.920518	-1.955137	-1.031592
H	4.457416	-1.244625	-3.009834
H	5.047838	-2.769182	0.949795
C	2.526439	-3.414662	1.534154
H	2.851671	-4.459335	1.538006
H	1.443549	-3.396057	1.637699
H	2.960359	-2.925853	2.410800
C	6.401890	-1.726926	-1.171189
H	6.869130	-2.551955	-1.718658
H	6.879659	-1.654032	-0.191901
H	6.605056	-0.805048	-1.721817
C	1.786209	-1.533274	-3.162876
H	1.384039	-0.516912	-3.101596
H	0.941367	-2.224385	-3.234236
H	2.355227	-1.603206	-4.091224
H	-3.686489	-3.308374	-2.142242
H	-3.107197	0.671808	3.237305
C	1.078921	2.374640	1.920243
C	0.113395	1.923999	2.903514
C	0.695221	2.999891	0.686126
H	2.071733	2.621193	2.277233
C	0.675361	1.579506	4.269881
O	-1.090787	1.797468	2.690128
O	1.733612	3.629984	0.103012
O	-0.390714	2.897007	0.114546
H	1.720197	1.264087	4.215529
H	0.626129	2.467649	4.908775
H	0.069610	0.791218	4.718728
Li	-1.335153	2.256324	-1.466850

C	1.476529	4.267083	-1.160165
O	-3.029913	1.882132	-0.663564
Cl	-1.450961	3.449560	-3.381673
C	2.779341	4.884511	-1.616658
H	1.098009	3.531097	-1.876754
H	0.690055	5.016177	-1.026472
C	-4.152534	1.530229	-1.484353
C	-3.437997	2.786805	0.383436
H	3.551234	4.117780	-1.723452
H	2.637273	5.371950	-2.583479
H	3.128390	5.629024	-0.897597
C	-5.276548	2.472362	-1.066543
H	-3.857255	1.627185	-2.532878
H	-4.422991	0.487106	-1.271368
C	-4.956001	2.682645	0.415503
H	-2.928148	2.484485	1.300184
H	-3.115777	3.800281	0.110594
H	-6.264901	2.045583	-1.247589
H	-5.197017	3.419210	-1.610285
H	-5.426190	3.570853	0.841953
H	-5.257921	1.804761	0.997277

Vibrational frequencies

-190.0927	23.8096	26.7424
31.4098	38.4241	42.2293
44.7631	51.0263	57.4426
60.2475	66.4147	70.8362
76.8526	81.4044	83.3897
85.3937	88.5527	92.0259
99.2046	104.4946	111.5031
114.3200	118.4477	120.4857
125.1825	132.2511	133.6250
137.1427	141.9022	147.0691
147.5142	150.8691	154.8131
161.9841	163.9000	169.0690
183.0896	188.5534	190.6670
207.4713	213.8076	215.6370
219.3778	236.9065	248.2439
252.3863	262.6224	271.0341
279.4331	285.3257	290.3611
299.3149	309.0706	327.3423
331.7184	339.6275	342.8591
350.6820	363.3942	375.9058
388.6795	401.7055	412.7252
417.0818	428.0022	430.4274

441.9445 455.4236 471.6505
475.2962 482.7368 493.0516
499.9570 503.1174 507.7472
528.9919 539.3357 557.2804
571.9733 574.0019 575.1403
583.8113 585.9072 592.6589
600.4147 619.1140 626.1686
633.0937 640.5496 653.6755
683.5600 693.7170 696.7833
706.0058 712.2990 726.9551
753.0772 754.7068 765.9336
774.5428 782.7936 784.8223
792.4265 811.0827 825.6079
828.3578 832.7415 845.2137
861.7759 862.5305 868.8634
874.1259 881.4389 889.3924
896.2978 899.4391 900.0972
923.4271 926.8647 932.2042
942.9371 944.6058 950.9600
960.8406 968.5844 970.3323
971.1857 976.3094 989.6727
995.1232 998.0539 1001.3422
1021.9721 1025.0603 1025.6506
1037.8428 1038.6118 1041.4882
1045.9660 1049.3073 1051.7344
1053.1543 1057.2997 1060.8404
1061.3464 1062.8402 1065.4699
1065.6760 1072.0502 1081.9300
1119.2737 1123.2803 1124.8602
1129.4616 1145.3284 1153.0434
1174.3125 1177.6843 1179.2649
1183.4291 1185.0604 1192.4868
1197.2478 1206.1302 1207.8959
1210.5605 1211.5058 1216.3164
1234.9350 1253.2522 1257.5256
1267.2298 1273.2954 1277.2057
1280.9751 1283.9733 1286.1600
1294.0997 1308.0362 1315.7828
1316.2363 1322.6042 1324.6565
1332.9788 1338.6213 1351.4094
1356.1104 1360.4577 1365.7863
1366.9371 1375.6762 1381.0237
1381.5893 1383.2071 1391.3842
1408.8520 1410.2724 1412.8070

1421.1073	1423.1490	1432.1818
1443.2870	1457.9577	1466.8369
1472.5380	1479.1222	1479.4959
1480.1409	1489.7600	1490.8018
1494.4717	1495.0661	1495.3179
1496.4584	1497.7763	1500.4522
1501.6018	1503.3556	1506.9159
1516.9878	1517.3025	1517.6913
1524.3272	1532.3701	1534.3465
1536.6008	1537.5284	1540.9261
1557.9123	1568.1234	1655.7292
1670.6682	1673.7879	1682.0761
1688.0658	1689.3336	1695.1330
1703.3693	1712.2080	1782.4834
2390.0394	3060.8162	3067.1466
3068.9397	3071.1571	3073.9754
3077.7687	3079.9176	3082.7902
3086.3394	3088.7441	3095.3392
3096.9553	3108.7865	3135.2044
3139.6414	3141.4617	3143.7069
3145.5273	3148.4776	3152.4109
3154.6797	3158.5929	3162.7175
3167.6208	3168.0977	3169.2051
3173.5524	3175.2233	3177.4759
3183.7665	3194.2718	3195.5619
3200.8840	3203.5033	3205.6272
3208.1500	3208.2473	3217.5091
3224.2105	3226.7330	3230.5636
3233.1510	3233.6132	3247.4730

TS5S

Zero-point correction= 0.792878

Thermal correction to Energy= 0.843117

Thermal correction to Enthalpy= 0.844061

Thermal correction to Gibbs Free Energy= 0.708838

Sum of electronic and zero-point Energies= -2725.336637

Sum of electronic and thermal Energies= -2725.286399

Sum of electronic and thermal Enthalpies= -2725.285455

Sum of electronic and thermal Free Energies= -2725.420678

Cartesian coordinates

C	-0.495266	0.259621	0.946298
C	0.418167	-0.510792	0.192915
C	0.541144	-0.687314	-1.189282
O	-0.453398	0.395031	2.173142

C	0.985599	-1.998811	-1.764508
C	0.926198	-2.222192	-3.144818
C	1.449649	-3.021237	-0.930372
C	1.323993	-3.441327	-3.680707
H	0.568541	-1.437507	-3.805587
C	1.860693	-4.235708	-1.471584
H	1.477272	-2.884941	0.144968
C	1.797235	-4.452234	-2.845970
H	1.267412	-3.599612	-4.752451
H	2.219573	-5.018972	-0.811789
H	2.111394	-5.403255	-3.263642
C	-0.374200	0.045048	-2.042295
N	-1.097877	0.608881	-2.749051
H	1.138355	-1.006925	0.835903
C	-1.870538	0.747003	0.441671
C	-4.051042	0.818601	0.623804
C	-3.010596	-1.307958	1.417536
H	-2.195139	-1.336252	2.148040
N	-3.705849	1.991628	0.186842
N	-2.345427	1.937179	0.072448
N	-2.955524	0.018919	0.787098
C	-5.413690	0.350284	1.041718
H	-6.144033	0.572521	0.262589
H	-5.697722	0.887323	1.957296
C	-4.377724	-1.477799	2.123028
O	-5.405255	-1.041397	1.243194
C	-3.813416	-3.496092	1.010946
C	-2.975770	-2.506920	0.490990
C	-2.248204	-2.720799	-0.668766
C	-2.343427	-3.960428	-1.301611
C	-3.162468	-4.958545	-0.775128
C	-3.908882	-4.730397	0.382625
C	-4.523734	-2.995114	2.247693
H	-1.627985	-1.941222	-1.090911
H	-3.231390	-5.918147	-1.277218
H	-4.563814	-5.501126	0.777378
H	-4.032196	-3.346249	3.161439
H	-5.577889	-3.276599	2.294789
C	-1.680342	3.111919	-0.442665
C	-0.761400	3.801981	0.355771
C	-2.108887	3.582746	-1.695550
C	-0.204216	4.965548	-0.180045
C	-1.519135	4.751362	-2.170577
C	-0.558115	5.448628	-1.436032

H	0.518117	5.513216	0.419961
H	-1.827997	5.129608	-3.141827
C	-3.195870	2.923484	-2.505408
H	-4.175993	3.290714	-2.188002
H	-3.190668	1.839218	-2.402431
H	-3.062235	3.164234	-3.561674
C	0.096618	6.680640	-2.001210
H	-0.585702	7.228167	-2.655163
H	0.974169	6.403898	-2.595459
H	0.433490	7.349835	-1.206769
C	-0.386433	3.387239	1.752450
H	0.511122	2.763361	1.733847
H	-1.178595	2.824730	2.248903
H	-0.165825	4.277098	2.345148
H	-4.430472	-0.935068	3.074715
H	-1.774661	-4.141114	-2.208834
C	1.459940	2.802329	-2.266180
C	1.933537	1.746653	-1.299999
H	1.790516	2.602802	-3.286172
H	0.365694	2.836982	-2.252364
H	1.826670	3.776047	-1.935106
C	2.335977	0.475105	-1.836694
C	3.291506	-0.353714	-1.122690
H	2.354437	0.364163	-2.915456
O	3.914802	-1.222103	-1.925383
O	1.879462	1.964519	-0.077069
O	3.510338	-0.326625	0.086533
C	4.831506	-2.127774	-1.287379
C	5.358111	-3.053824	-2.359662
H	5.628088	-1.547003	-0.813546
H	4.296103	-2.671973	-0.503205
H	6.053240	-3.772189	-1.919369
H	4.533726	-3.601279	-2.823022
H	5.884886	-2.489924	-3.132752
Li	2.809748	0.988906	1.325125
Cl	4.242042	2.403343	2.391967
O	2.437846	-0.389965	2.711098
C	1.955283	0.115021	3.970856
C	3.610615	-1.199145	2.921584
C	3.074207	-0.147575	4.969886
H	1.718637	1.174478	3.845161
H	1.038647	-0.424545	4.231547
C	3.670963	-1.447302	4.424455
H	3.509436	-2.108354	2.322464

H	4.486642	-0.639148	2.575091
H	2.706517	-0.231758	5.994524
H	3.812263	0.658022	4.916195
H	4.688144	-1.639369	4.770794
H	3.042144	-2.300623	4.699170

Vibrational frequencies

-257.3689	20.8982	22.7925
28.4458	35.5902	40.5897
46.1484	49.6577	51.1748
57.2987	60.7454	68.5157
72.7945	75.9178	84.8621
86.1695	89.5097	93.1695
95.4909	100.5760	104.4316
111.4669	114.2997	117.9821
120.8059	124.8697	131.7459
136.4170	143.7097	145.6382
152.2509	161.6926	166.4257
170.6418	175.8955	183.4595
196.2195	201.1970	204.7283
208.5731	219.9932	228.9683
231.2362	244.8878	259.5447
266.3667	275.3474	277.6821
282.1325	285.4935	286.6791
292.5824	302.8881	320.6829
325.2483	333.7062	348.8753
354.4817	363.9059	372.3836
393.4968	402.0959	405.8686
411.6531	416.7592	430.4898
433.9883	459.0745	466.8288
473.7368	486.3994	490.2677
496.3275	504.8421	515.7609
521.4978	529.2033	555.7324
574.8010	575.2264	580.8486
587.8241	588.5098	594.3177
607.9057	609.3161	627.8144
639.5192	643.4335	654.1147
679.7832	681.7523	704.3372
705.5778	710.7945	724.1282
747.5239	751.4958	761.9379
771.2452	786.8388	789.9668
791.5924	808.9917	814.5266
827.4202	840.8988	857.7605
860.1192	868.7111	871.9457
875.5610	883.3582	892.5422

893.6710	895.7395	904.3696
917.1654	918.0032	927.0125
938.7673	948.0357	952.1583
955.1862	971.4458	975.8081
977.6245	979.1071	983.5127
994.5913	1001.4809	1012.5858
1019.1389	1021.2219	1022.0150
1026.5734	1039.0054	1044.6062
1045.9329	1052.4007	1054.5312
1054.9930	1056.1448	1062.9155
1063.6729	1063.7150	1067.0250
1069.9020	1077.4205	1079.1423
1114.3729	1115.5376	1127.5877
1128.0930	1131.2772	1154.9194
1173.2251	1174.2745	1180.7215
1181.1707	1182.5675	1189.8464
1201.1158	1205.2458	1208.6021
1210.4951	1217.0834	1221.9972
1234.0433	1254.7574	1260.7457
1270.5805	1271.7649	1273.1173
1280.2211	1284.7337	1290.2773
1297.5802	1307.0511	1308.4293
1311.7991	1320.5405	1322.8327
1334.0699	1340.6884	1343.2845
1360.0708	1361.0079	1362.7961
1372.8814	1377.6547	1380.4191
1381.0212	1385.4439	1393.7687
1402.4030	1410.2678	1413.9526
1416.0030	1418.7403	1427.9688
1435.3524	1456.0232	1464.5772
1466.7419	1470.5378	1472.6947
1484.3251	1489.7514	1490.2801
1492.1390	1493.1379	1496.4614
1497.6543	1502.1591	1502.2449
1504.2460	1506.7969	1509.1633
1512.6139	1516.5404	1516.9373
1518.7683	1527.4060	1529.8309
1532.6356	1535.6591	1543.6020
1562.0133	1573.6295	1663.7845
1675.0021	1677.3733	1683.7163
1688.0928	1692.4409	1695.1181
1698.2893	1708.0550	1768.3288
2401.1135	3062.1366	3072.1149
3081.8679	3082.6526	3083.0454

3086.0097	3086.9129	3089.2384
3090.0266	3095.8267	3096.6545
3101.0341	3103.0452	3128.0119
3139.1317	3141.4372	3143.6064
3144.6470	3153.9840	3158.3345
3158.8825	3164.3535	3165.0385
3168.9652	3171.4631	3173.6830
3174.2220	3174.2880	3186.9874
3188.7903	3190.9508	3192.9531
3197.8341	3203.5691	3204.1581
3210.0263	3210.6557	3216.9584
3220.6328	3225.8506	3227.0674
3231.0799	3239.5283	3272.5053

TS5'R

Zero-point correction= 0.668412
Thermal correction to Energy= 0.709454
Thermal correction to Enthalpy= 0.710398
Thermal correction to Gibbs Free Energy= 0.596488
Sum of electronic and zero-point Energies= -2025.234539
Sum of electronic and thermal Energies= -2025.193497
Sum of electronic and thermal Enthalpies= -2025.192553
Sum of electronic and thermal Free Energies= -2025.306463
Cartesian coordinates

C	0.331859	-0.943496	1.696667
C	-0.828360	-0.108726	1.647322
C	-1.285976	0.568995	0.533278
O	0.944494	-1.284222	2.704154
C	-2.702864	0.877834	0.278603
C	-3.073303	1.670799	-0.817454
C	-3.694750	0.291600	1.076271
C	-4.416160	1.831215	-1.132589
H	-2.306720	2.181703	-1.394160
C	-5.036487	0.475159	0.767055
H	-3.418991	-0.350899	1.906189
C	-5.399145	1.232221	-0.346292
H	-4.697173	2.439582	-1.985459
H	-5.798905	0.004855	1.379942
H	-6.447750	1.360443	-0.595884
C	-0.401496	0.662336	-0.608016
N	0.330122	0.692101	-1.507367
H	-1.373842	-0.027020	2.581447
C	0.758179	-1.670308	0.426276
C	1.989910	-2.745311	-1.010259

C	3.271089	-1.594553	0.811166
H	3.082512	-1.817845	1.864352
N	0.759730	-3.008088	-1.352970
N	0.000237	-2.334857	-0.449140
N	2.030722	-1.939963	0.093398
C	3.256648	-3.266524	-1.619532
H	3.212522	-3.171302	-2.705154
H	3.364979	-4.328948	-1.360245
C	4.429072	-2.460623	0.259237
O	4.347197	-2.508548	-1.158400
C	5.177744	-0.223142	0.564536
C	3.782811	-0.181126	0.635442
C	3.095612	1.024917	0.611481
C	3.836131	2.205828	0.524642
C	5.228804	2.169121	0.464270
C	5.911090	0.952400	0.479860
C	5.677336	-1.648712	0.607552
H	2.010062	1.079131	0.632611
H	5.786794	3.097475	0.395101
H	6.994780	0.924029	0.418340
H	6.031473	-1.914905	1.609319
H	6.478426	-1.857780	-0.105020
C	-1.438644	-2.473316	-0.466184
C	-2.048358	-3.093025	0.634367
C	-2.160307	-2.007146	-1.571711
C	-3.438764	-3.175650	0.632336
C	-3.550248	-2.115079	-1.511409
C	-4.207033	-2.677574	-0.420777
H	-3.932286	-3.646650	1.478762
H	-4.132150	-1.735903	-2.348658
C	-1.542544	-1.419889	-2.815360
H	-1.831380	-2.023626	-3.680071
H	-0.457243	-1.368228	-2.777243
H	-1.924303	-0.406611	-2.971494
C	-5.709369	-2.766898	-0.396594
H	-6.056201	-3.611476	-1.000475
H	-6.154125	-1.856885	-0.807167
H	-6.081343	-2.905713	0.620810
C	-1.270150	-3.669135	1.790564
H	-1.137119	-2.936804	2.592899
H	-0.279606	-4.021507	1.491224
H	-1.814208	-4.517079	2.210208
H	4.422544	-3.476586	0.673379
H	3.306688	3.151693	0.495916

C	-1.924230	2.927712	3.002516
C	-1.757899	3.407670	1.564366
H	-2.690289	2.142562	3.014009
H	-1.004447	2.534550	3.439805
H	-2.298475	3.749998	3.617459
C	-0.517924	3.074238	0.931806
C	-0.135733	3.529988	-0.378077
H	0.284787	2.686299	1.548030
O	1.207528	3.341638	-0.570352
O	-2.706331	3.991616	1.028935
O	-0.840871	3.977619	-1.273016
C	1.705028	3.601503	-1.883610
C	2.013160	5.076224	-2.068986
H	2.608099	2.990345	-1.966207
H	0.974287	3.255089	-2.617637
H	2.444912	5.253017	-3.057941
H	1.095946	5.661532	-1.977175
H	2.727568	5.417145	-1.314395

Vibrational frequencies

-71.5307	23.6179	34.0228
40.7698	43.7987	49.8249
54.6176	59.0536	68.9778
71.2512	74.8323	85.1144
93.3458	100.6250	104.4310
109.4602	110.4196	124.8768
127.9546	133.8185	137.2492
146.0365	148.4695	153.4638
162.8893	175.8123	179.8601
183.7650	190.2059	199.5210
209.0587	213.7046	219.7742
243.9848	245.2582	250.2098
261.6817	268.3990	287.8972
299.5473	302.0102	319.1603
323.2867	329.9395	339.8659
351.3814	362.3977	365.8170
390.7869	395.2356	398.6590
413.0526	422.5949	433.9315
450.4751	464.2076	468.7281
483.7781	494.7778	496.4110
503.1467	529.0457	534.0551
557.9825	567.0134	575.8990
583.6229	585.2146	592.1072
600.8531	619.8939	626.8169
633.0596	638.5001	651.0773

684.1476	694.9536	704.8738
709.5251	724.1216	736.9523
750.1639	753.0189	756.2186
772.4996	776.0452	781.8944
799.7681	809.1873	817.3444
819.9151	832.6816	842.4541
869.9614	871.7685	879.4582
884.9738	890.3134	899.0548
919.6214	921.6140	954.3492
961.3400	961.8198	972.4276
976.6245	977.3106	988.6497
995.7926	1001.8621	1020.9867
1025.4622	1025.8114	1027.8346
1037.2111	1038.9164	1041.1871
1044.3250	1052.5872	1054.8312
1056.0459	1061.0187	1062.5636
1063.9611	1066.9580	1077.3434
1081.5852	1112.0601	1117.5484
1135.4349	1140.0914	1145.3546
1175.0806	1179.1796	1183.3227
1183.6540	1192.3910	1202.8620
1209.1069	1215.1012	1225.2895
1230.5120	1238.7132	1254.2702
1261.5520	1271.3924	1285.5025
1287.7193	1294.0811	1310.3449
1317.6161	1322.9964	1333.7907
1341.6504	1344.0390	1349.8597
1361.1318	1366.1434	1376.6961
1379.3397	1380.6181	1381.4501
1385.4781	1396.3832	1410.1722
1417.6276	1423.0069	1428.7471
1430.7201	1461.9446	1466.2393
1469.9545	1475.9331	1481.0198
1488.0531	1490.9024	1492.7058
1495.1406	1495.3787	1500.0881
1500.6904	1502.9708	1505.4865
1512.9088	1515.3778	1517.7204
1519.3861	1530.7641	1533.8285
1539.3800	1550.0470	1567.4271
1574.9838	1665.9178	1667.1459
1680.8491	1686.3618	1691.3922
1694.3816	1699.9958	1704.7445
1723.6788	1782.7784	2384.2579
3056.7595	3068.1306	3070.8986

3073.6149	3075.9960	3085.5701
3086.6609	3098.9436	3107.1624
3136.2756	3144.9054	3144.9836
3150.5576	3150.7399	3151.8780
3152.2651	3163.4414	3164.5527
3164.8790	3172.3381	3175.3939
3177.1694	3187.0437	3202.0808
3203.7266	3205.5902	3209.2967
3215.0724	3216.4624	3219.5605
3220.5866	3221.6921	3222.5163
3231.6415	3235.9293	3243.1307

TS5'S

Zero-point correction= 0.668042

Thermal correction to Energy= 0.709280

Thermal correction to Enthalpy= 0.710224

Thermal correction to Gibbs Free Energy= 0.594776

Sum of electronic and zero-point Energies= -2025.233177

Sum of electronic and thermal Energies= -2025.191939

Sum of electronic and thermal Enthalpies= -2025.190995

Sum of electronic and thermal Free Energies= -2025.306443

Cartesian coordinates

C	-0.462264	0.188693	-1.478194
C	0.814374	-0.257527	-1.040001
C	1.223287	-0.706115	0.201653
O	-0.760265	0.410263	-2.649912
C	2.644467	-0.632221	0.648696
C	3.011895	-1.069048	1.927357
C	3.624383	-0.089579	-0.188781
C	4.328497	-0.966851	2.357395
H	2.261560	-1.495743	2.586934
C	4.946244	-0.002873	0.238732
H	3.357131	0.288809	-1.169144
C	5.303246	-0.436037	1.513044
H	4.595473	-1.305872	3.352884
H	5.694382	0.419278	-0.424511
H	6.332267	-0.357623	1.848772
C	0.260856	-0.762144	1.277270
N	-0.472131	-0.796875	2.174236
H	1.524900	-0.329715	-1.855568
C	-1.484397	0.869352	-0.538071
C	-2.636705	2.633535	0.060648
C	-0.436031	3.143610	-0.996502
H	-0.103248	2.724513	-1.952016

N	-3.401079	1.618167	0.328284
N	-2.673387	0.523483	-0.044473
N	-1.445194	2.218774	-0.462595
C	-2.976048	4.092860	0.143536
H	-3.383994	4.329553	1.127290
H	-3.738806	4.310556	-0.616859
C	-1.084829	4.531633	-1.211604
O	-1.822915	4.874985	-0.046024
C	1.085883	4.814128	-0.301691
C	0.735875	3.477683	-0.094407
C	1.444284	2.680115	0.790086
C	2.546937	3.226303	1.448235
C	2.917701	4.551158	1.223476
C	2.182935	5.357989	0.352237
C	0.118520	5.474622	-1.257998
H	1.145983	1.658336	0.985930
H	3.776718	4.964906	1.741758
H	2.457051	6.397398	0.199294
H	0.524020	5.517027	-2.274748
H	-0.172161	6.484755	-0.961486
C	-3.274294	-0.771121	0.175604
C	-3.589663	-1.581832	-0.919534
C	-3.651293	-1.081731	1.491605
C	-4.231838	-2.790753	-0.647338
C	-4.289899	-2.302208	1.697658
C	-4.574217	-3.175090	0.646139
H	-4.481022	-3.440879	-1.482299
H	-4.579465	-2.571921	2.710187
C	-3.455576	-0.141048	2.652405
H	-4.311918	0.534982	2.734196
H	-2.555283	0.462995	2.549173
H	-3.375429	-0.711419	3.579675
C	-5.217388	-4.510907	0.907248
H	-5.853848	-4.479219	1.794266
H	-4.449134	-5.272905	1.077262
H	-5.819577	-4.833510	0.055079
C	-3.308214	-1.196525	-2.344747
H	-2.327171	-1.575478	-2.638532
H	-3.309457	-0.114500	-2.490684
H	-4.066195	-1.635486	-2.996672
H	-1.727072	4.564181	-2.099914
H	3.114691	2.609083	2.137651
C	-1.132629	-3.702270	0.595439
C	-0.177180	-3.118393	-0.431951

H	-1.806506	-4.402874	0.094689
H	-0.614556	-4.212900	1.409161
H	-1.747526	-2.900134	1.014819
C	1.211430	-3.099315	-0.084189
C	2.281779	-2.989874	-1.054872
H	1.502765	-3.523183	0.870874
O	3.468919	-3.368793	-0.504955
O	-0.633212	-2.620614	-1.471993
O	2.216182	-2.591196	-2.206792
C	4.606748	-3.260289	-1.361892
C	5.824175	-3.626302	-0.540831
H	4.478575	-3.929149	-2.219911
H	4.672933	-2.237418	-1.745908
H	6.724665	-3.566945	-1.157017
H	5.929886	-2.937623	0.301239
H	5.735941	-4.643644	-0.151768

Vibrational frequencies

-160.4646	17.8012	25.4548
26.8432	34.0792	49.3350
54.1203	60.1077	66.8339
73.1823	75.4006	85.3791
91.7939	101.7630	108.8157
113.2662	113.6169	116.0569
119.8069	124.3598	135.0364
143.7209	149.7163	156.7459
165.9008	170.3896	171.2468
186.2266	195.7217	197.9417
208.0105	216.6920	225.7357
237.5626	253.5739	260.5145
265.4247	268.2749	271.0618
288.4069	296.1266	296.8910
316.8531	328.9145	340.9126
345.4643	351.2916	355.1181
390.0709	394.5137	400.1849
412.6743	415.8055	428.3041
438.0019	459.1584	472.1352
486.9798	495.6255	501.9852
513.2315	519.9335	526.5837
554.5006	562.4500	573.3727
580.2637	588.1760	591.4090
604.7165	608.5625	626.8329
632.6749	639.4414	652.9122
679.5225	703.5317	707.3979
709.4830	726.4384	746.1835

748.4338	762.3266	765.2167
785.0882	786.6655	788.7624
806.0648	813.8048	823.9016
838.4675	840.2721	852.9142
867.7138	874.5730	877.3962
884.4260	898.6611	900.1656
916.9984	919.3869	946.2243
955.5980	967.9872	970.0670
977.4201	980.4313	993.9020
997.5086	1000.1054	1014.7274
1019.2785	1022.0644	1023.5280
1038.8614	1043.3864	1045.0370
1050.1868	1052.9896	1053.1786
1053.8396	1061.1959	1062.6639
1065.3444	1070.1233	1074.0340
1079.9474	1111.5546	1124.9178
1126.0284	1127.0853	1154.9149
1171.0978	1179.2363	1179.7292
1185.0499	1188.9304	1190.1979
1202.7537	1213.9314	1215.7825
1232.0727	1249.1368	1253.4209
1259.6246	1270.5598	1278.3163
1283.5498	1288.3384	1302.1009
1305.4053	1315.8006	1318.5699
1329.9633	1341.3572	1342.0741
1360.9175	1362.3654	1369.1792
1375.9238	1379.5137	1385.4786
1388.3484	1394.6051	1409.7981
1411.2513	1418.0271	1428.6750
1434.2187	1455.7281	1465.3767
1470.9838	1473.1753	1473.9790
1484.4627	1490.8344	1491.7525
1493.6279	1496.3216	1497.0188
1499.5725	1501.5074	1505.2158
1507.2187	1509.5669	1516.6815
1519.6050	1527.8522	1530.6332
1535.1958	1547.7854	1571.6272
1593.8717	1672.5651	1674.5413
1680.3776	1682.9922	1686.0041
1693.6186	1694.3944	1707.7934
1719.2812	1796.0235	2393.7562
3070.0452	3075.4634	3076.4529
3080.0613	3080.1927	3081.4285
3085.2141	3085.2329	3099.6449

3123.1841	3124.1851	3146.4394
3151.9114	3156.4462	3160.1840
3161.6748	3166.2402	3167.1520
3172.1331	3172.4342	3180.7232
3182.5225	3192.2381	3197.9682
3201.8908	3202.6829	3204.5099
3211.4672	3212.0272	3217.8480
3218.3899	3222.9428	3224.4973
3230.8353	3238.1480	3270.1382

M5R

Zero-point correction= 0.795184
Thermal correction to Energy= 0.845477
Thermal correction to Enthalpy= 0.846421
Thermal correction to Gibbs Free Energy= 0.711313
Sum of electronic and zero-point Energies= -2725.366053
Sum of electronic and thermal Energies= -2725.315759
Sum of electronic and thermal Enthalpies= -2725.314815
Sum of electronic and thermal Free Energies= -2725.449924
Cartesian coordinates

C	0.501106	-0.579494	1.048130
C	-0.175796	0.435884	0.421605
C	-0.943955	0.405408	-0.880787
O	1.223075	-0.520355	2.091147
C	-2.465965	0.177509	-0.768016
C	-3.220129	-0.142995	-1.899231
C	-3.111467	0.458758	0.434009
C	-4.609119	-0.164803	-1.832515
H	-2.721934	-0.372722	-2.839337
C	-4.503878	0.459917	0.492874
H	-2.521080	0.682776	1.317699
C	-5.255643	0.154101	-0.638848
H	-5.186449	-0.419677	-2.715494
H	-4.999560	0.687449	1.432080
H	-6.340367	0.154745	-0.590442
C	-0.349590	-0.591344	-1.798019
N	0.153358	-1.343704	-2.520279
H	-0.111964	1.397221	0.922165
C	0.502681	-1.991263	0.486549
C	1.261248	-3.917585	-0.207057
C	3.033319	-2.262107	0.433003
H	3.033414	-1.901968	1.466514
N	-0.022868	-4.084597	-0.098200
N	-0.483377	-2.878406	0.347657

N	1.633353	-2.654260	0.165760
C	2.289622	-4.921614	-0.627693
H	1.977294	-5.407677	-1.553195
H	2.396712	-5.684464	0.155911
C	3.940116	-3.509430	0.255658
O	3.505519	-4.259038	-0.869875
C	4.983757	-1.615488	-0.750020
C	3.669535	-1.233424	-0.475362
C	3.183441	-0.000322	-0.891634
C	4.030146	0.843734	-1.610140
C	5.334518	0.451874	-1.912808
C	5.820951	-0.781574	-1.481790
C	5.312477	-2.934995	-0.094772
H	2.176104	0.316003	-0.639672
H	5.979404	1.118080	-2.476787
H	6.841061	-1.080763	-1.703194
H	5.900420	-2.777596	0.815729
H	5.860566	-3.628651	-0.736757
C	-1.864257	-2.769436	0.745142
C	-2.151644	-2.520506	2.091930
C	-2.856495	-3.029998	-0.210155
C	-3.498912	-2.446630	2.451414
C	-4.179813	-2.953136	0.210104
C	-4.521350	-2.648378	1.528832
H	-3.747482	-2.244634	3.490140
H	-4.967448	-3.128146	-0.518953
C	-2.541600	-3.422293	-1.629065
H	-2.349950	-4.497925	-1.689932
H	-1.657444	-2.913590	-2.014860
H	-3.390123	-3.185896	-2.274585
C	-5.967792	-2.532917	1.926304
H	-6.534977	-3.412517	1.609891
H	-6.421503	-1.660857	1.442720
H	-6.078234	-2.419511	3.006536
C	-1.087581	-2.389672	3.150548
H	-0.643135	-1.392060	3.177601
H	-0.269180	-3.096857	2.983106
H	-1.522613	-2.601173	4.128921
H	3.941377	-4.146290	1.148991
H	3.670078	1.821656	-1.913010
C	-0.817346	1.799321	-1.667935
C	0.629721	2.202852	-1.948067
C	-1.574205	2.863207	-0.890584
H	-1.337489	1.661818	-2.617233

C	1.180216	1.867989	-3.304383
O	1.306380	2.761386	-1.103237
O	-2.766321	3.079270	-1.404981
O	-1.154764	3.432611	0.100958
H	0.436121	2.053053	-4.081795
H	2.079313	2.453891	-3.490913
H	1.431941	0.801399	-3.334284
Li	0.719995	3.868009	0.423993
C	-3.640766	3.960476	-0.658829
O	1.448234	3.031592	1.965965
Cl	1.295167	6.004395	0.102424
C	-4.954391	4.008385	-1.401696
H	-3.748852	3.543917	0.346959
H	-3.160879	4.938977	-0.583024
C	1.595732	3.851963	3.140997
C	2.674934	2.310356	1.700118
H	-5.385104	3.007028	-1.474898
H	-5.652384	4.652249	-0.862424
H	-4.816196	4.411370	-2.407154
C	3.094597	3.908259	3.400889
H	1.148502	4.826759	2.930725
H	1.062411	3.372952	3.970015
C	3.532357	2.515240	2.942266
H	2.414731	1.265736	1.516914
H	3.146365	2.745731	0.809631
H	3.328659	4.121330	4.445456
H	3.553311	4.677557	2.771010
H	4.599547	2.442647	2.725284
H	3.276258	1.767967	3.700580

Vibrational frequencies

21.2566	27.2850	33.9588
37.5288	43.8226	46.2904
48.0458	50.9815	54.9602
58.9578	67.3275	69.1855
74.9624	77.3537	80.6678
86.4395	92.0192	98.4818
102.3770	104.5713	110.5089
111.0595	121.0303	127.3446
128.2025	131.2508	138.4230
141.1101	148.3448	152.4459
156.0773	162.2872	168.1788
181.8324	185.6362	194.7779
198.5903	207.7667	210.7034
214.8389	222.2681	235.0370

239.5394 241.7433 250.2359
275.8755 283.2445 284.7511
289.4515 289.8049 293.8972
298.6937 315.3779 322.0812
329.6689 341.5834 351.5340
364.6077 377.4223 389.4839
393.9882 404.5058 424.5621
425.6942 434.6599 442.6880
454.6709 473.6723 481.6205
493.6037 500.6012 503.8843
516.4246 518.9381 525.8976
528.4105 554.8726 562.9467
575.2013 576.5416 584.3319
586.6090 586.9404 598.8997
615.6461 624.6092 635.5127
649.6171 664.3987 679.7062
684.3359 694.4010 702.0990
721.6210 723.8577 749.9329
754.2054 761.5671 767.3789
772.0965 786.4766 794.2181
797.9172 812.0774 819.4074
837.8105 847.3404 866.7445
868.4508 878.1311 881.7650
883.8550 885.8531 893.5022
904.4133 919.4332 922.7129
924.0051 925.9887 939.0733
951.2568 952.6198 956.7176
959.9454 966.7378 981.4901
985.3144 987.9107 996.3802
1003.6474 1008.8250 1017.3079
1024.5688 1025.4939 1026.8280
1029.9695 1039.4625 1042.2380
1048.0215 1054.0290 1059.3811
1060.5058 1062.1065 1063.7716
1067.7811 1069.9724 1074.0805
1075.8937 1083.0147 1098.8519
1116.8875 1117.4213 1122.0330
1133.3464 1152.8805 1162.0699
1176.5736 1180.1431 1180.1544
1182.9676 1187.8094 1196.6272
1204.0250 1206.6336 1208.1179
1208.6063 1213.0758 1215.9589
1218.7265 1237.9736 1251.7607
1265.6689 1278.4076 1285.2455

1288.0633	1289.9605	1291.5912
1305.5021	1311.0639	1312.1436
1329.9253	1330.8332	1334.5979
1338.5136	1341.2391	1345.8794
1348.6948	1360.7659	1365.5795
1366.6455	1376.6921	1382.6280
1390.5188	1391.1952	1391.9547
1403.1510	1406.5861	1414.2517
1415.8829	1422.6395	1426.7658
1427.0359	1430.6477	1456.6082
1457.0546	1464.5448	1465.7719
1469.2424	1473.4551	1481.8843
1490.1790	1490.4410	1494.3704
1495.1076	1495.4339	1498.3071
1499.9676	1500.3159	1502.3825
1505.0481	1507.5691	1518.1094
1520.1742	1520.5157	1521.2743
1531.0423	1536.4059	1539.8940
1544.0403	1574.8857	1674.3764
1677.6514	1681.1922	1685.5316
1691.6215	1696.2167	1701.2375
1704.6983	1793.5718	1841.4068
2401.0994	3063.9887	3067.1231
3069.3725	3073.4290	3079.9869
3080.0503	3081.9436	3083.2607
3083.4424	3085.0362	3092.3531
3092.7758	3107.6697	3127.7407
3139.0800	3147.3313	3147.3612
3148.5789	3148.8162	3153.8081
3154.1022	3158.1074	3164.2109
3167.2099	3168.4489	3168.8236
3171.2560	3172.4039	3176.0262
3179.4496	3184.1820	3192.0351
3199.8563	3200.6732	3201.9607
3207.8572	3207.9030	3213.5889
3218.2152	3219.9576	3224.2817
3228.9925	3231.7465	3236.5522

M5S

Zero-point correction= 0.794759

Thermal correction to Energy= 0.845264

Thermal correction to Enthalpy= 0.846208

Thermal correction to Gibbs Free Energy= 0.710542

Sum of electronic and zero-point Energies= -2725.359125

Sum of electronic and thermal Energies= -2725.308620
Sum of electronic and thermal Enthalpies= -2725.307676
Sum of electronic and thermal Free Energies= -2725.443342
Cartesian coordinates

C	-0.559725	0.340113	1.030099
C	0.448609	-0.323873	0.389106
C	0.732972	-0.613955	-1.056606
O	-0.792120	0.352154	2.279497
C	0.457533	-2.086577	-1.463026
C	0.346076	-2.436589	-2.810685
C	0.424926	-3.088583	-0.493024
C	0.215702	-3.770988	-3.184469
H	0.360744	-1.665882	-3.577368
C	0.303969	-4.425186	-0.869140
H	0.475563	-2.826666	0.558616
C	0.202173	-4.771304	-2.213792
H	0.127143	-4.027228	-4.235177
H	0.277941	-5.194690	-0.104258
H	0.104381	-5.812270	-2.504137
C	-0.049747	0.244823	-1.961510
N	-0.649457	0.871896	-2.725751
H	1.113829	-0.830306	1.081913
C	-1.621266	1.236513	0.377186
C	-3.622706	2.127723	0.282509
C	-3.546633	-0.198457	1.187470
H	-2.930281	-0.446435	2.057509
N	-2.818532	3.067645	-0.111123
N	-1.572878	2.502384	-0.057371
N	-2.932700	0.992100	0.589185
C	-5.106204	2.192563	0.490333
H	-5.582812	2.693042	-0.353285
H	-5.313156	2.765132	1.405417
C	-5.007790	0.112175	1.593334
O	-5.626989	0.887742	0.575023
C	-4.925101	-2.003474	0.502716
C	-3.706205	-1.373641	0.252043
C	-2.827688	-1.849925	-0.705873
C	-3.173943	-2.996241	-1.420557
C	-4.386090	-3.639194	-1.168164
C	-5.272045	-3.146287	-0.206892
C	-5.687368	-1.261062	1.577450
H	-1.888541	-1.344634	-0.896534
H	-4.649231	-4.528607	-1.731634
H	-6.220836	-3.642824	-0.027353

H	-5.572239	-1.747172	2.552295
H	-6.755084	-1.155577	1.372483
C	-0.462123	3.329607	-0.467851
C	0.586565	3.592564	0.421058
C	-0.559171	3.955395	-1.725809
C	1.585683	4.473423	-0.006002
C	0.466641	4.822915	-2.090115
C	1.547844	5.094356	-1.248537
H	2.409302	4.681035	0.672640
H	0.410753	5.310692	-3.060428
C	-1.729569	3.779602	-2.660039
H	-2.519390	4.494109	-2.412018
H	-2.152383	2.777613	-2.610142
H	-1.407068	3.964782	-3.686685
C	2.653232	6.013971	-1.694710
H	2.251116	6.906528	-2.180605
H	3.300492	5.510629	-2.421256
H	3.274019	6.324770	-0.852287
C	0.688318	3.011704	1.803809
H	1.309787	2.110395	1.777713
H	-0.276857	2.725064	2.222072
H	1.165410	3.734536	2.468761
H	-5.073250	0.633570	2.556239
H	-2.490500	-3.382889	-2.171130
C	2.772525	2.081629	-2.068507
C	2.732797	1.033347	-0.999437
H	3.255780	1.690840	-2.967286
H	1.742855	2.355480	-2.336113
H	3.292574	2.963830	-1.699453
C	2.273675	-0.357117	-1.426640
C	3.105068	-1.455518	-0.790481
H	2.365589	-0.463414	-2.509536
O	3.403215	-2.400363	-1.659425
O	3.030758	1.269249	0.156523
O	3.429246	-1.494221	0.382351
C	4.025578	-3.593942	-1.126725
C	4.111882	-4.586245	-2.261889
H	5.004601	-3.322755	-0.724331
H	3.398507	-3.958083	-0.307145
H	4.562967	-5.513232	-1.901716
H	3.112570	-4.807459	-2.645141
H	4.726014	-4.193261	-3.074863
Li	3.553585	0.020817	1.651852
Cl	5.663852	0.580648	2.216172

O	2.459402	-0.801367	3.040548
C	1.729355	-0.051013	4.033298
C	2.136174	-2.190241	3.158166
C	0.728817	-1.029686	4.662981
H	2.439986	0.354459	4.759832
H	1.211308	0.756631	3.513772
C	0.703091	-2.195384	3.667932
H	2.279372	-2.643728	2.174016
H	2.818839	-2.667638	3.873648
H	-0.251643	-0.567100	4.780923
H	1.082919	-1.370691	5.640190
H	0.422461	-3.146956	4.124159
H	0.012109	-1.958461	2.852397

Vibrational frequencies

20.0778	26.3001	30.7217
39.7612	43.0259	45.1011
56.3436	57.2775	58.7171
64.9616	67.9098	69.7408
71.8143	76.2934	79.2160
83.2042	88.6047	91.9907
98.2409	101.5447	102.9074
109.1814	115.7643	120.3175
124.7634	127.3335	131.0965
140.6255	146.4781	150.5794
156.9289	163.7584	166.7543
178.6712	180.0288	191.2836
197.3660	206.4103	211.7502
216.0452	218.7420	222.1789
229.3624	244.8792	255.7382
274.0056	281.6936	284.9953
288.0906	295.7322	297.4028
298.2700	317.7409	330.9017
336.7389	341.6930	352.2351
363.0558	380.5528	385.9896
402.3148	404.7375	414.8688
416.7306	428.6276	438.3946
447.3220	455.8527	465.9635
475.0787	485.5892	495.4178
501.5654	514.3331	521.5693
532.0117	546.9579	556.3336
576.3441	579.3922	581.6821
585.4784	587.5597	596.0488
609.3472	626.9029	636.3169
648.2743	669.6619	674.5986

695.3085 702.4594 710.8955
715.2838 726.8508 749.3804
753.6961 758.3134 766.0376
776.6221 787.1762 791.6952
808.9851 815.7765 833.8124
838.7734 843.6781 851.9626
867.4539 871.7950 878.2790
879.3234 891.9168 894.9528
900.0042 918.1283 918.7934
927.2797 941.0190 943.7160
950.9260 951.5164 955.4494
957.3663 969.4716 975.6202
978.4205 980.9545 984.8642
998.4955 999.7726 1016.7253
1020.0012 1021.0125 1022.1579
1023.8598 1038.2733 1043.4085
1049.7006 1054.3595 1058.5626
1062.4781 1063.8973 1065.5324
1067.0067 1070.5048 1072.4945
1073.9104 1082.4756 1095.7101
1120.1481 1121.8623 1128.6248
1133.5911 1150.4691 1171.7135
1172.2272 1177.1059 1180.9939
1183.5111 1187.5940 1197.0844
1197.4852 1200.9714 1203.6354
1209.7563 1211.8180 1218.5358
1234.3133 1237.9904 1259.4346
1274.0545 1275.1998 1280.7689
1285.5936 1286.1148 1288.7675
1306.7540 1309.1431 1314.1596
1322.0812 1325.7499 1331.4202
1333.7512 1337.5327 1346.3047
1349.4454 1351.9318 1362.7682
1367.7010 1376.1544 1382.6945
1383.7100 1387.0210 1388.8180
1400.9333 1404.8126 1413.0158
1416.2188 1418.4285 1421.7013
1425.2454 1427.9734 1454.7873
1456.6445 1461.0387 1461.5190
1464.0720 1467.7746 1476.9273
1483.0451 1485.7822 1489.0439
1490.5093 1493.8447 1497.9753
1498.0145 1500.3858 1501.2365
1502.6380 1505.1266 1515.8524

1519.8920	1523.6673	1525.3724
1530.4622	1540.6753	1543.7040
1544.7705	1556.0814	1674.9375
1676.4307	1686.5571	1687.9173
1691.3319	1693.9658	1710.3132
1717.7055	1801.6575	1850.6908
2414.6654	3063.4731	3063.9719
3064.1561	3065.7988	3076.6617
3079.8103	3081.9634	3087.7477
3090.8898	3095.9165	3099.8957
3104.4586	3104.5800	3127.6779
3135.5311	3142.7868	3149.9285
3151.7964	3154.1553	3154.3165
3154.8602	3155.0522	3165.3627
3170.8024	3172.8955	3174.1842
3174.3202	3174.6076	3182.6785
3190.5437	3192.9139	3194.2010
3195.2386	3196.9704	3205.1749
3206.4645	3211.5864	3214.7477
3218.4142	3220.0853	3225.4554
3235.7693	3236.0317	3254.7748

M5'R

Zero-point correction= 0.669928

Thermal correction to Energy= 0.711273

Thermal correction to Enthalpy= 0.712217

Thermal correction to Gibbs Free Energy= 0.597212

Sum of electronic and zero-point Energies= -2025.273414

Sum of electronic and thermal Energies= -2025.232069

Sum of electronic and thermal Enthalpies= -2025.231125

Sum of electronic and thermal Free Energies= -2025.346130

Cartesian coordinates

C	0.719175	-0.148069	1.480328
C	-0.206048	0.800056	1.133589
C	-0.852824	1.074109	-0.206042
O	1.327771	-0.294625	2.584314
C	-2.231061	0.423927	-0.448173
C	-2.775822	0.371398	-1.733111
C	-3.011213	0.048859	0.643917
C	-4.092163	-0.036380	-1.922149
H	-2.170663	0.654578	-2.591249
C	-4.338049	-0.333336	0.455301
H	-2.576380	0.071475	1.638824
C	-4.883756	-0.372207	-0.825288

H	-4.503890	-0.077587	-2.925660
H	-4.940400	-0.615513	1.314680
H	-5.918061	-0.672298	-0.970260
C	0.077638	0.722036	-1.300850
N	0.834522	0.486542	-2.145415
H	-0.443093	1.515323	1.912872
C	1.182076	-1.194968	0.477691
C	2.533413	-2.468239	-0.674207
C	3.673775	-0.757983	0.762555
H	3.494279	-0.797899	1.841105
N	1.355400	-2.985913	-0.853964
N	0.522311	-2.188162	-0.120811
N	2.479552	-1.380577	0.154447
C	3.844416	-2.954022	-1.212067
H	3.761165	-3.139897	-2.283895
H	4.117944	-3.892049	-0.708713
C	4.926747	-1.574602	0.349897
O	4.819912	-1.961637	-1.014479
C	5.403265	0.753534	0.168687
C	4.021961	0.652259	0.341688
C	3.205561	1.773194	0.264642
C	3.791741	3.003440	-0.028400
C	5.167516	3.103957	-0.238712
C	5.984826	1.978793	-0.134075
C	6.077532	-0.571620	0.431226
H	2.140021	1.704476	0.455689
H	5.608532	4.069271	-0.465787
H	7.058453	2.060277	-0.275874
H	6.522953	-0.586571	1.430721
H	6.855653	-0.830126	-0.291885
C	-0.848982	-2.595511	0.048238
C	-1.282893	-2.951783	1.329136
C	-1.650781	-2.726061	-1.093195
C	-2.608650	-3.373074	1.457017
C	-2.957673	-3.162219	-0.904939
C	-3.458765	-3.474292	0.360389
H	-2.973154	-3.647782	2.444064
H	-3.607128	-3.251304	-1.772222
C	-1.138685	-2.454214	-2.482384
H	-0.591195	-3.322598	-2.860542
H	-0.458180	-1.602561	-2.513041
H	-1.977698	-2.255542	-3.153339
C	-4.894244	-3.896984	0.518625
H	-5.148087	-4.701219	-0.180567

H	-5.559694	-3.052867	0.302067
H	-5.100045	-4.242769	1.535561
C	-0.375125	-2.952349	2.531456
H	-0.253039	-1.957065	2.965928
H	0.627351	-3.305603	2.271402
H	-0.782532	-3.619008	3.294351
H	5.065147	-2.462978	0.978110
H	3.165728	3.888776	-0.061197
C	-1.129394	2.635260	-0.399012
C	0.132617	3.500705	-0.301125
C	-2.199583	3.062706	0.595915
H	-1.556799	2.747221	-1.397629
C	0.647636	4.036871	-1.613046
O	0.671182	3.723662	0.759116
O	-3.371722	3.218813	-0.023737
O	-2.038448	3.215221	1.782260
H	-0.152487	4.561674	-2.143036
H	1.486392	4.710549	-1.442677
H	0.964413	3.200257	-2.245989
C	-4.504594	3.447996	0.835079
C	-5.737614	3.413705	-0.038399
H	-4.520134	2.662110	1.597677
H	-4.375673	4.409700	1.338794
H	-5.826490	2.439557	-0.525732
H	-6.627228	3.583176	0.572314
H	-5.689898	4.190781	-0.805648

Vibrational frequencies

21.2675	29.1368	36.3454
42.0945	48.5559	50.1477
58.8454	65.9628	69.8663
79.6234	87.5967	93.2378
94.5448	104.1725	112.0566
115.8251	117.5891	122.1307
124.3309	129.9751	143.4798
149.3425	156.3552	164.5347
169.4846	177.5143	183.7432
190.9089	203.4202	210.2608
212.3449	217.2513	235.1538
237.5807	259.9416	263.8255
276.1824	281.2737	284.9245
289.8739	294.3067	310.0362
318.8890	327.8583	343.2974
353.3384	364.3577	371.6654
392.2927	401.6192	417.7912

418.4694 428.4329 436.7769
452.7199 469.2325 481.7479
493.7856 500.8013 515.2612
518.5712 525.6972 555.1230
561.2950 567.8103 572.5590
584.7283 586.1143 596.7445
613.4698 625.4178 634.6326
648.0279 663.1370 676.7517
682.5248 701.2382 716.7795
724.0469 749.8452 753.1138
759.7637 763.0746 772.0311
780.2312 785.2792 800.0593
809.4803 811.2473 833.8127
846.1945 866.8297 870.0075
874.5516 881.3968 884.9481
902.3618 903.6118 919.5061
922.2119 944.4423 954.9711
963.0239 968.9347 979.4502
983.3702 986.7965 1001.7589
1006.4597 1013.7017 1018.7875
1022.0030 1023.6371 1025.4664
1040.1022 1042.3766 1047.7984
1054.2319 1059.1494 1060.9530
1063.7386 1068.5113 1071.2425
1075.1096 1077.0151 1081.0647
1103.3707 1113.4906 1118.4703
1132.0026 1153.5777 1163.7210
1176.2792 1177.2517 1181.0985
1184.6696 1186.2400 1196.9376
1202.9276 1204.5593 1214.6212
1218.0317 1234.7388 1247.6631
1259.6491 1265.7512 1281.1570
1287.5183 1301.3013 1304.7179
1306.7744 1323.4978 1333.4028
1336.1307 1340.2217 1343.4901
1351.7050 1364.6011 1366.8507
1374.9950 1380.6247 1381.0733
1385.9315 1401.8966 1404.4353
1410.0848 1415.2917 1418.5756
1422.3330 1431.1233 1444.4158
1455.9550 1467.8029 1469.4890
1475.2900 1480.2338 1480.8610
1488.7917 1489.9675 1491.9297
1493.2092 1498.2167 1499.6033

1503.1934	1503.4389	1509.7300
1517.5782	1523.6044	1523.9088
1537.2079	1539.5541	1544.0736
1573.0973	1673.8359	1675.9256
1681.4650	1688.6057	1692.5313
1698.1635	1706.2555	1716.0344
1844.8492	1881.1020	2395.2623
3051.2999	3063.7535	3075.2109
3075.2578	3075.8305	3079.6662
3088.1126	3097.7432	3104.7527
3119.7032	3128.2672	3143.4952
3145.9581	3146.7691	3146.7822
3150.4432	3152.3048	3154.0016
3164.2275	3167.0331	3168.8165
3171.1335	3188.7659	3189.2599
3191.6282	3193.4375	3196.9659
3203.9758	3204.8226	3207.3624
3218.1205	3218.2715	3225.8757
3229.4452	3233.1136	3243.0213

TS5Sb

Zero-point correction= 0.792603

Thermal correction to Energy= 0.842877

Thermal correction to Enthalpy= 0.843821

Thermal correction to Gibbs Free Energy= 0.706975

Sum of electronic and zero-point Energies= -2725.333574

Sum of electronic and thermal Energies= -2725.283300

Sum of electronic and thermal Enthalpies= -2725.282355

Sum of electronic and thermal Free Energies= -2725.419201

Cartesian coordinates

C	-0.469938	0.468587	0.921521
C	0.334918	-0.522614	0.319509
C	0.477573	-0.891612	-1.026374
O	-0.402010	0.821378	2.104193
C	0.745121	-2.322747	-1.389925
C	0.475615	-2.784758	-2.681747
C	1.249450	-3.214230	-0.434117
C	0.688549	-4.119883	-3.014053
H	0.092400	-2.102640	-3.434593
C	1.470303	-4.544940	-0.776859
H	1.485725	-2.881338	0.572872
C	1.186260	-5.005379	-2.060712
H	0.466673	-4.463566	-4.018313
H	1.862138	-5.225910	-0.028642

H	1.353654	-6.046550	-2.316946
C	-0.327162	-0.175093	-1.998960
N	-0.948368	0.381036	-2.802580
H	0.926779	-1.055521	1.060127
C	-1.810709	0.971166	0.332589
C	-3.982533	1.206713	0.493363
C	-3.072539	-0.835204	1.603196
H	-2.244499	-0.817735	2.318886
N	-3.568771	2.273874	-0.122428
N	-2.214331	2.115879	-0.220250
N	-2.938034	0.376136	0.781593
C	-5.366676	0.900352	0.987893
H	-6.094162	1.042500	0.188432
H	-5.599283	1.594962	1.806610
C	-4.431699	-0.801681	2.339917
O	-5.445919	-0.438915	1.410796
C	-4.023756	-2.998665	1.542394
C	-3.143690	-2.154908	0.862747
C	-2.470137	-2.579109	-0.270417
C	-2.653163	-3.891952	-0.706089
C	-3.507945	-4.749609	-0.014339
C	-4.207530	-4.305535	1.110047
C	-4.669093	-2.270334	2.699958
H	-1.826778	-1.906517	-0.822066
H	-3.642404	-5.768365	-0.361276
H	-4.891766	-4.968530	1.631190
H	-4.175883	-2.507473	3.648349
H	-5.736341	-2.471813	2.807502
C	-1.479747	3.153052	-0.905822
C	-0.545719	3.924842	-0.204982
C	-1.842354	3.420421	-2.234701
C	0.074491	4.963315	-0.901765
C	-1.165599	4.451101	-2.885695
C	-0.201530	5.227062	-2.240567
H	0.803025	5.573983	-0.374857
H	-1.415168	4.661921	-3.921837
C	-2.956752	2.700675	-2.948870
H	-3.911893	3.192368	-2.740004
H	-3.039048	1.657535	-2.646776
H	-2.782134	2.728295	-4.026731
C	0.541610	6.308328	-2.979168
H	-0.026225	6.662525	-3.841700
H	1.500447	5.925700	-3.344965
H	0.753044	7.157783	-2.325766

C	-0.175060	3.685163	1.232233
H	0.662150	2.982025	1.286955
H	-0.995721	3.264037	1.816391
H	0.137657	4.625001	1.692177
H	-4.431358	-0.117304	3.196791
H	-2.121519	-4.238427	-1.587439
C	1.888752	2.420336	-2.075616
C	2.249088	1.260043	-1.183626
H	2.402756	2.351646	-3.036393
H	0.808226	2.408417	-2.272813
H	2.136758	3.356618	-1.576811
C	2.348806	-0.041166	-1.796754
C	3.282044	-1.010163	-1.241369
H	2.236897	-0.094280	-2.875400
O	3.673805	-1.912615	-2.143647
O	2.353624	1.418946	0.043374
O	3.675648	-1.046548	-0.078874
C	4.556234	-2.946908	-1.669721
C	4.745332	-3.922502	-2.807518
H	5.498927	-2.486386	-1.357158
H	4.100160	-3.421067	-0.796391
H	5.405521	-4.734327	-2.491508
H	3.782999	-4.348723	-3.100487
H	5.192182	-3.428448	-3.673398
Li	3.019584	0.061650	1.352495
Cl	2.503719	-1.552893	2.969327
O	3.999374	1.424608	2.361317
C	4.832358	0.979706	3.448899
C	2.988009	2.330084	2.852498
C	4.053162	1.311706	4.712282
H	5.008742	-0.090364	3.318161
H	5.783890	1.523633	3.404282
C	3.354227	2.611116	4.307236
H	2.983199	3.218167	2.217308
H	2.009531	1.834990	2.774090
H	4.696469	1.416972	5.587647
H	3.316760	0.523937	4.892743
H	2.475303	2.839943	4.913732
H	4.049115	3.454588	4.371278

Vibrational frequencies

-286.0912	7.1805	23.1412
24.5457	32.8141	36.5920
42.4870	46.2212	50.5681
56.2408	60.8334	63.2391

65.6874 72.9618 81.0243
84.4967 85.0231 86.9194
94.0991 100.1218 107.0770
110.8644 114.5679 116.8199
120.0197 126.8667 132.5137
140.3191 143.5757 146.9570
152.7444 162.2046 173.3893
177.2154 179.0600 187.5749
201.1975 204.6527 207.1265
218.2958 221.8403 230.7388
236.4121 249.7573 257.7453
261.1443 264.7206 275.9617
281.4337 286.3225 287.1038
288.6433 295.4799 319.4951
323.9367 329.7240 347.9543
351.1517 365.1447 374.8530
393.5947 402.6245 409.5727
412.0296 420.9631 434.2230
442.4764 455.9704 460.0971
476.1119 485.2523 496.9547
507.8826 511.7463 521.1420
525.8022 528.1156 553.9728
573.0071 574.7164 580.1153
588.0162 588.3700 591.4754
606.3490 609.9730 628.3273
639.0971 650.3192 653.3015
679.5669 686.9075 703.7935
705.5706 713.8619 725.9082
750.0741 751.6162 762.1174
772.4891 785.7430 787.6453
791.9302 807.6092 818.0345
823.7185 839.5709 862.1177
866.3974 872.7194 877.5074
883.3035 891.7123 895.8155
896.6474 902.3618 917.8801
919.8479 921.5508 927.6687
936.6799 950.5158 950.6923
955.9617 969.3612 973.5400
978.9558 980.0392 983.1005
992.4140 1003.6143 1004.7289
1016.8365 1017.8799 1020.2010
1027.4166 1039.0213 1043.2476
1044.3701 1048.9445 1052.4830
1054.0685 1056.2653 1059.4689

1064.3893	1064.7610	1065.7615
1071.3785	1075.1195	1078.8809
1108.7811	1115.2141	1124.6137
1125.7724	1127.9974	1155.3353
1166.3682	1176.8168	1178.5796
1180.3877	1184.7310	1187.3266
1203.5622	1203.7509	1206.3878
1215.1953	1217.3360	1220.0823
1231.0466	1251.3528	1254.7099
1269.4444	1271.1839	1279.1875
1283.3362	1283.9022	1287.6709
1296.9667	1303.1917	1312.8035
1316.6329	1323.6314	1324.0132
1335.6100	1341.2794	1342.0757
1356.4349	1358.3991	1360.7339
1372.9604	1377.5858	1380.2459
1385.7821	1392.3357	1393.2366
1404.8562	1408.8304	1416.8311
1419.7570	1424.6548	1427.9719
1439.0328	1455.6943	1464.7990
1470.5984	1474.1657	1475.7621
1482.3163	1488.0820	1490.6934
1493.5662	1494.3755	1495.3436
1496.6920	1499.1523	1499.5211
1502.6741	1502.8940	1503.7547
1506.2139	1514.7165	1517.8744
1520.3997	1526.4389	1529.5754
1535.4932	1537.5332	1546.2814
1561.5314	1571.1426	1668.6761
1673.5093	1676.1587	1682.3902
1685.8786	1689.5226	1692.3484
1702.5869	1706.9967	1777.0969
2401.8283	3056.5264	3064.1528
3067.5934	3069.5766	3073.7024
3074.6997	3074.9496	3078.5363
3086.7952	3089.2545	3097.0317
3097.1725	3105.5230	3128.5770
3145.6147	3146.8597	3147.4573
3147.7584	3151.6141	3153.0058
3153.8681	3155.2403	3158.3748
3160.0290	3168.8978	3169.6153
3170.3019	3171.4307	3174.0008
3178.8924	3191.0361	3192.8848
3195.9697	3201.0959	3209.1008

3210.1841	3214.8403	3215.6173
3217.0043	3221.0288	3225.7665
3230.7461	3237.5367	3262.2756

M5'S

Zero-point correction= 0.670363
Thermal correction to Energy= 0.711609
Thermal correction to Enthalpy= 0.712553
Thermal correction to Gibbs Free Energy= 0.597882
Sum of electronic and zero-point Energies= -2025.264305
Sum of electronic and thermal Energies= -2025.223058
Sum of electronic and thermal Enthalpies= -2025.222114
Sum of electronic and thermal Free Energies= -2025.336786
Cartesian coordinates

C	-0.460619	-0.311985	-1.551069
C	0.694837	0.335876	-1.221311
C	1.340597	0.691329	0.088312
O	-0.986630	-0.408747	-2.703196
C	1.240207	2.200289	0.450023
C	1.444661	2.627066	1.764812
C	1.050240	3.153060	-0.551456
C	1.464274	3.984340	2.074036
H	1.587948	1.897230	2.557238
C	1.079322	4.512089	-0.242674
H	0.870707	2.834958	-1.572491
C	1.287319	4.933076	1.068150
H	1.619369	4.298623	3.101160
H	0.929806	5.241947	-1.031754
H	1.304323	5.991693	1.306413
C	0.768579	-0.059659	1.219402
N	0.357852	-0.591107	2.160950
H	1.207322	0.748068	-2.083516
C	-1.362123	-1.103857	-0.592875
C	-3.310148	-1.892147	0.037749
C	-3.379699	0.364196	-1.030182
H	-2.987666	0.515104	-2.040953
N	-2.465182	-2.841434	0.300336
N	-1.251170	-2.339240	-0.086829
N	-2.679163	-0.812660	-0.506107
C	-4.800516	-1.897606	0.196367
H	-5.074345	-2.323935	1.162325
H	-5.243632	-2.511533	-0.600400
C	-4.906772	0.106127	-1.040193
O	-5.281760	-0.575741	0.150613

C	-4.480310	2.279933	-0.163744
C	-3.257755	1.608777	-0.183131
C	-2.146199	2.110177	0.472718
C	-2.261583	3.320199	1.155934
C	-3.479615	4.000623	1.175431
C	-4.598700	3.484677	0.517730
C	-5.515076	1.509598	-0.952779
H	-1.203694	1.576588	0.450783
H	-3.560916	4.940424	1.712358
H	-5.546397	4.014046	0.546566
H	-5.638635	1.929199	-1.956907
H	-6.497512	1.468870	-0.476722
C	-0.097068	-3.181103	0.125144
C	0.717508	-3.545454	-0.952401
C	0.082381	-3.707048	1.419488
C	1.772032	-4.426402	-0.688852
C	1.145896	-4.582473	1.613661
C	2.003625	-4.953047	0.575443
H	2.418472	-4.711152	-1.515208
H	1.301604	-4.996273	2.607265
C	-0.840317	-3.414766	2.575703
H	-1.689185	-4.103934	2.566335
H	-1.229686	-2.398412	2.546250
H	-0.299505	-3.546009	3.515204
C	3.160837	-5.880464	0.836208
H	2.856765	-6.723489	1.462035
H	3.963265	-5.355019	1.365984
H	3.573945	-6.271027	-0.095976
C	0.517261	-3.066123	-2.363002
H	1.143161	-2.186220	-2.543277
H	-0.512915	-2.779092	-2.574222
H	0.818938	-3.852306	-3.058461
H	-5.227586	-0.467598	-1.918363
H	-1.394457	3.727223	1.668698
C	3.564353	-1.980142	0.872912
C	3.211704	-1.080522	-0.283218
H	4.325477	-1.511584	1.502773
H	2.671486	-2.138440	1.491732
H	3.914742	-2.939923	0.496365
C	2.902620	0.374680	0.085273
C	3.578287	1.363567	-0.852401
H	3.269527	0.579992	1.093575
O	4.220226	2.301417	-0.150213
O	3.169983	-1.466521	-1.428505

O	3.517660	1.348435	-2.057724
C	4.742801	3.405201	-0.913217
C	5.154940	4.471874	0.074923
H	5.581707	3.047731	-1.517485
H	3.959362	3.755783	-1.591541
H	5.561019	5.333670	-0.459342
H	4.289123	4.796645	0.657607
H	5.919183	4.094750	0.758237

Vibrational frequencies

26.9009	32.6499	40.8837
43.5874	46.8718	52.9936
56.1866	63.4498	69.8145
73.8021	79.4450	89.1787
94.2667	103.3044	105.9186
113.3375	115.5734	118.4660
119.2371	123.5251	137.2057
155.5303	162.6785	177.1378
179.8008	183.5694	184.7761
196.6943	209.1168	215.4415
218.1845	223.5524	228.3934
240.1294	253.1561	264.6156
272.3925	284.5832	286.8319
294.9120	300.3907	318.7490
325.4708	332.0304	349.8750
357.4729	366.0180	368.0225
399.4139	401.9626	409.5037
417.1528	427.6716	440.8346
455.3072	469.6253	484.6241
494.5914	501.3883	515.8343
523.0334	529.2832	549.0987
556.6453	570.8968	575.6585
581.5200	586.7201	595.0705
607.3892	626.3260	634.7678
648.3147	666.5854	675.1677
695.0677	702.8371	716.2153
727.5009	750.3092	754.1150
757.2975	765.6397	780.4345
781.8936	788.8076	798.5618
808.9241	822.2667	842.1512
846.6975	869.0455	871.4595
877.3457	879.0348	889.7806
899.7956	916.5439	921.1541
922.2078	946.4745	954.6399
956.2538	971.4208	977.7771

983.5040	987.5930	998.5427
1004.4303	1014.6848	1016.2686
1017.1584	1021.2188	1027.8373
1039.0001	1045.6865	1046.7399
1053.8595	1056.5670	1064.3525
1066.6499	1067.4604	1068.3923
1070.7732	1073.7389	1081.0475
1103.1462	1116.3536	1117.4039
1127.5140	1153.0897	1171.2548
1174.8289	1178.8742	1180.5259
1183.6525	1188.6471	1192.9269
1193.4022	1207.6574	1207.8833
1219.7606	1237.6714	1255.5296
1264.2836	1269.7575	1282.3009
1288.9385	1302.0553	1302.7805
1309.4983	1318.7792	1329.1321
1333.0979	1334.4364	1342.4255
1350.6377	1360.0556	1367.5088
1375.0678	1381.8010	1382.2007
1385.4150	1397.6749	1402.1916
1410.0143	1413.5564	1415.3392
1419.6215	1429.9709	1447.5460
1453.7689	1457.3445	1465.7165
1471.6853	1473.3587	1477.0486
1490.1864	1492.0706	1492.4616
1493.9197	1495.6272	1497.6832
1501.7894	1503.3451	1504.8971
1514.9743	1519.3944	1522.9976
1531.1693	1539.7001	1541.8989
1556.4777	1673.8408	1679.1518
1684.6817	1687.5355	1689.4421
1699.7795	1711.8789	1732.5012
1846.2739	1882.6087	2407.9393
3063.9956	3066.2834	3072.2318
3077.4966	3080.0173	3080.1043
3090.1667	3095.4540	3100.6580
3120.3947	3133.6553	3139.8526
3142.1176	3143.1181	3150.1904
3152.2351	3152.6775	3167.1092
3171.6538	3171.8106	3172.1560
3187.7757	3190.2250	3197.1025
3198.3375	3201.9963	3203.8965
3204.0474	3211.6411	3214.3230
3216.4854	3219.6260	3221.2679

3229.8035 3238.2493 3260.1296

TS6R

Zero-point correction= 0.844437

Thermal correction to Energy= 0.895845

Thermal correction to Enthalpy= 0.896789

Thermal correction to Gibbs Free Energy= 0.757795

Sum of electronic and zero-point Energies= -2407.658661

Sum of electronic and thermal Energies= -2407.607253

Sum of electronic and thermal Enthalpies= -2407.606309

Sum of electronic and thermal Free Energies= -2407.745303

Cartesian coordinates

C	0.847274	0.857491	0.438665
C	-0.047359	0.410652	-0.600240
C	0.044748	-0.937187	-1.346137
O	0.966185	2.037704	0.761589
C	-0.979755	-2.026421	-0.975934
C	-0.711238	-3.366105	-1.269437
C	-2.259529	-1.672785	-0.549899
C	-1.698076	-4.335411	-1.119097
H	0.274676	-3.660416	-1.622199
C	-3.252816	-2.640172	-0.415099
H	-2.506627	-0.633118	-0.373440
C	-2.975565	-3.975811	-0.694041
H	-1.468776	-5.371932	-1.344669
H	-4.245861	-2.341987	-0.091109
H	-3.748727	-4.730004	-0.586544
C	1.415238	-1.481489	-1.225101
N	2.504986	-1.861427	-1.129616
H	-0.091171	1.226094	-1.325993
C	1.712130	-0.076082	1.274248
C	3.467787	-0.881866	2.274640
C	3.842404	1.339355	1.163296
H	3.264610	2.198425	1.513868
N	2.497912	-1.691895	2.585612
N	1.407867	-1.175515	1.956446
N	3.023184	0.147037	1.488646
C	4.901379	-0.953749	2.701741
H	5.272086	-1.971789	2.576955
H	4.979673	-0.672732	3.761196
C	5.195986	1.235485	1.917950
O	5.663281	-0.103767	1.883466
C	5.583733	1.957722	-0.320018
C	4.257260	1.524079	-0.280705

C	3.499337	1.444532	-1.442014
C	4.098375	1.775879	-2.655845
C	5.431889	2.182044	-2.701702
C	6.182820	2.280933	-1.531375
C	6.160921	2.063948	1.070173
H	2.456788	1.150296	-1.427223
H	5.884894	2.434643	-3.654944
H	7.216632	2.610878	-1.563467
H	6.165800	3.104966	1.409613
H	7.175819	1.670844	1.163274
C	0.111777	-1.746624	2.210887
C	-0.858661	-0.944919	2.823056
C	-0.071933	-3.110771	1.943577
C	-2.092686	-1.543178	3.088943
C	-1.320866	-3.647411	2.233830
C	-2.346302	-2.879674	2.789317
H	-2.862220	-0.951775	3.579435
H	-1.500647	-4.697045	2.015006
C	1.024270	-3.990788	1.404260
H	1.684949	-4.310254	2.215284
H	1.642637	-3.477725	0.664617
H	0.589551	-4.877835	0.940251
C	-3.687227	-3.502974	3.065371
H	-3.592379	-4.337754	3.765450
H	-4.114935	-3.900030	2.139073
H	-4.386755	-2.778406	3.485964
C	-0.598433	0.473423	3.267814
H	-0.701961	1.201488	2.458520
H	0.407184	0.584762	3.685092
H	-1.315478	0.746407	4.044171
H	5.111745	1.576566	2.957070
H	3.505343	1.739922	-3.563000
C	-0.182453	-0.714165	-2.904734
C	0.863425	0.193526	-3.568294
C	-1.599830	-0.187818	-3.098026
H	-0.131380	-1.702248	-3.364915
C	1.828940	-0.501564	-4.489027
O	0.902163	1.384225	-3.345241
O	-2.374954	-1.129626	-3.627667
O	-1.980598	0.911010	-2.770679
H	1.284185	-1.101756	-5.223229
H	2.461546	0.226051	-4.995440
H	2.449086	-1.188971	-3.901259
C	-3.784699	-0.829549	-3.687805

C	-4.491430	-2.112772	-4.057887
H	-4.095873	-0.456189	-2.707126
H	-3.940930	-0.035312	-4.422708
H	-4.298559	-2.878441	-3.302004
H	-5.567869	-1.937775	-4.114552
H	-4.146976	-2.479244	-5.027244
C	-3.238824	1.347968	1.180663
C	-4.198684	2.265755	1.536474
C	-4.130970	3.586428	1.017300
C	-3.050521	3.866187	0.140360
C	-2.142798	2.877126	-0.154895
H	-3.268548	0.331762	1.566132
H	-4.991369	1.960797	2.205886
H	-2.920729	4.843454	-0.303561
H	-1.305467	3.066219	-0.820104
C	-4.938511	5.864638	0.780602
C	-6.134105	4.199003	2.248051
H	-4.994086	5.841621	-0.312638
H	-5.762963	6.468908	1.153029
H	-3.998592	6.342681	1.075825
H	-6.761042	3.397592	1.843272
H	-5.752730	3.887897	3.226290
H	-6.754168	5.082163	2.386735
N	-5.044462	4.524259	1.339389
N	-2.222779	1.636781	0.350916
H	-1.234500	0.825948	-0.039593

Vibrational frequencies

-1240.5893	13.0756	19.9730
24.5550	30.4163	32.2180
37.9062	42.7293	47.9883
55.4103	59.7211	64.7001
71.3567	73.9621	74.9173
79.5961	82.6032	91.4910
92.8778	100.5081	104.4866
105.7207	110.3623	113.3763
121.5550	128.2693	132.5456
134.4836	136.8284	141.8119
145.3989	148.5956	158.2645
165.9067	174.2946	183.5975
184.4735	201.6280	204.4864
206.7345	208.6541	218.9708
223.5729	240.3301	252.0894
260.2831	266.8971	271.7170
279.3239	283.6769	287.3894

293.4944 294.6003 299.3457
315.2774 327.0221 343.3833
353.3162 364.3822 370.2629
379.9309 391.3000 402.1533
414.6990 416.3119 426.1640
431.9663 435.2352 443.2825
463.3855 481.2885 485.8285
490.9059 500.8464 505.6583
516.8554 520.5543 531.5423
543.4224 550.3332 560.9280
564.6197 569.1590 579.5606
584.6493 589.4578 610.5768
625.3789 633.3285 637.7797
654.6268 666.0925 671.6230
685.7690 692.2820 706.1207
720.7691 726.3877 744.8193
745.5836 752.0165 759.3077
765.6780 776.7421 780.9716
786.3792 803.6548 807.4201
812.3579 840.4846 842.2528
847.6027 853.4715 867.0458
881.1417 881.7384 885.4577
891.7527 898.7146 919.0805
922.7335 928.7217 952.0412
956.4088 959.3282 966.5201
975.4685 981.5809 982.7593
986.5964 988.4606 991.5090
1006.4094 1010.8850 1014.2796
1015.9882 1023.7740 1025.3033
1030.9418 1031.6460 1036.3366
1042.0342 1047.1880 1049.1636
1055.4649 1061.4243 1062.4252
1063.9192 1068.8574 1069.4870
1073.0317 1077.1041 1086.2380
1093.5197 1097.6826 1111.7627
1121.5961 1126.3760 1136.8639
1139.7252 1143.6186 1151.6323
1154.9777 1167.9437 1178.0202
1178.5701 1182.3141 1186.0083
1188.4702 1194.6464 1206.2001
1213.3977 1215.3765 1216.5323
1228.5566 1237.0406 1251.8235
1255.3724 1261.5707 1271.6531
1281.5524 1289.3209 1290.3859

1297.3449	1306.6402	1309.8900
1321.1487	1337.2274	1340.7464
1341.3085	1349.5145	1356.7432
1363.6523	1365.8921	1366.7820
1376.2199	1376.7668	1378.0692
1382.9263	1387.0372	1390.9800
1398.9998	1413.8034	1415.3477
1419.7827	1423.3766	1428.9731
1437.7941	1444.6702	1446.0810
1452.0309	1455.7521	1461.1330
1466.4787	1474.0661	1474.8544
1475.8227	1488.9462	1489.7466
1491.8053	1491.8890	1492.3668
1493.1036	1498.2572	1500.8223
1500.9390	1503.4694	1503.9404
1507.9777	1517.2677	1520.3716
1522.5703	1525.0634	1528.0820
1536.1004	1536.8961	1537.5442
1548.6163	1595.4736	1601.7261
1607.9837	1666.4748	1675.0157
1680.3506	1681.3637	1685.8578
1692.4506	1693.6808	1706.3203
1713.2573	1746.6265	1840.1159
1873.8671	2396.3553	3056.1235
3063.5015	3067.5984	3070.9371
3072.8538	3076.5457	3080.2206
3081.0055	3090.9223	3096.6593
3099.7018	3123.0068	3128.4900
3139.4584	3140.9199	3144.3306
3146.6848	3148.0471	3151.3668
3153.6384	3155.1769	3155.9105
3165.9150	3168.3467	3172.4038
3174.9533	3175.6042	3178.3394
3189.1418	3194.1591	3195.2317
3197.1751	3198.0730	3201.4936
3203.7438	3207.7214	3207.9249
3223.8927	3225.9862	3227.4353
3241.0123	3242.5340	3257.6834
3266.8714	3269.0583	3282.9296

TS6R[b]

Zero-point correction= 0.830803

Thermal correction to Energy= 0.881855

Thermal correction to Enthalpy= 0.882799

Thermal correction to Gibbs Free Energy= 0.744589
Sum of electronic and zero-point Energies= -2407.198908
Sum of electronic and thermal Energies= -2407.147856
Sum of electronic and thermal Enthalpies= -2407.146912
Sum of electronic and thermal Free Energies= -2407.285122
Cartesian coordinates

C	-2.244893	0.409058	1.462914
C	-0.915362	0.303439	1.754132
C	0.322447	0.201569	0.874473
O	-3.229043	0.434212	2.279979
C	0.956552	1.561106	0.471338
C	1.850538	1.638658	-0.600510
C	0.738356	2.699986	1.245326
C	2.547734	2.815595	-0.864485
H	2.003604	0.773137	-1.239984
C	1.444927	3.872341	0.992527
H	0.029890	2.648031	2.064274
C	2.361625	3.932871	-0.054437
H	3.238534	2.853583	-1.701780
H	1.269433	4.745169	1.615273
H	2.912504	4.848556	-0.249285
C	-0.011926	-0.499494	-0.388925
N	-0.276304	-0.977671	-1.410874
C	-2.776250	0.511584	0.037756
C	-4.141695	0.196215	-1.647613
C	-4.463465	-1.380082	0.262069
H	-4.617931	-0.994113	1.275004
N	-3.503837	1.289594	-1.937686
N	-2.663408	1.481046	-0.874580
N	-3.738091	-0.309999	-0.444169
C	-5.264891	-0.434690	-2.413401
H	-4.975270	-0.577091	-3.455826
H	-6.134342	0.236954	-2.378070
C	-5.799664	-1.655864	-0.469056
O	-5.569491	-1.695607	-1.872921
C	-4.797340	-3.722591	0.131796
C	-3.813804	-2.743271	0.286189
C	-2.484929	-3.074194	0.492474
C	-2.141045	-4.426986	0.527032
C	-3.114991	-5.412660	0.367041
C	-4.454316	-5.067276	0.172117
C	-6.155054	-3.083502	-0.049927
H	-1.716622	-2.321466	0.630677
H	-2.831065	-6.460358	0.394368

H	-5.211245	-5.835948	0.046281
H	-6.715320	-3.070060	0.891517
H	-6.776395	-3.562067	-0.810584
C	-2.001084	2.758331	-0.782478
C	-2.480506	3.673469	0.161473
C	-1.037069	3.085891	-1.741217
C	-1.880515	4.932747	0.187204
C	-0.488439	4.363110	-1.680670
C	-0.880061	5.289467	-0.714203
H	-2.225988	5.659148	0.918563
H	0.279434	4.634665	-2.401331
C	-0.641061	2.137476	-2.839414
H	-1.367189	2.183463	-3.657769
H	-0.599925	1.104235	-2.492036
H	0.339988	2.412795	-3.232435
C	-0.210031	6.634837	-0.641808
H	-0.091973	7.073838	-1.635899
H	0.791827	6.528976	-0.209912
H	-0.775094	7.330854	-0.018359
C	-3.650782	3.364035	1.058485
H	-3.441110	2.572705	1.783496
H	-4.506410	3.027733	0.460831
H	-3.951607	4.265050	1.595861
H	-6.570790	-0.910857	-0.234764
H	-1.101741	-4.691966	0.688872
C	1.448249	-0.613908	1.579396
C	1.221414	-2.042094	1.786933
C	2.120104	0.109044	2.682034
H	2.579006	-0.840697	0.633418
C	2.141860	-2.827147	2.710461
O	0.359802	-2.662281	1.161642
O	3.398832	-0.319083	2.847445
O	1.663407	0.995367	3.375792
H	2.137171	-2.421214	3.725754
H	1.795029	-3.860201	2.724458
H	3.173999	-2.784264	2.352467
C	4.092409	0.196305	3.990862
C	5.442484	-0.485622	4.036632
H	4.183120	1.282116	3.894589
H	3.501735	-0.010120	4.889045
H	6.014225	-0.272634	3.129776
H	6.013408	-0.129355	4.897063
H	5.321213	-1.568230	4.124079
C	4.655647	-0.461095	-0.138220

C	5.656393	-0.731640	-1.039632
C	5.459610	-1.735637	-2.026752
C	4.206510	-2.404844	-2.017049
C	3.264102	-2.063503	-1.076701
H	4.762804	0.296278	0.631534
H	6.579533	-0.171928	-0.980253
H	3.973192	-3.179622	-2.733983
H	2.290106	-2.543588	-1.035587
C	6.174987	-3.064369	-3.931392
C	7.688404	-1.329962	-2.903956
H	5.314520	-2.809607	-4.558479
H	7.052263	-3.146535	-4.569564
H	5.994293	-4.037887	-3.463793
H	7.549101	-0.257346	-3.074903
H	8.198389	-1.470650	-1.945368
H	8.326380	-1.723664	-3.692297
N	6.415821	-2.036261	-2.928747
N	3.483893	-1.114201	-0.152568
H	-0.700321	0.265540	2.817021

Vibrational frequencies

-925.8465	9.2425	14.4907
27.3900	32.6998	35.2653
43.2605	46.4082	49.8799
53.6560	57.5047	61.9299
67.8505	73.8095	77.9358
81.7624	87.2922	94.2766
95.9002	99.7342	105.7701
108.8092	114.6122	118.3135
123.9891	127.8193	132.5186
136.6162	149.0798	154.6475
158.6810	167.7997	172.0914
177.7782	186.4427	187.7761
199.6405	202.9467	204.2813
212.1270	226.4020	228.9294
238.2405	242.8063	258.6161
263.5694	267.2925	270.3601
275.9116	285.9106	288.2364
293.3177	297.2805	310.8145
316.1590	327.9770	336.0857
346.3485	355.9497	366.7440
389.0123	398.7610	402.8521
412.0801	425.7690	428.6183
432.2167	434.0776	443.1355
458.5529	484.2275	489.2179

491.3006 494.8855 502.2056
515.4144 525.3566 535.1740
537.2914 552.7228 559.1853
573.7724 580.0276 585.2623
588.3702 594.0569 596.0983
608.4326 624.3877 636.1716
650.7415 666.2065 667.8850
677.7326 703.6604 709.7756
720.6181 726.9237 741.3618
743.9987 754.1151 755.8859
775.8342 778.0660 785.0826
794.0455 802.3754 808.4785
812.9289 822.0959 834.1995
837.6311 844.0927 848.5989
871.5317 872.3096 877.8228
882.4228 884.8456 908.3162
911.3700 913.9965 932.9977
948.2148 960.6869 969.1236
979.4931 985.6632 986.2779
991.3991 993.1731 997.8185
1000.1527 1011.4626 1016.0339
1017.7698 1020.6087 1037.7285
1038.2072 1039.1682 1041.9892
1046.8149 1053.5479 1061.9346
1064.1650 1065.0578 1066.3093
1067.5298 1068.1485 1074.8014
1076.3792 1078.9160 1082.5018
1095.7601 1110.3454 1117.1173
1129.1015 1137.0191 1146.2617
1150.0361 1153.2716 1160.8048
1165.1123 1166.5995 1170.6283
1177.0385 1183.5108 1189.0043
1193.8681 1198.9119 1202.6067
1205.2669 1214.7149 1215.4161
1236.1833 1253.4596 1255.0759
1268.3098 1278.6555 1281.5508
1285.4280 1286.2148 1291.4169
1298.9136 1302.1233 1322.2707
1330.3712 1336.0202 1337.1025
1341.4607 1346.0541 1356.8406
1359.9247 1361.6873 1372.3800
1377.0869 1381.2996 1385.2061
1385.3640 1390.1512 1399.7344
1408.1718 1416.9154 1417.6195

1424.1595	1439.2617	1440.6404
1445.5796	1449.9694	1455.7932
1468.8042	1470.0442	1473.2476
1477.9599	1491.0898	1492.5019
1493.0475	1493.2502	1493.6837
1495.0494	1496.4969	1497.2556
1499.2291	1500.7930	1502.0042
1502.9236	1503.8667	1508.6045
1514.8093	1524.0137	1524.4520
1532.4109	1535.9095	1538.9574
1540.7074	1541.2535	1565.8827
1591.6537	1609.8225	1671.2800
1673.3286	1679.5129	1681.3555
1686.5593	1689.6037	1698.7802
1709.6594	1712.0730	1715.5935
1743.5651	1819.3780	2385.7262
3058.6871	3061.0185	3061.8072
3067.5956	3069.1588	3072.9634
3074.5174	3078.1529	3079.7697
3094.7604	3096.6252	3116.7194
3129.9609	3133.0550	3133.4841
3138.7979	3141.8472	3143.4961
3146.3453	3152.0899	3162.2362
3164.7452	3166.5743	3166.6044
3167.9288	3185.2892	3187.8688
3188.7379	3189.5434	3190.9285
3193.8843	3200.0638	3202.1910
3202.6697	3211.7600	3214.2626
3214.5670	3224.4802	3226.4386
3233.2536	3238.1962	3246.5853
3264.7240	3265.0795	3267.3956

TS6R[c]

Zero-point correction= 0.665346

Thermal correction to Energy= 0.706230

Thermal correction to Enthalpy= 0.707174

Thermal correction to Gibbs Free Energy= 0.593427

Sum of electronic and zero-point Energies= -2025.212414

Sum of electronic and thermal Energies= -2025.171530

Sum of electronic and thermal Enthalpies= -2025.170586

Sum of electronic and thermal Free Energies= -2025.284333

Cartesian coordinates

C	0.090589	-0.747544	1.681977
C	-0.362462	0.582126	1.482404

C	-0.738546	1.315778	0.170574
O	0.522909	-1.216273	2.743683
C	-2.206908	1.523186	-0.189073
C	-2.535363	1.971622	-1.471830
C	-3.220259	1.317508	0.744126
C	-3.863197	2.209481	-1.814659
H	-1.740476	2.145687	-2.192859
C	-4.545745	1.575834	0.405911
H	-2.970886	0.969586	1.740390
C	-4.873096	2.017837	-0.873119
H	-4.107067	2.554371	-2.814745
H	-5.326836	1.415637	1.143686
H	-5.908629	2.214345	-1.134808
C	-0.058615	0.615630	-0.937753
N	0.512945	0.029167	-1.755653
C	0.167184	-1.749602	0.538900
C	0.917520	-3.320251	-0.767032
C	2.629629	-2.337625	0.786616
H	2.480669	-2.368688	1.870028
N	-0.361896	-3.268276	-1.001159
N	-0.819424	-2.288011	-0.172851
N	1.281949	-2.416559	0.193215
C	1.932609	-4.256580	-1.347522
H	1.806064	-4.320528	-2.428853
H	1.789361	-5.255518	-0.912540
C	3.464340	-3.549583	0.297052
O	3.223431	-3.763403	-1.086538
C	4.798879	-1.581816	0.199707
C	3.483988	-1.152299	0.386353
C	3.151345	0.190988	0.284514
C	4.150599	1.108154	-0.036597
C	5.462931	0.681416	-0.236987
C	5.796954	-0.667729	-0.114703
C	4.911975	-3.072021	0.419654
H	2.136551	0.533879	0.440403
H	6.231991	1.405230	-0.487463
H	6.819583	-0.999395	-0.267075
H	5.299141	-3.291850	1.420395
H	5.543353	-3.582928	-0.310727
C	-2.232902	-2.010095	-0.103338
C	-2.895547	-2.216688	1.113588
C	-2.901938	-1.630108	-1.278258
C	-4.268966	-1.968822	1.143693
C	-4.270755	-1.401354	-1.181983

C	-4.969688	-1.557322	0.014612
H	-4.800649	-2.117535	2.080200
H	-4.805931	-1.082062	-2.073282
C	-2.237522	-1.513853	-2.625458
H	-2.376518	-2.442864	-3.187465
H	-1.169571	-1.318933	-2.559412
H	-2.703099	-0.701632	-3.189081
C	-6.450349	-1.292463	0.064735
H	-7.002148	-2.063908	-0.481164
H	-6.679122	-0.329916	-0.402492
H	-6.817419	-1.274971	1.092955
C	-2.219941	-2.720422	2.363841
H	-1.914157	-1.895814	3.013925
H	-1.327688	-3.313380	2.150523
H	-2.917573	-3.346269	2.923533
H	3.242119	-4.461992	0.864166
H	3.892526	2.159371	-0.118104
C	0.104168	2.600757	0.480131
C	-0.438166	3.496280	1.510551
C	0.886901	3.188032	-0.623994
H	0.612966	1.568381	1.384760
C	0.218950	4.844733	1.750581
O	-1.381835	3.157743	2.223389
O	1.988182	3.836493	-0.189333
O	0.620875	3.097626	-1.808076
H	0.220909	5.455446	0.843687
H	-0.342702	5.350445	2.535618
H	1.259916	4.719422	2.055263
C	2.736134	4.536777	-1.196119
C	3.843282	5.286410	-0.488344
H	3.124971	3.809793	-1.915953
H	2.063718	5.211714	-1.733999
H	4.501652	4.597363	0.047373
H	4.441447	5.838987	-1.216247
H	3.427358	5.996025	0.230911
H	-0.815396	1.032525	2.362102

Vibrational frequencies

-1572.3543	25.6552	33.9521
37.4125	41.1093	48.2799
53.5132	56.6627	67.4641
72.2056	80.3456	84.7488
86.0428	96.3592	98.3831
105.9742	107.7507	114.5350
129.2639	131.3336	141.2381

144.4800 156.8301 160.2670
165.3086 182.1855 188.9557
197.9676 207.3354 211.5125
215.0715 222.3817 228.0064
237.9947 243.8267 248.9814
270.5620 282.7140 290.1659
294.0823 304.8453 308.0530
318.6437 327.5446 349.4564
350.7435 357.1436 364.4478
391.3921 396.0999 401.0126
407.1010 414.0754 434.8885
449.2839 459.0195 485.1359
491.9948 501.3697 510.4299
517.7887 523.9894 527.5355
536.9557 559.4382 575.2069
583.5330 585.6339 603.9749
606.4743 625.8184 632.2461
634.4675 642.7222 649.5557
693.7071 698.5385 707.4138
712.1083 726.8583 738.0419
746.5240 754.9961 762.4418
773.5227 787.6749 790.8529
808.4943 817.6575 828.9081
844.3919 860.0360 865.2940
873.1799 880.5338 882.2631
882.8251 898.3378 916.0377
917.1690 919.3185 942.3788
956.4233 969.1930 972.7048
980.8801 983.9619 993.5262
998.1838 1018.0668 1018.8449
1020.9115 1025.4406 1039.4235
1043.4035 1044.7090 1049.7051
1052.0301 1057.5519 1061.5719
1062.6717 1064.9584 1065.8990
1067.9541 1070.7412 1073.8347
1082.8007 1115.0075 1116.0543
1139.8176 1150.9122 1161.9926
1172.4272 1173.8778 1178.3404
1181.6879 1187.4409 1191.5797
1206.9010 1210.9186 1219.2617
1236.1777 1240.5503 1251.2964
1255.4825 1271.7713 1287.4343
1289.6434 1292.1738 1303.3338
1306.4737 1316.5831 1326.8496

1337.3005	1341.4645	1343.2492
1346.6381	1356.4670	1362.6663
1366.0780	1377.5955	1379.8884
1390.1741	1399.9367	1403.6083
1414.0223	1417.6568	1417.7923
1421.5764	1429.8522	1442.3731
1459.0015	1467.1386	1468.5345
1472.7905	1474.0698	1484.0640
1489.8046	1491.5734	1493.4674
1498.1115	1500.4485	1503.5978
1509.2442	1516.6316	1516.7876
1519.7082	1526.8736	1531.2052
1535.5920	1539.0910	1549.3005
1588.1422	1671.1650	1677.2080
1684.4948	1686.3217	1693.7286
1698.5491	1706.8452	1708.6156
1737.8693	1744.1440	1801.7689
2403.3740	3068.4741	3069.1879
3076.3949	3077.0880	3079.3826
3084.8524	3086.5230	3094.3311
3096.3693	3130.6841	3139.5102
3141.0691	3148.4071	3149.5639
3153.3203	3161.0794	3162.3370
3163.3551	3169.7864	3173.0513
3178.9557	3191.6263	3195.7554
3196.1509	3196.9213	3199.5892
3199.7446	3208.6913	3211.7359
3214.8453	3214.9543	3222.0176
3223.4608	3232.9300	3265.6952

TS6R[d]

Zero-point correction= 0.665554

Thermal correction to Energy= 0.705875

Thermal correction to Enthalpy= 0.706820

Thermal correction to Gibbs Free Energy= 0.593998

Sum of electronic and zero-point Energies= -2025.211170

Sum of electronic and thermal Energies= -2025.170848

Sum of electronic and thermal Enthalpies= -2025.169904

Sum of electronic and thermal Free Energies= -2025.282726

Cartesian coordinates

C	-0.769309	-0.670023	-1.641229
C	0.184725	0.405749	-1.683511
C	0.902924	1.078049	-0.497911
O	-1.383986	-1.081787	-2.625594

C	2.348713	0.622156	-0.249029
C	2.891292	0.680176	1.040138
C	3.175512	0.242139	-1.307088
C	4.229501	0.372363	1.266367
H	2.263783	0.969871	1.878540
C	4.512123	-0.073719	-1.077597
H	2.798201	0.230639	-2.321753
C	5.046942	-0.008109	0.206188
H	4.626224	0.423759	2.276041
H	5.139737	-0.362428	-1.915134
H	6.091290	-0.249832	0.377806
C	0.108246	0.887143	0.729299
N	-0.560494	0.757344	1.665608
H	0.841367	0.293831	-2.548357
C	-1.174748	-1.387653	-0.364840
C	-2.395623	-2.331685	1.167036
C	-3.672071	-0.938223	-0.491936
H	-3.630614	-1.192470	-1.555437
N	-1.194990	-2.799654	1.353950
N	-0.443954	-2.208796	0.383764
N	-2.431837	-1.475830	0.099495
C	-3.653958	-2.668065	1.907127
H	-3.475467	-2.629763	2.982356
H	-3.971965	-3.683846	1.633756
C	-4.885397	-1.616321	0.197887
O	-4.641209	-1.717392	1.593402
C	-5.295999	0.718297	-0.010333
C	-3.940214	0.537668	-0.289973
C	-3.087520	1.624062	-0.431373
C	-3.603652	2.906609	-0.248417
C	-4.954177	3.090158	0.048204
C	-5.811969	1.996567	0.161431
C	-6.019717	-0.606613	0.022340
H	-2.039351	1.491878	-0.676102
H	-5.341565	4.093854	0.189096
H	-6.864483	2.141715	0.384598
H	-6.543880	-0.787968	-0.922074
H	-6.741155	-0.700903	0.836907
C	0.937250	-2.581908	0.202399
C	1.323558	-3.175438	-1.008387
C	1.818450	-2.407407	1.277578
C	2.671698	-3.500327	-1.154535
C	3.147709	-2.767036	1.074208
C	3.599362	-3.288255	-0.137249

H	2.996131	-3.954840	-2.087573
H	3.853904	-2.621376	1.887253
C	1.381726	-1.896041	2.624779
H	0.964002	-2.712743	3.221407
H	0.617376	-1.121801	2.548433
H	2.242047	-1.486684	3.158741
C	5.053563	-3.614240	-0.341880
H	5.557922	-3.791157	0.610470
H	5.558339	-2.777267	-0.835705
H	5.176879	-4.497051	-0.973727
C	0.368366	-3.539247	-2.117643
H	0.390073	-2.804546	-2.926415
H	-0.665423	-3.620759	-1.776264
H	0.662825	-4.504012	-2.535601
H	-5.096843	-2.607833	-0.221087
H	-2.949224	3.768234	-0.336741
C	0.863143	2.686962	-0.760388
C	0.851707	2.879190	-2.278284
C	1.972896	3.381078	-0.002715
H	-0.079426	3.046381	-0.336397
C	-0.465632	2.923937	-2.788331
O	1.883256	2.631132	-2.923807
O	1.672560	3.405532	1.308885
O	2.981016	3.858152	-0.458077
H	-1.261534	3.362267	-2.194039
H	-0.593237	2.935470	-3.866997
H	-0.433199	1.397410	-2.240698
C	2.699202	3.922854	2.171709
C	2.215626	3.750421	3.594049
H	3.623293	3.368340	1.977555
H	2.876078	4.972349	1.920040
H	2.040118	2.694737	3.816873
H	2.965282	4.132413	4.290375
H	1.282822	4.295971	3.753130

Vibrational frequencies

-1126.7526	20.0534	27.1483
32.6887	39.4570	42.0369
47.9056	56.5116	68.0292
79.5193	82.8438	89.2215
92.4480	97.1480	110.7043
121.3390	125.5456	130.9882
135.3814	141.9212	145.5375
149.1469	160.8848	168.4284
171.6303	178.4551	190.9564

195.3062 203.5010 213.5354
219.8332 226.9597 236.1516
240.4934 253.4697 259.6266
285.3929 287.7365 289.7166
293.6394 304.5852 321.0177
330.5487 338.4778 343.2428
350.0923 368.7005 393.8252
401.5647 412.6181 417.5074
430.8553 439.3125 451.4868
468.8030 482.0781 491.8977
499.8764 505.0350 517.9938
527.0657 535.9680 560.2481
577.2171 582.6996 583.8597
586.7251 589.0166 597.3408
626.2021 627.9093 637.6606
646.8422 656.5432 673.0063
697.4457 703.7370 709.9061
723.0262 734.0905 746.5862
754.9449 755.1905 759.5518
779.2618 789.3552 793.0531
806.6543 812.4130 826.4150
845.2690 855.4354 860.2730
866.3332 877.6306 889.9771
890.2326 896.6060 902.4143
914.3668 921.2900 934.4612
941.3352 954.1316 956.7070
968.4623 979.0200 981.3165
986.4702 1000.8313 1017.1086
1021.3991 1022.1039 1027.3116
1039.3218 1042.2201 1043.1256
1046.6993 1049.2780 1052.0201
1057.8395 1062.3274 1064.4436
1066.7236 1068.4477 1076.8507
1082.1879 1105.7420 1118.1376
1121.3847 1138.7151 1153.7228
1170.0843 1176.8440 1180.0459
1184.9201 1187.5628 1193.4429
1208.8536 1210.9164 1213.4407
1217.4965 1223.7673 1237.3632
1255.1270 1256.6494 1265.5590
1277.5104 1285.5859 1290.2417
1304.5695 1308.3644 1319.6296
1321.5591 1334.0408 1341.3632
1344.3844 1347.3495 1360.6548

1367.2661	1374.5366	1380.0991
1385.1534	1387.6743	1391.7212
1411.3587	1419.3232	1419.9370
1420.2525	1429.3644	1445.6019
1450.3053	1458.5130	1465.8650
1472.5838	1473.6562	1488.2299
1488.3882	1488.8839	1491.9114
1493.9226	1494.3500	1498.2502
1502.7335	1506.9891	1517.7279
1519.1307	1528.8631	1531.3511
1537.6249	1539.3332	1543.7481
1553.0242	1589.6590	1670.0349
1672.7010	1682.8788	1685.9088
1694.4588	1695.6883	1706.7634
1731.1731	1738.6711	1879.5687
2395.7018	3062.0118	3072.7513
3077.5926	3079.0818	3079.8505
3087.7296	3092.6912	3102.9963
3115.6819	3136.5046	3139.2199
3143.0302	3145.3714	3150.8176
3151.6106	3157.1311	3159.3737
3164.4167	3164.5464	3167.1588
3170.1252	3171.8101	3193.0581
3194.7765	3198.4370	3199.9535
3206.6715	3212.3077	3212.4118
3218.6180	3226.8024	3230.9389
3239.3941	3245.6923	3255.4193

TS6S

Zero-point correction= 0.843528

Thermal correction to Energy= 0.895166

Thermal correction to Enthalpy= 0.896111

Thermal correction to Gibbs Free Energy= 0.756266

Sum of electronic and zero-point Energies= -2407.652444

Sum of electronic and thermal Energies= -2407.600806

Sum of electronic and thermal Enthalpies= -2407.599861

Sum of electronic and thermal Free Energies= -2407.739706

Cartesian coordinates

C	0.619053	-0.550155	-1.142473
C	0.243965	0.753943	-0.673655
C	0.895253	1.540895	0.468511
O	0.286358	-0.986648	-2.240640
C	-0.140663	2.293882	1.326994
C	0.070030	2.516449	2.688617

C	-1.268673	2.847610	0.714156
C	-0.844933	3.259096	3.432039
H	0.947078	2.106192	3.181105
C	-2.181429	3.589910	1.458422
H	-1.436530	2.714481	-0.350301
C	-1.976308	3.792931	2.821570
H	-0.669696	3.416827	4.491138
H	-3.054282	4.008936	0.967893
H	-2.690325	4.367682	3.401903
C	1.690570	0.670189	1.348828
N	2.341780	0.040842	2.067608
H	0.158681	1.391291	-1.557839
C	1.131111	-1.731751	-0.277797
C	0.941101	-3.778336	0.475067
C	-1.215435	-2.570021	0.159536
H	-1.521070	-2.055291	-0.758365
N	2.215724	-3.595999	0.295757
N	2.325649	-2.315785	-0.168500
N	0.243727	-2.652983	0.140420
C	0.209464	-5.035432	0.851824
H	0.683211	-5.504051	1.715115
H	0.259239	-5.728336	0.000530
C	-1.817918	-3.990381	0.210238
O	-1.123945	-4.741257	1.197403
C	-3.031599	-2.552882	1.661457
C	-1.819676	-1.918662	1.383226
C	-1.367086	-0.855027	2.147342
C	-2.177681	-0.386823	3.183544
C	-3.412946	-0.984979	3.435561
C	-3.844323	-2.080037	2.682472
C	-3.232027	-3.735959	0.740548
H	-0.398973	-0.401578	1.966734
H	-4.035876	-0.610234	4.241104
H	-4.789904	-2.564315	2.906325
H	-3.900314	-3.485369	-0.091470
H	-3.624995	-4.622333	1.242875
C	3.650503	-1.793366	-0.416055
C	4.022859	-1.441981	-1.717529
C	4.550005	-1.782721	0.664464
C	5.322482	-0.961583	-1.898821
C	5.829919	-1.294664	0.418285
C	6.229797	-0.863655	-0.848866
H	5.629773	-0.674713	-2.901317
H	6.540718	-1.267156	1.240486

C	4.227427	-2.349089	2.023335
H	4.474809	-3.414728	2.044480
H	3.177774	-2.240053	2.287309
H	4.823574	-1.842711	2.784693
C	7.607772	-0.297721	-1.064585
H	8.350820	-0.826078	-0.462762
H	7.635531	0.756784	-0.768268
H	7.901431	-0.356831	-2.114459
C	3.131435	-1.606423	-2.918781
H	2.620512	-0.668981	-3.150584
H	2.371156	-2.375146	-2.771246
H	3.741448	-1.884468	-3.780466
H	-1.780817	-4.500413	-0.759890
H	-1.842875	0.450174	3.788088
C	4.432096	2.051643	-0.376071
C	3.034953	1.983075	-0.926040
H	4.663480	3.064868	-0.036858
H	4.495512	1.386687	0.495932
H	5.142659	1.721223	-1.132063
C	1.942062	2.616513	-0.054306
C	1.185325	3.709181	-0.795688
H	2.391576	3.072594	0.830652
O	1.072166	4.792277	-0.032918
O	2.760773	1.444961	-1.975454
O	0.702414	3.592253	-1.897528
C	0.195288	5.828354	-0.522662
C	-0.052193	6.772895	0.630468
H	0.676387	6.317750	-1.373815
H	-0.727861	5.357021	-0.872558
H	-0.713983	7.580411	0.310245
H	-0.525967	6.237152	1.457410
H	0.884781	7.209579	0.982753
C	-2.648311	0.176651	-2.240525
C	-3.904826	-0.013207	-2.766106
C	-5.032145	-0.021688	-1.903497
C	-4.770557	0.188050	-0.523554
C	-3.476334	0.369044	-0.093346
H	-1.767879	0.177955	-2.875872
H	-4.007738	-0.153036	-3.833370
H	-5.567079	0.212747	0.208022
H	-3.260593	0.535091	0.957962
C	-7.411931	-0.201031	-1.451093
C	-6.506487	-0.417982	-3.793920
H	-7.504010	0.769024	-0.951317

H	-8.325771	-0.387120	-2.011316
H	-7.309865	-0.980932	-0.689460
H	-6.185021	0.453515	-4.373956
H	-5.967670	-1.299813	-4.155556
H	-7.569728	-0.572091	-3.965602
N	-6.282627	-0.215757	-2.369441
N	-2.419549	0.354446	-0.925490
H	-1.120312	0.523212	-0.580227

Vibrational frequencies

-1340.0672	13.5142	14.5429
23.3212	31.6400	35.3582
43.1624	44.7422	50.3376
54.5551	57.2978	59.4580
68.0020	70.9245	75.9062
81.3233	83.2999	87.8788
91.4263	93.6377	97.6940
100.5145	106.2884	109.2254
112.6209	119.5813	121.4284
129.4208	136.3091	139.3352
145.1065	156.2545	163.4223
164.7780	176.4540	184.6110
190.3208	196.4501	208.2950
211.2005	212.5793	215.7602
224.9647	234.8981	239.5580
247.9849	256.8384	264.7088
270.2179	278.2172	288.4718
291.7004	292.5367	292.8448
319.3199	326.1290	340.1896
346.0528	359.6300	374.0144
377.6827	397.2380	410.2114
418.0993	421.6126	423.9322
428.6408	434.1415	453.9821
465.8879	483.6558	486.5403
493.6910	496.1264	502.5618
515.8978	520.1533	526.5655
545.1862	553.1657	558.1640
559.7987	564.4921	579.4185
582.4644	586.8400	604.5575
612.1895	627.1117	637.8594
650.4351	668.5667	670.7926
675.6284	704.8908	706.2757
721.5480	723.2247	742.9682
744.7627	748.4787	759.0361
762.8947	779.5077	781.1401

783.5013 793.4468 807.6994
822.7072 831.6709 840.5762
851.4879 854.5871 873.0446
873.8997 875.3076 879.7160
884.3442 897.8776 916.1130
917.9506 920.9315 935.9919
952.5650 954.4086 965.4243
968.5151 976.7474 979.9659
985.2468 991.7664 994.8232
1008.1081 1008.8530 1012.9592
1015.2319 1018.9855 1021.8905
1023.3733 1028.7531 1037.5918
1040.1165 1042.5211 1048.6344
1050.9878 1053.3935 1062.2582
1063.5119 1065.2643 1070.9555
1072.4136 1077.5271 1079.2669
1092.9466 1100.6601 1112.9623
1114.7212 1121.8046 1127.7136
1142.8143 1149.1807 1152.5453
1159.7271 1169.1467 1174.4708
1177.7140 1180.6253 1184.3200
1187.2941 1192.5876 1203.7407
1211.3419 1216.2144 1219.6334
1226.3114 1235.8216 1254.3498
1256.8808 1262.8544 1272.8831
1279.0837 1286.1449 1286.8233
1289.3004 1307.9747 1315.3064
1315.8701 1332.5255 1335.9059
1337.9544 1344.4862 1354.5308
1361.5517 1364.2292 1367.7108
1379.2350 1381.8317 1383.0422
1385.3794 1386.8234 1391.0306
1403.2896 1413.9872 1416.2528
1417.6081 1419.2803 1426.2031
1428.0833 1444.0682 1449.8911
1455.8020 1462.6698 1462.9347
1463.5416 1467.2740 1468.9118
1473.7790 1489.8938 1490.5624
1490.7642 1493.1401 1493.4447
1494.2203 1495.6337 1500.6181
1502.3787 1502.7377 1503.4431
1505.0264 1516.2301 1517.3005
1520.1403 1521.9652 1524.1737
1531.8039 1536.0058 1537.9851

1550.2769	1569.5786	1589.9381
1606.1151	1648.7239	1671.8020
1676.7411	1682.9118	1684.7065
1692.9135	1693.9982	1706.4383
1707.7527	1753.4844	1839.3512
1873.8728	2419.8200	3060.3603
3061.7574	3068.2176	3069.8675
3071.9344	3080.3275	3083.4700
3085.0725	3092.3571	3102.5054
3110.0657	3119.8195	3130.4923
3131.5376	3136.0544	3136.7890
3140.3189	3141.4947	3151.5897
3153.7499	3158.6319	3167.0494
3169.2306	3170.3151	3171.1711
3175.1581	3185.4685	3190.2896
3193.1005	3198.5837	3198.8854
3201.4487	3202.0675	3202.5089
3206.1494	3206.7207	3217.3484
3217.8786	3224.2572	3227.6507
3231.3194	3234.2420	3244.1582
3254.4537	3258.6423	3266.8654

TS6'R

Zero-point correction= 0.969366

Thermal correction to Energy= 1.029502

Thermal correction to Enthalpy= 1.030447

Thermal correction to Gibbs Free Energy= 0.872964

Sum of electronic and zero-point Energies= -3107.745941

Sum of electronic and thermal Energies= -3107.685805

Sum of electronic and thermal Enthalpies= -3107.684861

Sum of electronic and thermal Free Energies= -3107.842344

Cartesian coordinates

C	-0.777852	-0.324272	-0.804679
C	0.014577	0.107736	0.330900
C	-0.006384	-0.581238	1.717763
O	-1.037072	0.403774	-1.759237
C	1.232286	-1.420432	2.084929
C	1.138264	-2.445310	3.028148
C	2.492424	-1.030989	1.631389
C	2.283132	-3.097356	3.477380
H	0.168285	-2.745534	3.417304
C	3.638482	-1.681209	2.082128
H	2.590665	-0.181208	0.965941
C	3.537464	-2.722110	3.002046

H	2.190708	-3.897742	4.204263
H	4.611649	-1.358208	1.723300
H	4.430151	-3.228804	3.354524
C	-1.220177	-1.416566	1.845824
N	-2.193061	-2.039471	1.920848
H	-0.154646	1.185477	0.420427
C	-1.347806	-1.726468	-0.965485
C	-2.805439	-3.299910	-1.320502
C	-3.665960	-0.981872	-1.753796
H	-3.181026	-0.397809	-2.540446
N	-1.682988	-3.919588	-1.095136
N	-0.780556	-2.926012	-0.880677
N	-2.638950	-1.941891	-1.282313
C	-4.143645	-3.898903	-1.627142
H	-4.362159	-4.691925	-0.910764
H	-4.127900	-4.325659	-2.639437
C	-4.867848	-1.782889	-2.324876
O	-5.128489	-2.905565	-1.498399
C	-5.667334	0.036440	-1.005372
C	-4.302396	-0.066856	-0.730247
C	-3.716150	0.716867	0.256410
C	-4.518104	1.599646	0.978483
C	-5.886378	1.686054	0.720863
C	-6.469684	0.904816	-0.274559
C	-6.053818	-0.830713	-2.178615
H	-2.651970	0.673278	0.462699
H	-6.498070	2.374452	1.294450
H	-7.532394	0.979125	-0.483495
H	-6.169133	-0.227192	-3.084974
H	-6.975788	-1.396835	-2.027979
C	0.616459	-3.250068	-0.754155
C	1.499715	-2.747984	-1.717994
C	1.002647	-4.146570	0.252601
C	2.846198	-3.089433	-1.575347
C	2.357275	-4.447333	0.341013
C	3.295773	-3.908757	-0.542482
H	3.556124	-2.718192	-2.310593
H	2.690607	-5.121892	1.125557
C	0.017136	-4.808298	1.178953
H	-0.446636	-5.665656	0.682899
H	-0.788159	-4.136173	1.483013
H	0.531616	-5.162495	2.073988
C	4.757239	-4.221565	-0.374362
H	4.916140	-5.293154	-0.229717

H	5.147896	-3.711114	0.512880
H	5.338549	-3.896616	-1.239167
C	1.047965	-1.955894	-2.920772
H	0.911290	-0.892798	-2.706561
H	0.104725	-2.340406	-3.320724
H	1.801770	-2.034117	-3.705983
H	-4.685724	-2.110513	-3.355860
H	-4.063728	2.237545	1.729053
C	-0.119120	0.486764	2.902130
C	-1.390562	1.339879	2.851666
C	1.136448	1.344198	2.894039
H	-0.117320	-0.092445	3.826730
C	-2.523445	0.928058	3.742813
O	-1.465591	2.303700	2.109135
O	1.968420	0.989370	3.843676
O	1.358344	2.222506	2.078158
H	-2.150187	0.646684	4.729849
H	-3.243829	1.740201	3.826466
H	-3.015494	0.047356	3.312735
Li	0.008540	3.549151	1.557907
C	3.273000	1.624494	3.843493
O	-0.334564	3.701396	-0.324930
Cl	-0.053351	5.418959	2.744892
C	4.093463	0.929823	4.903577
H	3.699962	1.505021	2.843532
H	3.132849	2.689647	4.040659
C	0.235693	4.904113	-0.891828
C	-1.718286	3.567245	-0.729521
H	4.178414	-0.136235	4.677730
H	5.094680	1.364589	4.930050
H	3.636363	1.049832	5.887742
C	-0.952205	5.702163	-1.408927
H	0.798909	5.414085	-0.106869
H	0.916271	4.614048	-1.702006
C	-1.907090	4.588429	-1.843870
H	-1.874261	2.531701	-1.043756
H	-2.355560	3.787881	0.134580
H	-0.675302	6.380907	-2.217112
H	-1.393085	6.284215	-0.593797
H	-2.944567	4.914129	-1.932515
H	-1.588019	4.167268	-2.802969
C	3.329751	0.175242	-1.472424
C	4.138875	0.588570	-2.503921
C	3.734656	1.679013	-3.319157

C	2.492817	2.282998	-2.989986
C	1.753539	1.794436	-1.937036
H	3.623743	-0.662131	-0.847097
H	5.076391	0.074855	-2.667801
H	2.104101	3.118875	-3.556170
H	0.796464	2.232524	-1.664701
C	4.051984	3.251641	-5.144394
C	5.749177	1.452773	-4.655930
H	3.931440	4.145146	-4.523129
H	4.803148	3.460211	-5.903376
H	3.101904	3.040965	-5.646618
H	6.455632	1.535283	-3.823290
H	5.591547	0.392985	-4.880749
H	6.191617	1.925029	-5.530206
N	4.489697	2.114269	-4.347160
N	2.152070	0.754049	-1.181245
H	1.200279	0.280419	-0.321851

Vibrational frequencies

-1340.5457	8.8071	21.4219
27.2814	34.0029	38.2035
40.2979	42.6520	44.0530
48.3996	48.7651	53.9094
58.9497	62.2552	67.5542
70.1803	71.7558	77.5718
80.0680	82.9980	89.4752
91.3358	95.5182	97.5119
100.7361	103.3504	109.1570
112.8742	117.1090	119.4219
125.5340	129.5492	133.2635
136.0136	138.1455	146.8724
148.2351	153.3992	154.9650
160.4979	165.7138	175.7825
184.7526	187.4858	194.2606
199.2159	208.2576	208.8348
213.6122	220.4429	227.5003
232.7561	237.6042	243.9437
245.7261	257.3920	274.0964
276.7311	279.3411	286.2457
289.6929	290.2886	292.9089
298.2138	302.3499	312.1942
321.7733	327.0338	340.9941
354.0002	367.5811	370.4424
380.6646	389.4965	405.1753
420.1709	427.5339	436.0932

439.4611	443.4036	447.7941
460.9005	482.4556	486.1343
492.4481	494.3908	500.0814
506.4341	519.1584	522.7423
527.4570	533.7477	551.9321
555.6476	562.1186	565.7656
574.4607	577.7118	584.3117
586.0712	588.9094	609.7083
627.1996	629.0529	637.1217
654.6187	665.7144	669.3781
674.0173	686.2580	690.2735
703.5869	722.8079	731.5458
743.2590	744.6147	751.8635
760.6086	764.8452	776.9402
785.6590	788.5849	799.4971
805.3338	816.5279	836.6229
839.5983	845.8813	846.8904
862.2133	864.7065	876.4673
881.2954	889.5003	891.8468
896.8802	898.5469	909.8376
920.3881	924.7661	930.8996
935.4939	937.1243	950.9755
960.0423	963.5047	965.6392
974.7096	982.0673	983.9232
987.5509	988.7218	992.0937
1003.3250	1008.5309	1017.1267
1023.4658	1026.0163	1028.1859
1031.9089	1034.0466	1037.2530
1038.8865	1040.8690	1042.3832
1048.3316	1055.1251	1057.9333
1062.0505	1062.8999	1064.2094
1068.0304	1069.7665	1073.5102
1075.7058	1085.0072	1094.4697
1099.3370	1108.7984	1109.7694
1121.9533	1122.2485	1138.3889
1141.3317	1148.3622	1150.8845
1152.8861	1168.3786	1173.9151
1180.6587	1182.2987	1185.2575
1186.4046	1195.5106	1204.0172
1206.6025	1211.4577	1211.8244
1215.6819	1218.1064	1219.7735
1228.9048	1236.1975	1252.2533
1259.5459	1269.3710	1279.8020
1282.4807	1284.0146	1287.8837

1290.5897	1294.1705	1302.1116
1311.2621	1312.4380	1325.3638
1326.4216	1336.3692	1342.6784
1344.5687	1349.2196	1353.8381
1356.9767	1357.6102	1366.7689
1368.3051	1370.3409	1377.6643
1378.5243	1386.9003	1389.7091
1390.1954	1393.2641	1394.6600
1406.0145	1412.1464	1420.2162
1423.3906	1423.6921	1429.0030
1432.1744	1449.3379	1453.5554
1455.1435	1457.5420	1462.3633
1465.9963	1467.0637	1477.0042
1486.0489	1489.0840	1490.6218
1491.5822	1491.9407	1493.0830
1494.4180	1495.5343	1499.1724
1501.7439	1502.1897	1503.3957
1505.0276	1505.4753	1507.7482
1518.0002	1519.7514	1521.2908
1521.8218	1525.5665	1527.2003
1532.7445	1534.6444	1537.6705
1539.6836	1548.6131	1593.4314
1601.1982	1610.8404	1664.2140
1670.2899	1681.1264	1681.4923
1684.9337	1694.0792	1695.1899
1703.8735	1710.5194	1752.3303
1793.8610	1840.7123	2402.8304
3059.0000	3065.0102	3066.4595
3068.9371	3072.3709	3072.4684
3081.2053	3081.5885	3087.1750
3087.4262	3089.8992	3090.1930
3097.9702	3103.6228	3108.1364
3127.2758	3128.2832	3129.7572
3137.9057	3141.9194	3149.4505
3151.1623	3155.4029	3156.8973
3157.1487	3157.1845	3157.9416
3161.7590	3162.6032	3167.3806
3169.6428	3173.1447	3176.5613
3177.1307	3177.5786	3182.7306
3194.6527	3196.9855	3199.4804
3205.8693	3206.2467	3206.2675
3208.7907	3208.9003	3218.4793
3221.6418	3226.8733	3230.7213
3231.5279	3231.7865	3241.5634

3252.6335 3253.2939 3264.5182

TS6'S

Zero-point correction= 0.969230

Thermal correction to Energy= 1.029346

Thermal correction to Enthalpy= 1.030290

Thermal correction to Gibbs Free Energy= 0.871662

Sum of electronic and zero-point Energies= -3107.740433

Sum of electronic and thermal Energies= -3107.680317

Sum of electronic and thermal Enthalpies= -3107.679373

Sum of electronic and thermal Free Energies= -3107.838001

Cartesian coordinates

C	0.515289	-0.506630	-0.821073
C	0.231347	0.413258	0.252730
C	0.878722	0.445677	1.640612
O	0.207253	-0.281164	-1.985548
C	-0.143400	0.774488	2.746911
C	-0.004317	0.255451	4.034459
C	-1.180247	1.674192	2.481672
C	-0.905172	0.608806	5.036843
H	0.802852	-0.433741	4.263491
C	-2.079610	2.024543	3.484168
H	-1.293992	2.111734	1.493483
C	-1.949124	1.488112	4.763599
H	-0.788547	0.189964	6.030697
H	-2.883175	2.719326	3.261449
H	-2.653822	1.758172	5.542854
C	1.525805	-0.837138	1.961951
N	2.063758	-1.818238	2.250977
H	0.200870	1.411535	-0.192806
C	0.872022	-2.008710	-0.683476
C	0.469192	-4.120680	-1.087955
C	-1.559773	-2.714734	-0.741659
H	-1.777524	-1.777538	-1.267824
N	1.762710	-4.000827	-1.142063
N	2.005718	-2.682210	-0.884031
N	-0.112612	-2.918202	-0.802322
C	-0.383501	-5.314902	-1.409732
H	0.006884	-6.202379	-0.910350
H	-0.350118	-5.475293	-2.496248
C	-2.283057	-3.898248	-1.421907
O	-1.702102	-5.110015	-0.960354
C	-3.432787	-3.295683	0.568690
C	-2.161639	-2.725511	0.645094

C	-1.655145	-2.242189	1.840682
C	-2.466336	-2.290149	2.976477
C	-3.756819	-2.815234	2.896431
C	-4.245784	-3.331756	1.693631
C	-3.693146	-3.813829	-0.828154
H	-0.646828	-1.852069	1.909575
H	-4.379370	-2.842711	3.784603
H	-5.237808	-3.770671	1.645129
H	-4.297564	-3.105092	-1.406826
H	-4.185366	-4.788262	-0.852192
C	3.384029	-2.248548	-0.826046
C	3.860837	-1.320095	-1.759343
C	4.221087	-2.900329	0.096978
C	5.212783	-0.975482	-1.680344
C	5.557748	-2.512379	0.124461
C	6.069911	-1.545516	-0.744234
H	5.601311	-0.251663	-2.392340
H	6.222800	-2.994954	0.836345
C	3.766620	-4.033797	0.980972
H	3.879597	-4.983487	0.449906
H	2.726539	-3.939043	1.286509
H	4.383590	-4.067752	1.880774
C	7.510879	-1.121603	-0.655049
H	8.150866	-1.956900	-0.361960
H	7.629440	-0.335310	0.099025
H	7.867194	-0.723441	-1.606955
C	3.025378	-0.728172	-2.862999
H	2.614673	0.241898	-2.568407
H	2.191507	-1.371275	-3.147955
H	3.655095	-0.569140	-3.740322
H	-2.246956	-3.844801	-2.516432
H	-2.087793	-1.910953	3.920297
C	4.458529	0.696621	1.274492
C	3.173241	1.249653	0.747749
H	4.766738	1.242498	2.169754
H	4.302364	-0.351584	1.563045
H	5.222434	0.747554	0.500928
C	2.060909	1.514061	1.761751
C	1.491478	2.913001	1.604268
H	2.454191	1.426481	2.776344
O	1.283918	3.483021	2.769527
O	2.991762	1.468073	-0.437641
O	1.223109	3.426440	0.533027
C	0.585431	4.753835	2.762905

C	0.228687	5.058773	4.198237
H	1.246448	5.502211	2.318854
H	-0.299587	4.649292	2.128552
H	-0.311618	6.005841	4.245458
H	-0.408420	4.267844	4.602441
H	1.127892	5.139145	4.812240
Li	1.901065	2.902203	-1.269674
Cl	3.091001	4.437967	-2.341164
O	0.144521	2.781983	-2.061281
C	0.199853	2.533995	-3.484571
C	-0.635288	3.968194	-1.792851
C	-0.337112	3.802470	-4.132844
H	1.236967	2.313740	-3.750376
H	-0.420742	1.657193	-3.703144
C	-1.359766	4.273729	-3.096442
H	-1.300113	3.748681	-0.951059
H	0.048919	4.777071	-1.512304
H	-0.767945	3.615928	-5.118180
H	0.468481	4.536396	-4.225926
H	-1.616206	5.330241	-3.187105
H	-2.281466	3.685111	-3.168068
C	-2.566511	1.038218	-1.372988
C	-3.780549	1.233569	-1.991146
C	-4.973831	0.827544	-1.337392
C	-4.818935	0.248755	-0.049679
C	-3.560191	0.094528	0.484281
H	-1.634673	1.343367	-1.844575
H	-3.800473	1.686434	-2.973710
H	-5.671739	-0.074260	0.532042
H	-3.428997	-0.341250	1.470135
C	-7.382772	0.545278	-1.203042
C	-6.299596	1.605148	-3.218543
H	-7.507286	1.080800	-0.255703
H	-8.252128	0.744003	-1.825984
H	-7.344029	-0.529322	-0.996654
H	-5.890792	2.620978	-3.212939
H	-5.773303	1.018712	-3.979472
H	-7.350771	1.660093	-3.494308
N	-6.186450	0.986755	-1.905551
N	-2.439414	0.464626	-0.160888
H	-1.124566	0.295092	0.238855

Vibrational frequencies

-1372.3208	3.8047	21.1381
25.5693	30.9676	33.7350

37.9387 42.8438 43.6861
47.3362 52.8774 54.0509
57.7065 63.2203 65.7896
68.6967 74.9239 77.3204
80.2012 82.9372 86.0096
88.5387 90.6591 95.6659
98.7487 103.3119 106.4114
109.3452 113.2158 118.5133
123.3572 126.4465 129.5817
131.5748 135.6588 136.2473
141.6809 148.2091 158.3330
162.4147 166.3912 177.9024
182.8019 189.2018 199.4753
204.5960 212.6665 217.2268
222.2931 225.9109 229.9892
241.3515 248.0078 254.0612
261.6436 264.8807 271.9957
276.0776 277.6841 281.4257
289.0078 290.3743 296.0866
298.2342 298.9065 313.9867
321.3177 329.7269 344.6509
352.4513 364.4557 378.4788
384.7959 400.1624 409.8618
421.4663 423.5567 429.6955
433.8551 443.6258 457.7772
466.5679 486.2546 488.6091
494.2124 494.8650 501.4109
502.4447 517.8034 520.5995
527.8245 531.3017 553.4197
556.0483 560.7046 564.2970
579.0299 579.6634 581.2129
585.2046 588.5788 607.4919
613.5191 630.1327 638.7616
651.3091 670.2634 672.4712
681.3198 688.2745 705.3602
710.1267 723.0294 725.1529
744.4758 746.5372 751.1303
756.3858 769.3935 781.2714
783.4163 786.9443 793.3162
810.3967 814.3907 840.0537
844.6468 854.5340 858.1088
861.5949 873.9472 875.4799
879.0459 882.5465 891.0656
892.0172 900.7456 916.1625

921.9164	926.9485	928.2271
931.7893	951.1193	954.3988
954.9206	959.6710	969.6778
974.9229	980.1462	980.9961
982.6779	985.9906	990.8576
1006.1711	1013.2739	1015.1413
1016.6441	1019.6587	1024.6143
1027.5170	1030.0481	1031.7550
1036.6505	1041.6722	1046.7235
1049.6741	1050.9757	1056.3327
1057.5630	1059.4597	1065.7196
1068.1714	1069.0887	1069.9733
1076.4976	1077.1695	1093.1550
1097.4248	1111.1218	1114.5602
1114.7849	1125.4192	1128.3189
1138.8696	1145.1775	1150.7856
1159.1096	1173.7658	1174.1312
1176.5834	1178.7726	1181.5545
1184.6124	1187.3465	1206.3976
1207.9190	1208.0551	1211.3978
1213.1974	1218.4158	1224.4119
1227.2671	1234.2658	1252.8223
1256.1340	1262.4184	1272.6256
1274.5353	1283.4984	1285.6299
1288.0750	1292.4245	1297.8649
1306.5575	1308.9117	1317.1142
1324.4290	1330.6211	1336.6965
1339.7063	1341.5403	1355.9416
1358.7706	1361.8758	1364.4052
1371.4982	1375.1547	1378.4796
1380.4849	1385.0574	1387.4479
1388.4693	1390.0344	1403.7672
1407.6204	1419.1540	1421.2078
1423.6340	1425.7893	1431.5905
1437.4973	1446.9476	1453.1109
1455.0096	1461.9173	1463.0401
1465.5240	1467.4944	1474.0583
1484.0018	1487.2557	1489.5039
1491.7709	1492.2530	1492.9542
1494.3000	1497.6974	1499.7665
1500.2580	1501.7995	1502.4069
1503.1571	1503.3737	1508.4821
1516.1477	1516.4986	1519.6307
1519.9387	1522.3619	1523.9663

1530.5631	1532.8359	1535.6022
1539.0886	1553.0823	1571.9666
1588.0992	1607.3714	1641.1630
1670.0197	1676.4705	1682.1402
1682.6282	1690.1660	1695.8976
1701.1006	1703.9971	1761.4672
1795.4069	1841.6893	2417.4793
3054.4184	3060.7170	3063.5765
3065.8888	3072.0135	3078.2442
3078.4656	3078.8833	3083.1108
3085.4876	3085.7160	3087.6742
3103.8150	3104.5237	3107.3384
3109.6282	3120.8948	3121.9535
3134.2894	3142.2338	3142.8615
3148.8135	3150.1587	3152.6278
3153.6431	3154.9858	3159.4844
3162.4053	3163.6451	3170.3028
3172.1814	3173.5218	3175.6300
3178.4896	3180.3773	3194.1965
3198.8893	3203.4967	3204.6550
3207.0712	3209.4648	3211.2778
3216.5721	3217.8181	3220.6146
3231.5116	3232.2851	3235.6914
3241.8238	3244.1855	3247.5512
3249.8617	3261.2142	3270.9049

M6R

Zero-point correction= 0.849576

Thermal correction to Energy= 0.901070

Thermal correction to Enthalpy= 0.902014

Thermal correction to Gibbs Free Energy= 0.763119

Sum of electronic and zero-point Energies= -2407.679343

Sum of electronic and thermal Energies= -2407.627850

Sum of electronic and thermal Enthalpies= -2407.626905

Sum of electronic and thermal Free Energies= -2407.765800

Cartesian coordinates

C	1.191767	0.707561	-0.547438
C	-0.077221	-0.112855	-0.630268
C	0.023165	-1.669222	-0.460616
O	1.585628	1.393085	-1.459388
C	-0.988467	-2.230204	0.556149
C	-0.705251	-3.403091	1.258804
C	-2.260312	-1.660848	0.655847
C	-1.674555	-3.991595	2.066195

H	0.277060	-3.863566	1.184317
C	-3.234222	-2.267133	1.446305
H	-2.505340	-0.754194	0.108087
C	-2.945708	-3.428441	2.158478
H	-1.435002	-4.895428	2.616648
H	-4.223686	-1.822494	1.509346
H	-3.705841	-3.892902	2.778709
C	1.388106	-2.039899	-0.040873
N	2.454778	-2.310778	0.316037
H	-0.490887	0.114897	-1.613702
C	2.011220	0.799508	0.732907
C	3.652412	1.200936	2.104512
C	4.179440	1.781528	-0.265521
H	3.568570	2.475948	-0.844227
N	2.659713	0.815652	2.858493
N	1.646348	0.574136	1.995725
N	3.293268	1.224729	0.787222
C	5.003663	1.662803	2.559011
H	5.410789	0.951448	3.279614
H	4.891892	2.639634	3.050149
C	5.365117	2.521222	0.402798
O	5.878398	1.730972	1.464322
C	6.168230	1.234498	-1.421668
C	4.875385	0.777531	-1.157005
C	4.391501	-0.393129	-1.717156
C	5.234985	-1.121089	-2.556055
C	6.526151	-0.671514	-2.829294
C	7.002989	0.512689	-2.263861
C	6.435125	2.528774	-0.689725
H	3.388907	-0.747872	-1.516790
H	7.170185	-1.252338	-3.482535
H	8.011942	0.856423	-2.471102
H	6.297133	3.393707	-1.347426
H	7.430722	2.591728	-0.245242
C	0.337017	0.307728	2.540672
C	-0.643512	1.296810	2.385844
C	0.155122	-0.851740	3.302086
C	-1.886233	1.045603	2.962809
C	-1.105938	-1.040469	3.862558
C	-2.135273	-0.115022	3.696952
H	-2.670713	1.788826	2.845135
H	-1.288289	-1.944442	4.439022
C	1.259373	-1.844295	3.552667
H	1.840943	-1.544971	4.432077

H	1.948911	-1.922634	2.709260
H	0.830686	-2.832497	3.742061
C	-3.481939	-0.355982	4.323768
H	-3.478124	-0.045629	5.373804
H	-3.737768	-1.417977	4.292244
H	-4.265125	0.207687	3.812358
C	-0.383432	2.592335	1.660571
H	-0.402945	2.469110	0.572531
H	0.578711	3.027743	1.944386
H	-1.167533	3.312311	1.901272
H	5.083689	3.515745	0.770035
H	4.876265	-2.045235	-2.999352
C	-0.256334	-2.409959	-1.817397
C	0.661302	-1.961518	-2.956812
C	-1.716928	-2.218101	-2.208566
H	-0.090646	-3.481289	-1.653905
C	0.348087	-2.492006	-4.327921
O	1.591821	-1.220972	-2.732640
O	-2.447863	-3.286282	-1.933948
O	-2.141782	-1.188100	-2.684649
H	-0.520254	-1.950117	-4.717796
H	1.200227	-2.329043	-4.986125
H	0.087876	-3.553343	-4.288995
C	-3.876055	-3.133728	-2.093641
C	-4.518807	-4.367375	-1.505920
H	-4.178154	-2.221006	-1.568248
H	-4.094776	-3.007393	-3.157217
H	-4.258540	-4.457972	-0.447168
H	-5.603715	-4.295203	-1.595490
H	-4.185189	-5.266416	-2.029766
C	-4.053973	1.457697	0.308891
C	-5.151916	2.202595	-0.080450
C	-5.017693	3.124137	-1.145025
C	-3.737944	3.200386	-1.742111
C	-2.718725	2.397498	-1.262312
H	-4.156024	0.746612	1.130103
H	-6.094554	2.065986	0.433409
H	-3.537567	3.869970	-2.568486
H	-1.735503	2.458510	-1.728475
C	-5.872678	4.807160	-2.680229
C	-7.353934	3.768273	-0.929295
H	-5.578305	4.277766	-3.593768
H	-6.811091	5.324222	-2.872340
H	-5.107041	5.558068	-2.453997

H	-7.761284	2.755022	-1.033448
H	-7.293966	4.007735	0.138468
H	-8.047807	4.464567	-1.395506
N	-6.057144	3.888688	-1.570801
N	-2.838324	1.531221	-0.248566
H	-0.787568	0.286782	0.099730

Vibrational frequencies

10.6723	16.4605	26.8748
32.7911	34.9105	43.6537
45.7487	49.6075	53.4738
57.3070	64.5791	71.5520
74.5410	77.7883	80.0845
86.2491	95.3655	95.9932
105.1366	112.0671	114.9290
116.7123	118.9506	122.1967
126.3781	130.6430	131.2128
137.8661	143.1024	152.6176
156.1693	164.2545	166.0035
167.4863	178.5175	186.6572
197.0082	200.6266	210.1042
220.6388	225.7214	233.0231
238.4015	251.0232	260.5568
264.1067	266.4846	274.4063
283.2528	285.8891	288.1254
289.9580	296.8447	304.7301
323.7418	338.4187	352.3871
363.9405	370.6937	380.7031
390.5606	396.4640	407.8842
417.9268	425.4072	427.2820
428.4153	430.8096	444.0627
472.0167	478.6934	486.5677
492.5438	501.4154	504.2180
518.3757	526.3130	536.9247
552.3595	556.6042	557.7399
568.6887	571.1278	583.2373
585.0520	590.2426	615.4882
628.2275	632.4134	647.9319
653.0061	670.1234	680.9727
694.9801	712.4928	720.5007
722.3804	732.0586	749.2045
754.3073	758.3052	768.1796
774.1908	779.3809	783.1587
793.4822	806.7764	814.2728
827.9701	838.1587	841.6157

847.7175 859.2106 868.6222
878.1647 883.2723 893.7590
894.7029 907.7965 914.1131
919.4909 932.9404 957.4360
959.4737 966.7974 977.6893
984.2423 986.1279 991.0135
994.3219 994.6527 1009.4720
1012.0479 1014.8130 1017.2305
1022.0330 1024.4548 1025.6314
1032.1813 1032.6539 1039.4616
1045.6533 1051.7544 1053.6434
1054.5378 1063.0125 1065.3666
1066.1235 1068.2386 1076.8889
1079.6555 1081.4384 1093.0427
1100.1598 1113.6230 1113.9032
1118.0055 1138.8781 1144.6161
1148.4276 1151.6215 1153.1365
1161.3607 1174.3147 1177.8379
1183.4848 1186.4178 1187.5346
1192.1012 1204.9742 1211.4441
1212.2872 1222.4306 1226.8475
1239.6147 1243.1036 1248.5917
1255.4910 1262.4875 1268.5641
1286.2723 1288.2587 1289.1819
1306.0719 1311.3893 1311.8895
1313.1750 1332.7179 1335.9306
1338.2965 1348.2081 1351.3590
1357.5255 1359.5176 1366.4100
1377.2657 1380.6996 1381.1563
1384.8837 1392.2504 1400.4256
1409.5550 1410.6712 1415.6929
1418.9546 1424.3106 1430.9278
1435.5228 1450.5766 1452.4033
1454.2599 1463.2669 1469.0864
1471.0962 1473.0159 1477.8986
1488.8361 1491.2866 1492.6802
1493.0946 1493.8073 1494.8737
1495.0294 1495.6267 1501.2424
1502.6860 1504.4483 1506.4852
1510.5536 1517.2689 1519.5211
1521.8677 1524.8632 1527.6363
1532.7686 1535.1858 1540.5800
1555.0020 1576.0173 1590.8608
1627.1392 1662.2810 1675.0879

1684.5025	1684.8851	1690.5989
1693.6458	1694.7101	1707.5914
1842.2815	1854.7650	1872.0286
2408.1059	3045.8069	3054.0347
3066.0598	3070.5959	3072.4010
3075.7810	3076.2547	3078.0519
3086.3628	3095.5436	3097.8819
3106.9524	3107.1608	3111.9114
3127.6315	3141.2222	3144.5738
3146.5421	3148.8337	3153.9802
3154.0878	3155.4365	3159.9189
3164.9529	3166.8384	3170.5024
3171.9462	3173.5586	3173.7846
3179.5747	3182.3951	3183.9294
3195.4503	3197.5392	3198.0719
3199.6842	3206.0232	3206.4960
3210.7918	3213.5080	3213.8987
3217.1625	3228.7065	3232.3042
3250.8116	3252.6846	3271.2335

M6R[b]

Zero-point correction= 0.835267

Thermal correction to Energy= 0.886669

Thermal correction to Enthalpy= 0.887614

Thermal correction to Gibbs Free Energy= 0.748656

Sum of electronic and zero-point Energies= -2407.197481

Sum of electronic and thermal Energies= -2407.146079

Sum of electronic and thermal Enthalpies= -2407.145135

Sum of electronic and thermal Free Energies= -2407.284092

Cartesian coordinates

C	-2.308898	0.404358	1.483032
C	-0.984408	0.453047	1.811100
C	0.280624	0.391698	0.963655
O	-3.319226	0.379221	2.267676
C	0.800144	1.772502	0.473335
C	1.729785	1.847390	-0.567460
C	0.439999	2.945210	1.134227
C	2.316863	3.061339	-0.916559
H	1.992879	0.948566	-1.120139
C	1.037772	4.156741	0.799646
H	-0.294133	2.891802	1.930782
C	1.985483	4.220443	-0.218878
H	3.035710	3.097570	-1.730093
H	0.754346	5.057808	1.336611

H	2.451300	5.167343	-0.476773
C	0.024706	-0.397944	-0.268634
N	-0.196560	-0.916809	-1.281531
C	-2.793972	0.360962	0.038700
C	-4.036342	-0.219926	-1.670220
C	-4.265559	-1.692621	0.334219
H	-4.517295	-1.255693	1.306018
N	-3.514841	0.919625	-2.011271
N	-2.750845	1.276644	-0.933653
N	-3.633881	-0.596023	-0.419961
C	-5.038365	-1.030419	-2.435090
H	-4.682887	-1.203020	-3.452295
H	-5.983152	-0.470306	-2.481984
C	-5.519907	-2.176420	-0.433131
O	-5.214306	-2.281302	-1.819102
C	-4.319718	-4.062280	0.367594
C	-3.466265	-2.964162	0.496630
C	-2.122669	-3.121383	0.793969
C	-1.627480	-4.418129	0.943784
C	-2.470723	-5.520874	0.811510
C	-3.827643	-5.351034	0.526411
C	-5.729541	-3.605013	0.071302
H	-1.449123	-2.279176	0.907940
H	-2.069961	-6.523139	0.929626
H	-4.483456	-6.210712	0.422505
H	-6.342553	-3.597420	0.979201
H	-6.244252	-4.203925	-0.683767
C	-2.226190	2.619959	-0.914847
C	-2.805950	3.538022	-0.032587
C	-1.283023	2.985648	-1.882457
C	-2.334393	4.851143	-0.078717
C	-0.866857	4.312853	-1.895827
C	-1.363275	5.252657	-0.991885
H	-2.758575	5.580391	0.606956
H	-0.119790	4.617183	-2.625189
C	-0.767880	2.018022	-2.912529
H	-1.485134	1.921345	-3.734092
H	-0.610202	1.023658	-2.493022
H	0.178757	2.380088	-3.319288
C	-0.832888	6.660799	-1.000432
H	-0.801456	7.066804	-2.015098
H	0.191406	6.675518	-0.611188
H	-1.441147	7.322042	-0.379926
C	-3.944988	3.170822	0.882153

H	-3.645280	2.502115	1.693431
H	-4.732998	2.652894	0.323384
H	-4.377467	4.076364	1.311233
H	-6.383375	-1.514709	-0.287533
H	-0.572367	-4.538743	1.163963
C	1.432322	-0.286580	1.749905
C	1.461526	-1.706320	1.886160
C	2.141732	0.562413	2.693840
H	2.956466	-0.558324	0.628686
C	2.437219	-2.392322	2.842311
O	0.732000	-2.460197	1.208890
O	3.439213	0.160845	2.876570
O	1.721366	1.554439	3.265038
H	2.461470	-1.925988	3.829233
H	2.119217	-3.431833	2.927672
H	3.457075	-2.360319	2.447420
C	4.146564	0.795281	3.945840
C	5.436736	0.029252	4.148548
H	4.331434	1.842588	3.686148
H	3.523796	0.784967	4.845489
H	6.040354	0.036971	3.237172
H	6.020751	0.482630	4.952822
H	5.225992	-1.009740	4.414152
C	4.860712	-0.326719	-0.220248
C	5.735457	-0.740015	-1.188207
C	5.360281	-1.785129	-2.082240
C	4.066330	-2.353899	-1.904875
C	3.245926	-1.887388	-0.913802
H	5.089518	0.463753	0.484636
H	6.700174	-0.257892	-1.255376
H	3.709028	-3.154068	-2.536776
H	2.251077	-2.279437	-0.722436
C	5.766943	-3.274578	-3.955011
C	7.511105	-1.618060	-3.195405
H	4.864116	-2.985411	-4.501230
H	6.560759	-3.456781	-4.675634
H	5.571242	-4.203581	-3.410604
H	7.437416	-0.550161	-3.423678
H	8.102239	-1.747742	-2.283623
H	8.029616	-2.111613	-4.014030
N	6.188266	-2.213609	-3.047229
N	3.646341	-0.893244	-0.094237
H	-0.791057	0.501106	2.878320

Vibrational frequencies

12.7710	16.9355	27.8571
29.6011	37.2978	43.6118
47.5879	48.5082	51.0256
58.6394	59.3943	64.0584
69.9720	73.3994	77.7769
84.8163	87.7873	94.1761
95.1895	97.3015	97.9001
108.6676	115.1325	121.2405
131.0389	134.9160	135.3008
136.1670	146.5238	155.2877
164.7766	170.0444	176.4901
184.8224	192.8611	196.9654
201.9142	205.0834	211.0225
211.9491	225.6796	229.8448
238.1139	253.2776	259.4085
261.1745	268.1926	276.9126
281.4476	288.4224	294.5940
296.4164	312.7812	319.0129
330.0867	342.2364	344.5632
357.6575	370.3768	394.0052
399.5542	402.5760	403.8019
412.2837	432.5188	433.0774
441.7261	442.8402	458.9759
480.7843	485.1095	492.0605
495.6082	502.5377	516.1222
526.0799	530.1853	531.3473
548.5855	551.8645	559.3280
573.5526	584.9400	586.6426
594.8888	598.2863	607.0859
626.3906	635.0744	642.1842
649.8430	658.2601	666.4748
679.2591	703.5397	721.3355
728.0431	734.8024	745.8289
754.6593	758.7271	770.1063
774.1184	776.1531	783.0073
794.6321	801.7938	804.6898
813.3500	817.0118	839.1250
843.8581	846.0201	864.3348
871.0158	876.5733	877.0609
884.6372	906.7039	908.9959
911.1358	926.6248	945.5395
957.1011	968.7990	977.5624
978.7238	981.6876	985.9399
993.1924	997.1615	1001.4030

1007.0473 1013.3257 1016.8796
1018.6654 1019.3768 1037.6388
1039.3626 1039.9389 1040.9381
1048.8795 1052.8487 1058.6727
1062.3245 1064.8481 1067.2402
1070.7287 1072.8199 1075.6637
1079.6557 1083.6835 1091.8641
1095.2901 1106.4858 1112.1375
1117.4586 1128.9632 1138.2975
1143.5931 1148.1783 1151.5351
1159.8446 1166.2122 1167.8416
1175.3231 1180.7372 1191.5140
1191.8759 1197.3723 1202.9746
1206.2343 1212.8569 1214.3625
1234.5262 1239.7413 1253.2818
1261.7163 1279.7203 1281.2361
1285.7709 1289.5154 1302.8363
1304.6835 1308.9544 1319.0797
1330.6369 1337.2224 1337.8934
1343.4734 1343.9501 1359.2759
1361.2707 1369.8392 1377.0578
1377.9869 1380.0183 1380.1958
1385.6775 1404.3042 1406.0876
1417.2344 1420.9426 1427.7568
1435.7409 1439.7700 1448.0757
1454.0756 1454.9830 1466.1126
1466.8236 1471.7798 1474.6142
1480.8377 1489.0438 1491.3499
1492.7163 1494.4326 1495.9957
1496.1818 1498.3423 1498.3703
1502.4715 1503.8436 1504.5025
1505.2196 1509.3756 1513.5745
1513.7863 1524.0834 1533.4796
1535.6219 1535.8558 1537.7958
1543.3624 1567.2553 1590.1423
1616.7108 1651.5088 1660.2972
1673.6323 1680.3110 1684.0389
1687.2842 1691.4941 1697.5902
1708.1028 1709.4347 1727.2984
1783.5664 2383.0358 2833.3460
3058.2795 3062.4356 3065.2888
3065.5958 3071.0201 3071.3160
3079.3249 3079.4759 3086.1546
3089.6001 3094.9932 3130.6973

3131.1271	3132.4253	3134.2353
3136.5482	3137.6762	3146.0105
3149.4778	3155.7637	3163.8982
3164.2466	3167.6983	3168.1577
3170.2782	3178.9116	3185.7598
3187.0212	3196.4815	3197.1018
3198.8433	3203.6165	3207.4312
3207.4970	3210.4797	3214.2965
3216.7595	3219.4176	3231.1525
3231.5706	3245.1252	3246.1354
3257.3320	3272.2748	3275.5743

M6S

Zero-point correction= 0.848360
Thermal correction to Energy= 0.900434
Thermal correction to Enthalpy= 0.901379
Thermal correction to Gibbs Free Energy= 0.759698
Sum of electronic and zero-point Energies= -2407.669830
Sum of electronic and thermal Energies= -2407.617756
Sum of electronic and thermal Enthalpies= -2407.616812
Sum of electronic and thermal Free Energies= -2407.758492
Cartesian coordinates

C	0.920835	-0.524334	-1.176456
C	0.361872	0.772972	-0.666044
C	1.145058	1.668725	0.326054
O	0.889588	-0.826908	-2.341131
C	0.167474	2.477391	1.202064
C	0.569254	2.944532	2.454386
C	-1.098273	2.817236	0.715564
C	-0.287467	3.731036	3.220141
H	1.550143	2.689260	2.845431
C	-1.950703	3.607510	1.484472
H	-1.443512	2.458758	-0.251263
C	-1.551075	4.063546	2.738499
H	0.035991	4.080454	4.194877
H	-2.933889	3.858177	1.098697
H	-2.219649	4.673578	3.336766
C	2.005306	0.861307	1.208135
N	2.677973	0.288171	1.953132
H	0.128650	1.350117	-1.564081
C	1.203318	-1.732326	-0.251515
C	0.690473	-3.687148	0.579389
C	-1.262212	-2.187402	0.195413
H	-1.501658	-1.635245	-0.721737

N	1.983860	-3.698693	0.439142
N	2.295975	-2.477058	-0.077306
N	0.174333	-2.486838	0.179187
C	-0.222286	-4.815609	0.966177
H	0.162787	-5.324111	1.850732
H	-0.251175	-5.529481	0.131091
C	-2.068013	-3.502987	0.258621
O	-1.506783	-4.328464	1.270952
C	-3.057209	-1.898426	1.699167
C	-1.767691	-1.445006	1.413609
C	-1.176398	-0.435244	2.154901
C	-1.921681	0.176760	3.164734
C	-3.224043	-0.245591	3.429330
C	-3.796169	-1.297372	2.708390
C	-3.431517	-3.032361	0.771980
H	-0.146975	-0.134856	1.985841
H	-3.792805	0.236024	4.218029
H	-4.800652	-1.640263	2.937596
H	-4.039197	-2.664476	-0.065167
H	-3.967297	-3.848546	1.260823
C	3.697218	-2.139034	-0.215772
C	4.256942	-1.978107	-1.483165
C	4.448169	-2.082986	0.969721
C	5.614546	-1.653273	-1.538988
C	5.793537	-1.751424	0.849053
C	6.390542	-1.516677	-0.393534
H	6.071832	-1.518945	-2.515521
H	6.396674	-1.690321	1.751488
C	3.880644	-2.437057	2.320131
H	3.948365	-3.517325	2.480587
H	2.836661	-2.140742	2.427384
H	4.449716	-1.934787	3.103862
C	7.845506	-1.137697	-0.476583
H	8.453214	-1.773615	0.173903
H	7.989860	-0.101249	-0.151941
H	8.220868	-1.227137	-1.499494
C	3.491729	-2.151977	-2.765881
H	3.160436	-1.180893	-3.142036
H	2.607577	-2.781675	-2.645618
H	4.140895	-2.608376	-3.516536
H	-2.097419	-4.030727	-0.702163
H	-1.477565	0.982790	3.741024
C	3.916776	2.856225	-2.233554
C	3.058456	1.978225	-1.370065

H	3.291297	3.293329	-3.018257
H	4.339692	3.677308	-1.648519
H	4.708289	2.261467	-2.687182
C	2.089909	2.675558	-0.414327
C	1.245161	3.713897	-1.140877
H	2.686925	3.200552	0.340349
O	1.118383	4.824231	-0.432522
O	3.124951	0.766817	-1.392144
O	0.719008	3.507772	-2.212328
C	0.158311	5.787522	-0.923873
C	-0.043196	6.803890	0.175033
H	0.552803	6.229330	-1.842598
H	-0.763883	5.251608	-1.165872
H	-0.771872	7.551104	-0.146229
H	-0.418269	6.311230	1.075814
H	0.894411	7.311105	0.411953
C	-3.122153	-0.113230	-2.320319
C	-4.392813	-0.559789	-2.634406
C	-5.426982	-0.433942	-1.675375
C	-5.060270	0.146274	-0.438485
C	-3.751548	0.551198	-0.241132
H	-2.326417	-0.210407	-3.057352
H	-4.573363	-0.995518	-3.608306
H	-5.777803	0.276684	0.361361
H	-3.463983	0.984029	0.717807
C	-7.713012	-0.730102	-0.898972
C	-7.019552	-1.447830	-3.211160
H	-7.865948	0.315693	-0.609509
H	-8.654413	-1.118543	-1.283246
H	-7.445278	-1.301481	-0.002218
H	-6.821739	-0.752779	-4.034778
H	-6.443027	-2.363895	-3.386073
H	-8.077842	-1.702012	-3.227212
N	-6.695199	-0.850455	-1.927646
N	-2.771339	0.438103	-1.148226
H	-0.612485	0.513353	-0.230117

Vibrational frequencies

12.9871	16.7472	21.6923
32.1149	33.2137	38.2262
43.9934	45.9593	50.1622
53.5427	57.0151	60.8839
63.6236	66.3130	69.2000
79.1312	82.1652	83.4636
85.9056	91.6003	96.1144

99.7927	103.8671	109.7217
118.3054	122.2990	126.9827
136.3941	141.3413	150.3208
153.8640	154.8892	159.4120
174.4817	176.9826	191.0229
194.2250	205.5503	212.5492
219.2828	220.9119	223.3728
233.8739	238.9069	259.1211
262.6966	266.2167	268.4540
277.7256	283.6062	288.5376
293.7348	299.1709	310.2436
322.8356	333.0213	346.7886
354.0038	365.6318	375.5951
393.1096	394.8783	405.0531
414.4759	416.8543	427.1736
431.2487	442.0962	462.9715
471.2050	479.0706	486.6784
491.6942	499.3260	502.0590
515.2506	523.2272	526.0723
550.3950	551.8386	560.2357
569.0335	572.2499	578.9843
584.1468	591.0008	612.0363
623.9374	627.8464	640.5881
650.7634	671.0826	678.3539
693.9455	705.2041	720.4740
722.6052	737.3125	746.3787
751.5922	757.3400	771.7216
777.5218	778.3290	790.4608
793.8769	803.6741	813.6669
835.2681	839.8620	840.1395
849.7173	860.8490	875.4106
877.0020	878.9618	891.3058
897.6486	905.8507	914.5118
924.9716	925.9982	956.3160
962.4442	963.9664	971.1142
980.3746	985.4181	989.9401
990.8286	1000.4600	1007.0139
1011.2271	1015.5524	1016.3271
1023.4478	1028.0169	1031.2909
1032.5595	1034.8520	1045.4523
1046.6525	1048.6196	1050.7069
1055.4520	1058.6602	1062.7846
1067.4342	1068.8385	1075.1567
1076.8293	1079.6426	1093.3165

1097.2194 1103.7064 1112.1458
1119.4197 1124.9183 1141.6002
1145.8428 1149.4122 1150.4507
1160.8987 1174.9399 1177.1200
1182.4798 1183.3659 1185.8604
1196.7149 1205.1863 1210.5373
1211.9482 1218.5377 1220.9975
1233.0385 1236.7198 1250.5078
1253.3206 1262.0474 1263.4728
1282.4237 1284.2850 1288.3355
1298.9577 1309.4765 1314.4817
1321.5309 1326.8421 1334.2587
1336.1002 1343.2203 1352.3157
1356.7923 1367.9717 1373.4874
1376.0270 1377.9931 1380.5237
1384.7850 1388.0943 1394.9879
1401.8650 1406.4776 1412.2524
1416.2219 1422.6934 1431.3525
1433.0503 1448.8890 1454.3769
1461.3008 1467.1093 1469.8214
1471.8504 1473.6063 1474.0754
1475.9986 1486.7067 1487.8575
1491.5524 1491.9846 1493.3391
1493.3581 1494.5448 1498.7124
1500.3274 1501.8438 1502.4510
1505.3156 1509.4633 1515.1727
1520.0325 1523.1283 1525.5476
1527.1186 1535.4744 1536.5706
1552.8004 1574.4703 1586.9410
1622.1312 1668.3107 1677.4556
1680.5906 1689.5852 1691.1432
1691.9436 1695.5752 1702.6029
1842.5854 1852.3494 1864.1226
2417.2599 3047.5431 3054.7215
3061.5594 3067.1920 3072.1044
3075.7338 3077.3923 3079.1709
3080.6643 3088.5941 3101.4296
3103.2083 3109.5030 3109.6196
3111.1645 3113.8517 3134.4947
3150.7797 3154.4575 3155.8748
3157.5597 3159.3229 3162.9121
3163.1069 3164.1693 3169.1593
3171.4694 3176.9366 3178.6996
3181.8708 3188.5902 3193.6657

3199.5036	3200.8351	3202.6981
3204.2390	3206.9557	3208.2521
3214.1515	3217.3144	3217.6155
3224.9723	3226.2255	3233.6413
3240.0824	3257.4582	3263.0799

TS7R

Zero-point correction= 0.844364
Thermal correction to Energy= 0.895753
Thermal correction to Enthalpy= 0.896697
Thermal correction to Gibbs Free Energy= 0.757855
Sum of electronic and zero-point Energies= -2407.662993
Sum of electronic and thermal Energies= -2407.611604
Sum of electronic and thermal Enthalpies= -2407.610660
Sum of electronic and thermal Free Energies= -2407.749502
Cartesian coordinates

C	-2.055695	0.406464	1.435000
C	-0.711368	1.062420	1.669448
C	0.519821	0.546817	0.829485
O	-2.621383	-0.258496	2.267929
C	1.319954	1.697480	0.172600
C	1.975265	1.488121	-1.046625
C	1.492253	2.923453	0.819706
C	2.786026	2.474008	-1.600982
H	1.852398	0.548454	-1.577499
C	2.318135	3.902865	0.272337
H	1.016581	3.110655	1.774882
C	2.967707	3.685227	-0.938619
H	3.278344	2.288247	-2.550383
H	2.444300	4.845084	0.796901
H	3.607720	4.452330	-1.363328
C	0.020960	-0.310484	-0.270507
N	-0.362418	-0.938594	-1.164545
H	-0.497852	0.911752	2.727321
C	-2.837012	0.619916	0.140994
C	-4.357335	0.406179	-1.404807
C	-4.611251	-1.232904	0.455696
H	-4.715520	-0.929183	1.498848
N	-3.654590	1.447225	-1.755354
N	-2.719077	1.572841	-0.786749
N	-3.901320	-0.126988	-0.233830
C	-5.576081	-0.128180	-2.093216
H	-5.388307	-0.202889	-3.165182
H	-6.405634	0.573760	-1.926951

C	-6.002906	-1.441216	-0.194280
O	-5.876832	-1.409191	-1.607952
C	-4.998066	-3.553481	0.208120
C	-3.982521	-2.603138	0.335884
C	-2.647778	-2.967165	0.387160
C	-2.333054	-4.324171	0.304073
C	-3.338701	-5.281610	0.178464
C	-4.681874	-4.902922	0.130160
C	-6.351757	-2.882777	0.179680
H	-1.856359	-2.237355	0.497164
H	-3.076199	-6.332740	0.113511
H	-5.463146	-5.649118	0.023212
H	-6.829976	-2.910618	1.164862
H	-7.044985	-3.307282	-0.549645
C	-1.896838	2.759853	-0.808110
C	-2.145795	3.741071	0.161257
C	-1.007533	2.932851	-1.872414
C	-1.387253	4.906220	0.087964
C	-0.290386	4.127134	-1.902392
C	-0.457726	5.114934	-0.933211
H	-1.543763	5.678874	0.835805
H	0.429990	4.280162	-2.701664
C	-0.848583	1.918966	-2.972748
H	-1.597267	2.092303	-3.752004
H	-0.970526	0.895740	-2.614675
H	0.142849	2.012983	-3.420811
C	0.332987	6.393048	-1.005411
H	-0.167825	7.117495	-1.655669
H	1.328687	6.208025	-1.415978
H	0.440945	6.848520	-0.018670
C	-3.202350	3.575770	1.225343
H	-2.885931	2.912183	2.038366
H	-4.131555	3.174919	0.809190
H	-3.427335	4.543175	1.675552
H	-6.737062	-0.697511	0.139561
H	-1.292309	-4.629131	0.343696
C	1.497042	-0.320957	1.655530
C	0.928209	-1.574839	2.163694
C	2.291862	0.430933	2.658908
H	2.515342	-0.843843	0.743335
C	1.766010	-2.461885	3.063166
O	-0.197244	-1.940564	1.828045
O	3.474663	-0.165966	2.900904
O	1.958481	1.453925	3.225008

H	1.915326	-1.989113	4.038802
H	1.240843	-3.407278	3.196153
H	2.757112	-2.628752	2.634454
C	4.254147	0.382910	3.977474
C	5.477314	-0.492852	4.130734
H	4.513436	1.416563	3.732654
H	3.641567	0.396061	4.883863
H	6.063721	-0.501364	3.208776
H	6.106954	-0.113940	4.938657
H	5.187355	-1.519089	4.368590
C	4.561789	-0.753467	-0.205733
C	5.474441	-1.222845	-1.119077
C	5.138714	-2.334471	-1.939495
C	3.842852	-2.890552	-1.761806
C	2.998344	-2.349943	-0.822745
H	4.781277	0.092147	0.438658
H	6.436751	-0.735729	-1.194088
H	3.502320	-3.731205	-2.349934
H	1.997336	-2.743029	-0.664083
C	5.624400	-3.976451	-3.662896
C	7.322977	-2.235737	-2.999103
H	4.761875	-3.739285	-4.294250
H	6.459880	-4.242222	-4.306804
H	5.378952	-4.843619	-3.041460
H	7.246065	-1.185228	-3.297738
H	7.897379	-2.297125	-2.068986
H	7.864847	-2.772763	-3.774516
N	6.004905	-2.834763	-2.842524
N	3.348247	-1.306705	-0.053848
H	-0.826378	2.133650	1.495776

Vibrational frequencies

-931.5579	13.1786	17.5961
25.9001	31.4034	31.8820
34.6063	39.4356	51.0226
53.7593	62.1284	66.7797
69.7117	73.7213	78.6000
82.2488	88.8140	90.0212
95.0632	100.5871	103.0628
107.2988	113.8383	116.1474
120.5932	127.9237	133.6795
136.2283	139.1501	142.1010
159.6280	162.5466	168.9907
178.5572	185.9493	191.8011
193.6336	201.3742	205.2642

210.0834	216.6130	224.1034
233.3499	236.8268	240.2654
248.6441	252.2194	265.8859
274.2036	276.4151	289.9201
292.9379	298.5754	304.0393
314.8907	326.9367	334.4326
343.0288	355.9999	366.6957
388.0801	391.5310	398.7734
408.7668	416.5825	425.9539
427.7320	428.0487	435.2939
443.1007	478.5744	482.2523
490.7155	495.7248	508.2962
518.4604	528.7960	533.1980
537.2425	554.8513	556.8507
560.7039	577.7586	583.3531
585.2534	587.8931	594.7246
606.0807	630.6258	632.2850
647.5356	651.7117	668.0252
671.7858	699.8292	714.5032
716.0161	725.1499	728.4812
743.1191	747.0698	752.8798
765.5389	770.2050	783.0756
798.2593	805.4811	806.8851
814.4202	824.4069	842.3652
843.6855	854.6910	861.4385
865.2727	870.0129	877.9314
881.2352	898.6259	906.0974
920.6174	923.0498	929.6290
948.2495	961.8137	968.8430
977.7770	983.1572	984.6756
987.3680	990.6730	996.3268
1002.0373	1005.6064	1018.9597
1020.9976	1022.0951	1022.7206
1031.2268	1040.8562	1043.5323
1048.4271	1049.2720	1058.0289
1059.2327	1062.0652	1064.4596
1065.6792	1070.7657	1071.2831
1078.7698	1080.8463	1082.8874
1098.3477	1105.4739	1119.6268
1131.2854	1132.2967	1139.6878
1144.6505	1148.4295	1152.5596
1154.5262	1158.2391	1176.5170
1179.9532	1183.8194	1187.3226
1189.2880	1194.6187	1214.9935

1215.8065	1219.7480	1224.9276
1227.1686	1241.9733	1243.2046
1251.6089	1260.5683	1277.1845
1279.0512	1285.0221	1287.5050
1295.9458	1300.8206	1309.7152
1320.5233	1327.8260	1333.9314
1341.4728	1343.3277	1351.5219
1353.4275	1356.7500	1362.3660
1368.3530	1372.9359	1380.4482
1382.6071	1383.7493	1395.2080
1404.4798	1410.4515	1421.0363
1423.2422	1425.9867	1433.9160
1442.0251	1445.4211	1451.2203
1457.1659	1463.1400	1466.5980
1468.2379	1473.5621	1474.9903
1484.0052	1484.5030	1490.1793
1491.9593	1492.2146	1494.7670
1495.6454	1497.1349	1501.7462
1502.8797	1504.5888	1505.0164
1509.5199	1514.2130	1517.2486
1522.1991	1523.6492	1533.5838
1535.2559	1539.5314	1540.8203
1550.5341	1569.0476	1591.6911
1612.0601	1661.0133	1670.9298
1675.9343	1683.1876	1688.1832
1694.5848	1695.0771	1709.6676
1709.8241	1750.7390	1814.1344
1855.1367	2398.5361	3058.4517
3062.5277	3064.4092	3070.8245
3072.3074	3080.2308	3082.6498
3084.8905	3086.5613	3099.8172
3102.7312	3127.5330	3131.0389
3134.4401	3134.9312	3146.1726
3148.3725	3155.1383	3159.1891
3160.8579	3161.4507	3165.8642
3171.3336	3172.2255	3172.4441
3175.3213	3188.9432	3193.4688
3193.9674	3200.1781	3201.6570
3205.5543	3206.4700	3210.1250
3210.5168	3215.0930	3216.5284
3221.0378	3224.7609	3225.6982
3232.0767	3233.9631	3250.5357
3267.8704	3273.3868	3285.3352

TS7R[b]

Zero-point correction= 0.831902

Thermal correction to Energy= 0.882336

Thermal correction to Enthalpy= 0.883280

Thermal correction to Gibbs Free Energy= 0.748123

Sum of electronic and zero-point Energies= -2407.173253

Sum of electronic and thermal Energies= -2407.122818

Sum of electronic and thermal Enthalpies= -2407.121874

Sum of electronic and thermal Free Energies= -2407.257031

Cartesian coordinates

C	-0.512926	0.434024	1.052282
C	0.075483	-0.620121	0.288879
C	-0.395648	-1.151621	-1.114579
O	-0.464552	0.514157	2.288605
C	0.629913	-0.923370	-2.251861
C	0.232381	-0.521270	-3.531184
C	1.989451	-1.173510	-2.034925
C	1.160015	-0.364249	-4.559687
H	-0.810302	-0.297145	-3.735276
C	2.917605	-1.007964	-3.059660
H	2.300815	-1.548124	-1.068430
C	2.511364	-0.597926	-4.328256
H	0.819410	-0.043614	-5.539969
H	3.967302	-1.213031	-2.864686
H	3.238133	-0.469099	-5.124336
C	-1.596120	-0.356952	-1.455895
N	-2.508414	0.318886	-1.685259
H	0.183944	-1.455458	0.977276
C	-1.202618	1.646794	0.451068
C	-2.692157	3.198570	0.146077
C	-3.288328	1.504148	1.913143
H	-2.652256	1.418389	2.798088
N	-1.696886	3.530957	-0.624190
N	-0.770886	2.553754	-0.418183
N	-2.419076	2.056750	0.849108
C	-3.986174	3.921275	0.351912
H	-4.383796	4.250888	-0.608626
H	-3.815344	4.801414	0.988100
C	-4.455884	2.499323	2.163823
O	-4.912818	3.038953	0.932523
C	-5.317506	0.281853	2.061978
C	-3.997247	0.195141	1.615301
C	-3.504070	-0.996764	1.094584
C	-4.368641	-2.082191	0.952839

C	-5.698034	-1.980726	1.364462
C	-6.176642	-0.803365	1.937960
C	-5.587338	1.623187	2.699125
H	-2.468975	-1.115096	0.795980
H	-6.363724	-2.830031	1.247400
H	-7.205110	-0.731834	2.279074
H	-5.527720	1.552247	3.790459
H	-6.555437	2.056991	2.438503
C	0.513302	2.611188	-1.066741
C	1.652046	2.752682	-0.263869
C	0.561781	2.591326	-2.466030
C	2.886326	2.763657	-0.911687
C	1.824447	2.594702	-3.054027
C	2.994007	2.644378	-2.296826
H	3.786841	2.866694	-0.311381
H	1.891684	2.545961	-4.137665
C	-0.669482	2.632418	-3.331157
H	-1.017110	3.665134	-3.433905
H	-1.491438	2.048608	-2.915130
H	-0.433340	2.248357	-4.325655
C	4.338098	2.560587	-2.968104
H	4.369485	3.174236	-3.871851
H	4.535143	1.525108	-3.268733
H	5.140793	2.880934	-2.300366
C	1.574771	2.963726	1.227434
H	1.299217	2.058554	1.773104
H	0.837513	3.734629	1.474614
H	2.547297	3.290132	1.600527
H	-4.160241	3.311165	2.840148
H	-3.990775	-3.001197	0.512279
C	-0.803903	-2.644718	-0.951036
C	-2.014831	-3.212278	-1.487297
C	0.167292	-3.466245	-0.287800
C	-2.704908	-2.598572	-2.709704
O	-2.555647	-4.242739	-1.052821
O	-0.173689	-4.775624	-0.121383
O	1.286660	-3.096211	0.097931
H	-2.055402	-1.987599	-3.336700
H	-3.071770	-3.443043	-3.296393
H	-3.567086	-1.997535	-2.407971
C	0.832405	-5.596413	0.461761
C	0.257299	-6.994304	0.565969
H	1.736033	-5.578749	-0.157195
H	1.109263	-5.202605	1.445638

H	-0.010834	-7.373368	-0.423084
H	0.989041	-7.672603	1.012090
H	-0.641543	-6.992857	1.187155
C	3.791151	0.084389	0.474187
C	4.964551	0.221092	1.181098
C	4.962199	0.034455	2.587508
C	3.716747	-0.302822	3.176768
C	2.598173	-0.415118	2.383203
H	3.769884	0.220558	-0.602509
H	5.871577	0.460994	0.642863
H	3.621579	-0.475561	4.239860
H	1.626691	-0.655433	2.805580
C	6.041900	-0.051014	4.762866
C	7.344002	0.507829	2.678394
H	5.732198	-1.074592	4.999404
H	7.035213	0.111122	5.176358
H	5.349189	0.645616	5.246718
H	7.638729	-0.258200	1.952982
H	7.274510	1.471332	2.162267
H	8.122332	0.581507	3.435242
N	6.086132	0.167532	3.324923
N	2.619972	-0.216709	1.054437
H	1.427337	-0.321654	0.469699

Vibrational frequencies

-1300.4822	13.3037	21.1274
28.8383	36.4928	39.3986
39.8339	47.9572	53.8125
63.1436	64.3812	70.3626
75.1222	80.5937	83.0486
86.4934	91.6833	96.9759
102.5332	106.9627	109.3428
113.4788	114.2726	118.7716
130.0775	132.7803	137.5319
140.1626	151.9575	161.7777
168.7152	172.5729	177.3854
186.0560	187.0161	204.2652
207.3048	215.9113	216.6715
217.2225	230.9375	237.7257
247.9178	258.6842	263.4692
267.4753	273.1414	275.5538
282.9388	288.7837	290.3527
292.5609	300.9960	315.5397
322.6311	325.4571	336.5109
353.5522	373.4183	373.9035

393.2729 401.8633 416.3439
426.1591 432.1387 436.7628
438.6157 443.2943 446.9212
464.9102 477.0512 482.3559
490.1335 493.9745 506.1729
519.1102 521.3569 532.4597
535.8738 547.1498 562.4928
564.8736 581.2007 585.0428
588.9938 594.2880 611.1232
629.1998 631.6484 637.8648
639.8970 661.9213 670.4288
671.3006 685.3297 702.8757
725.5919 726.9043 745.6687
750.1233 751.1441 757.3405
770.5548 776.3163 784.6232
787.9037 796.7445 810.1824
824.4363 827.6341 838.8631
844.5939 850.4498 861.3830
868.4542 875.6269 881.4284
893.9044 896.9470 913.1642
915.0712 923.5045 931.1603
954.8453 966.7826 970.0500
978.2663 983.0330 985.6444
988.2248 991.4586 998.8082
1013.5295 1015.5783 1020.6192
1025.3953 1034.3248 1036.6211
1040.0069 1041.4772 1042.9144
1044.6392 1047.3827 1052.0769
1058.0056 1062.5381 1063.9661
1065.5607 1068.8958 1070.5572
1077.9112 1081.7388 1083.1271
1090.5153 1107.1434 1120.3307
1121.2903 1134.9577 1139.7422
1141.4489 1146.6096 1155.2776
1163.7489 1179.1108 1180.1231
1184.9419 1187.0522 1189.1241
1201.2065 1208.2268 1211.4563
1214.2559 1218.9426 1229.5983
1234.9812 1249.4851 1258.3808
1259.9160 1282.5441 1287.1951
1287.7139 1299.3353 1300.7785
1306.2414 1307.6743 1317.0828
1334.7555 1341.0788 1344.0312
1347.0100 1353.1537 1355.5740

1362.2505	1369.1909	1375.1734
1376.1953	1377.1243	1383.2746
1386.3959	1387.7994	1398.5337
1409.6454	1413.5321	1416.7171
1422.3853	1432.3062	1442.6171
1444.4078	1452.5448	1458.4388
1465.2244	1471.4297	1474.9756
1481.9027	1488.9379	1490.1108
1490.7436	1494.1031	1494.5022
1494.5818	1495.6487	1498.2452
1498.9046	1501.7157	1502.1361
1506.0206	1510.1852	1519.9260
1520.6160	1521.9029	1527.3825
1534.5503	1534.7366	1538.1365
1541.6688	1550.6831	1587.8579
1598.2803	1602.8166	1647.0673
1656.4918	1671.9318	1675.1269
1680.9738	1685.6228	1692.1898
1696.8065	1700.3662	1705.1671
1711.4254	1717.5011	2392.2169
3057.1749	3063.4314	3065.1066
3069.3678	3075.9042	3077.4984
3078.0160	3080.4494	3083.5068
3087.0205	3094.3466	3117.0134
3122.7926	3128.0081	3137.3591
3144.8554	3149.0479	3149.8767
3156.9122	3162.1540	3163.9078
3165.0626	3170.9772	3176.0475
3176.4587	3181.0523	3192.4817
3192.9424	3193.8830	3196.8329
3199.4009	3200.0951	3202.6928
3203.0193	3207.2674	3212.2270
3219.6626	3223.4221	3229.0223
3229.2549	3230.3135	3236.8501
3262.3294	3264.9973	3266.2529

TS7S

Zero-point correction= 0.844271

Thermal correction to Energy= 0.895748

Thermal correction to Enthalpy= 0.896692

Thermal correction to Gibbs Free Energy= 0.756940

Sum of electronic and zero-point Energies= -2407.649968

Sum of electronic and thermal Energies= -2407.598492

Sum of electronic and thermal Enthalpies= -2407.597547

Sum of electronic and thermal Free Energies= -2407.737300

Cartesian coordinates

C	-1.865866	0.533228	1.676326
C	-1.317470	-0.871187	1.582560
C	0.035133	-1.157691	0.865199
O	-2.447083	0.921554	2.660096
C	0.077017	-2.626683	0.405571
C	0.666542	-2.993004	-0.805448
C	-0.417903	-3.625074	1.249165
C	0.752508	-4.334754	-1.170759
H	1.058805	-2.233291	-1.474918
C	-0.324884	-4.965694	0.885582
H	-0.863130	-3.370091	2.206273
C	0.257288	-5.325749	-0.327462
H	1.208828	-4.601979	-2.118515
H	-0.713691	-5.727419	1.553277
H	0.323576	-6.370443	-0.612601
C	0.118812	-0.310999	-0.341135
N	0.174824	0.284382	-1.330838
H	-1.242055	-1.206859	2.619868
C	-2.162881	1.394611	0.422716
C	-3.535628	2.226033	-1.065249
C	-4.272185	0.053699	-0.089951
H	-4.314493	-0.173798	0.981474
N	-2.591434	3.108659	-0.933459
N	-1.738466	2.585349	-0.006585
N	-3.303812	1.148435	-0.255815
C	-4.817411	2.352623	-1.836384
H	-4.610127	2.639451	-2.868162
H	-5.420465	3.140401	-1.364314
C	-5.660444	0.527384	-0.581241
O	-5.502875	1.124673	-1.860066
C	-5.309961	-1.716177	-1.258008
C	-4.056802	-1.198661	-0.919235
C	-2.888894	-1.835854	-1.310897
C	-2.984156	-3.043757	-2.003677
C	-4.231974	-3.583503	-2.309098
C	-5.404707	-2.915366	-1.950259
C	-6.411741	-0.786684	-0.799942
H	-1.913314	-1.400841	-1.126180
H	-4.293614	-4.521956	-2.850221
H	-6.374799	-3.320224	-2.221759
H	-6.861268	-1.124311	0.140158
H	-7.207569	-0.656789	-1.536153

C	-0.566723	3.373306	0.322383
C	-0.475950	3.957700	1.589872
C	0.384789	3.584454	-0.681975
C	0.670997	4.694475	1.873419
C	1.522635	4.314335	-0.331149
C	1.692474	4.861878	0.939086
H	0.766556	5.147814	2.857052
H	2.284414	4.477290	-1.090545
C	0.218095	3.164254	-2.120078
H	-0.044108	4.042880	-2.717897
H	-0.548322	2.408716	-2.264590
H	1.158881	2.760281	-2.501738
C	2.918837	5.668966	1.275680
H	2.740879	6.732857	1.089358
H	3.772312	5.363559	0.666585
H	3.185799	5.558943	2.329136
C	-1.536097	3.806777	2.644527
H	-1.301022	2.955493	3.287689
H	-2.528321	3.639241	2.219882
H	-1.572916	4.707486	3.260325
H	-6.140846	1.221676	0.118396
H	-2.075718	-3.555661	-2.305756
C	2.095497	0.820531	3.536712
C	1.133695	0.464080	2.430047
H	1.710921	0.415386	4.476878
H	3.083177	0.383908	3.368029
H	2.166197	1.906077	3.610178
C	1.247225	-0.824697	1.772779
C	1.716900	-1.960732	2.626926
H	2.314704	-0.620303	0.874102
O	2.509143	-2.800181	1.941471
O	0.313354	1.306018	2.040095
O	1.439810	-2.133099	3.795815
C	2.861134	-4.023705	2.610571
C	3.619624	-4.871247	1.615247
H	3.457319	-3.783050	3.495003
H	1.938374	-4.510420	2.942644
H	3.899709	-5.822415	2.073270
H	2.994440	-5.074350	0.741485
H	4.531904	-4.363789	1.290892
C	3.908257	-1.358842	-0.637045
C	4.770747	-1.102852	-1.677120
C	4.914899	0.225904	-2.159172
C	4.134157	1.224706	-1.517221

C	3.295787	0.868487	-0.488140
H	3.764762	-2.361086	-0.243303
H	5.326086	-1.923400	-2.110076
H	4.176044	2.261082	-1.824091
H	2.667557	1.606907	0.007311
C	5.871307	1.899005	-3.638278
C	6.509872	-0.531691	-3.828656
H	6.208525	2.555471	-2.829634
H	6.607154	1.938099	-4.438648
H	4.918731	2.276650	-4.024859
H	7.202427	-1.009628	-3.127773
H	5.846927	-1.296421	-4.246071
H	7.087502	-0.098387	-4.642421
N	5.746468	0.523744	-3.177933
N	3.185928	-0.394347	-0.046014
H	-2.105385	-1.469031	1.105472

Vibrational frequencies

-1084.5142	11.5965	20.5407
23.6749	31.6097	35.3465
38.7930	39.5854	43.1842
48.1036	52.3593	62.0571
66.6512	68.8777	72.7768
76.5908	80.6668	81.5140
88.7798	94.3281	97.0378
104.7450	107.5100	111.6572
116.2279	123.3284	127.2846
130.5841	138.4139	141.3683
148.2554	155.7099	166.3096
178.4969	183.0520	185.1175
189.0428	203.8590	208.4139
214.7469	218.3749	229.1070
238.3973	239.5693	249.8244
260.7740	265.2653	273.1840
274.8222	286.3557	288.2431
292.4517	295.6551	302.8817
315.8268	327.2271	338.9549
349.4910	357.9586	373.8169
385.7612	398.9269	408.8965
416.6875	417.7026	424.7646
434.8725	442.9375	450.6913
463.3004	477.2794	484.0990
489.2570	499.6271	503.4669
515.9042	523.6868	529.3352
532.3274	541.9030	552.7244

565.6223 577.4681 580.5541
581.6567 585.7073 588.1010
615.1562 627.9372 631.0633
640.8309 652.3410 669.0239
676.6919 684.3824 706.4498
720.4338 726.8667 742.7868
744.5011 748.9352 752.0249
770.1442 770.3164 787.3673
789.2220 798.4223 810.0119
813.1637 838.5183 838.9487
844.9305 849.7614 871.1768
874.6868 875.9685 879.6011
893.8873 900.2580 910.6647
922.2732 927.0879 942.8709
948.2314 963.3061 968.4748
971.2933 979.1856 984.3732
986.1285 993.0449 1006.1642
1012.1213 1016.6998 1017.1266
1019.6303 1024.0430 1029.6682
1033.0172 1042.7333 1043.4844
1047.2870 1052.4106 1057.5139
1060.4231 1061.2953 1061.8385
1063.4302 1067.8430 1067.9896
1075.7052 1078.8567 1092.1783
1093.2657 1113.4159 1114.8050
1118.4202 1124.6465 1141.6414
1146.9782 1149.7101 1154.2662
1158.2107 1164.6003 1179.0804
1179.3996 1182.4279 1184.0828
1185.8895 1196.4304 1208.1117
1214.1419 1218.6954 1219.5511
1234.0246 1235.7254 1247.7468
1253.8073 1263.9384 1281.6587
1286.7018 1287.5473 1290.8244
1303.1589 1307.1973 1309.0427
1317.1232 1326.2660 1335.8712
1340.3221 1342.2527 1346.7111
1356.3793 1359.0957 1366.7787
1371.6014 1376.7966 1381.1311
1383.0558 1386.6318 1396.4526
1403.3558 1410.0959 1415.4837
1421.5183 1434.3009 1436.0106
1444.5098 1445.0766 1453.8316
1457.2360 1466.4404 1466.8904

1467.6927	1475.9918	1477.4680
1483.3602	1490.4816	1490.5034
1491.9345	1492.6014	1494.8452
1498.0518	1499.9839	1500.2155
1501.1383	1502.7521	1503.2124
1505.4967	1507.0858	1517.4304
1518.5419	1522.0939	1525.4596
1532.6371	1539.0542	1539.5787
1550.4516	1571.6380	1589.0966
1608.5441	1659.6747	1670.8486
1676.6861	1682.9304	1688.2542
1694.8897	1695.1320	1706.6369
1712.0120	1730.1662	1823.4737
1837.9856	2413.4322	3061.2537
3067.6563	3072.3982	3072.5669
3073.3711	3078.8478	3085.7712
3089.4685	3092.1173	3095.0859
3100.0293	3106.7317	3112.7509
3129.2239	3132.1246	3143.9746
3145.1406	3152.1942	3157.3210
3162.8052	3163.6367	3166.3371
3167.7352	3168.1094	3174.5793
3177.0595	3179.0157	3191.3084
3193.8136	3196.1462	3201.8363
3203.8163	3204.2338	3205.5614
3205.9872	3209.6314	3211.6176
3220.0913	3224.1660	3226.3457
3230.9867	3235.1490	3239.9577
3257.8099	3263.3450	3269.5370

M7R

Zero-point correction= 0.671505

Thermal correction to Energy= 0.712243

Thermal correction to Enthalpy= 0.713187

Thermal correction to Gibbs Free Energy= 0.598387

Sum of electronic and zero-point Energies= -2025.280701

Sum of electronic and thermal Energies= -2025.239963

Sum of electronic and thermal Enthalpies= -2025.239019

Sum of electronic and thermal Free Energies= -2025.353819

Cartesian coordinates

C	0.473482	0.331148	-1.622545
C	-1.037121	0.195045	-1.435498
C	-1.539450	-0.818816	-0.386207
O	0.874299	0.815271	-2.731558

C	-3.069718	-0.791269	-0.466634
C	-3.799228	0.086866	0.333412
C	-3.738153	-1.575773	-1.408202
C	-5.186337	0.157427	0.215893
H	-3.285614	0.718468	1.055408
C	-5.122986	-1.506141	-1.523173
H	-3.175081	-2.252636	-2.046470
C	-5.853154	-0.642136	-0.707608
H	-5.744624	0.835719	0.853488
H	-5.632220	-2.129341	-2.251270
H	-6.933519	-0.591935	-0.795118
C	-1.107272	-0.471840	0.985305
N	-0.734965	-0.316972	2.070470
H	-1.398264	-0.159607	-2.405223
C	1.226485	1.198190	-0.522234
C	2.971757	2.312188	0.217176
C	3.509593	0.096558	-0.770009
H	3.197788	-0.253042	-1.757178
N	1.958220	3.082462	0.470528
N	0.877459	2.377279	0.011611
N	2.568761	1.146018	-0.371848
C	4.429104	2.617582	0.397763
H	4.595440	3.091114	1.366052
H	4.737714	3.314889	-0.394265
C	4.948303	0.656011	-0.810541
O	5.187347	1.433412	0.356323
C	4.966318	-1.476036	0.228210
C	3.639475	-1.041500	0.221154
C	2.685534	-1.619048	1.047210
C	3.073898	-2.682629	1.863434
C	4.388783	-3.148162	1.844706
C	5.348451	-2.542037	1.031967
C	5.807905	-0.604613	-0.678825
H	1.663667	-1.249112	1.073161
H	4.673501	-3.977796	2.483804
H	6.378721	-2.884831	1.044806
H	5.950997	-1.064647	-1.662752
H	6.790133	-0.362122	-0.267029
C	-0.432332	2.934220	0.244727
C	-1.121046	3.529347	-0.820423
C	-0.919078	2.922163	1.554279
C	-2.409334	3.990270	-0.564211
C	-2.215587	3.402223	1.756006
C	-2.983081	3.907281	0.708230

H	-2.975965	4.436338	-1.377721
H	-2.626871	3.384293	2.762177
C	-0.064916	2.512188	2.723970
H	0.521884	3.373050	3.060879
H	0.626262	1.707455	2.473483
H	-0.689536	2.171847	3.551087
C	-4.399793	4.365559	0.932545
H	-4.588033	5.320122	0.434443
H	-4.617091	4.480034	1.996241
H	-5.104546	3.636859	0.519306
C	-0.483460	3.694069	-2.174042
H	-0.144186	2.741295	-2.592986
H	0.397143	4.340677	-2.092536
H	-1.185860	4.161002	-2.866298
H	5.147677	1.248909	-1.711929
H	2.345722	-3.145843	2.521189
C	-0.889377	-2.163164	-0.683957
C	0.375212	-2.174129	-1.181407
C	-1.562088	-3.405897	-0.277642
C	1.182364	-3.402015	-1.487907
O	1.076868	-1.066847	-1.424607
O	-2.385430	-3.176047	0.758438
O	-1.432461	-4.503096	-0.785848
H	0.884350	-4.249188	-0.874167
H	1.034524	-3.675665	-2.537063
H	2.237838	-3.169510	-1.335979
C	-3.347620	-4.194462	1.064595
C	-4.434906	-3.532317	1.882557
H	-3.733984	-4.603288	0.126425
H	-2.851151	-5.003947	1.608086
H	-4.895865	-2.723926	1.306963
H	-5.203447	-4.263186	2.144865
H	-4.023080	-3.113789	2.803897
H	-1.489511	1.170192	-1.257535

Vibrational frequencies

20.1408	24.9552	28.5537
34.2794	38.8349	47.1484
58.8150	63.2744	65.4873
74.2206	76.3950	80.6264
90.2434	98.3863	106.6250
111.8203	115.7631	123.5991
127.1803	134.7234	141.1051
153.3599	163.5865	175.5017
180.3382	189.8530	198.8537

206.8375 215.7864 223.2103
238.4465 247.9767 253.0181
263.1573 270.2652 273.8424
279.6501 287.6787 293.1533
298.9774 321.2012 327.8966
333.2095 338.1017 341.5855
383.7453 389.9767 390.7273
414.6825 418.2998 420.7202
445.1596 453.2341 456.2619
469.2348 483.4696 494.5266
499.7702 505.7251 510.7073
531.0630 532.7740 540.5653
556.6391 579.7627 584.1321
587.7144 591.5982 604.6232
624.2029 629.1141 636.3903
645.4337 659.5152 679.4874
698.6223 702.7347 718.8964
729.4622 730.9057 752.3199
756.3226 765.7649 775.9530
782.6402 792.7993 805.3852
812.7121 840.5084 842.0295
871.7836 872.7141 874.9969
877.9976 880.8180 900.1013
910.3489 911.2867 924.2589
941.3034 946.9104 965.6537
968.8723 982.2316 991.5586
1001.5838 1010.2453 1017.2047
1019.5103 1021.0746 1024.6110
1030.0290 1037.9972 1042.8403
1048.5386 1050.4396 1055.3171
1058.8401 1063.5713 1066.2944
1068.4749 1071.3289 1072.0366
1078.7330 1080.7430 1111.5190
1115.9356 1117.4428 1125.0267
1135.6509 1148.6137 1167.4824
1175.7811 1178.0638 1184.0227
1188.2692 1190.0983 1203.0053
1205.8114 1206.3184 1217.9304
1236.3298 1254.5933 1256.9969
1259.7628 1282.3364 1285.5163
1288.5638 1307.9068 1309.4845
1312.5747 1321.0691 1334.9770
1338.4744 1341.6725 1343.8031
1356.6951 1359.3890 1360.6848

1365.8444	1370.8820	1379.1155
1386.2779	1406.3256	1412.4067
1417.4714	1420.5295	1426.7305
1442.6208	1444.3541	1451.7627
1459.5909	1465.0609	1473.1947
1476.8693	1477.5645	1480.5735
1483.3364	1488.0789	1492.3646
1493.5894	1493.9973	1497.6532
1500.6712	1503.4477	1506.9842
1519.1786	1521.1424	1524.4556
1526.4678	1532.4317	1537.9867
1547.1045	1561.7421	1676.8705
1681.2981	1684.1692	1685.2615
1686.6930	1694.4444	1696.3325
1706.8386	1820.8721	2398.8401
3061.8888	3062.8571	3072.0419
3073.3551	3079.6936	3083.0804
3092.2722	3097.8524	3102.8091
3122.0569	3132.6367	3140.3897
3143.6190	3145.1345	3152.8440
3158.3420	3159.3426	3160.1479
3166.3840	3167.8049	3171.5329
3178.2752	3182.8919	3185.1659
3191.0733	3193.3475	3198.2366
3201.0088	3205.1622	3208.9670
3211.0700	3214.2356	3214.8136
3219.7190	3230.6292	3230.6659

M7S

Zero-point correction= 0.671945

Thermal correction to Energy= 0.712428

Thermal correction to Enthalpy= 0.713372

Thermal correction to Gibbs Free Energy= 0.597700

Sum of electronic and zero-point Energies= -2025.285709

Sum of electronic and thermal Energies= -2025.245225

Sum of electronic and thermal Enthalpies= -2025.244281

Sum of electronic and thermal Free Energies= -2025.359953

Cartesian coordinates

C	-0.238995	-0.625457	-1.676299
C	-0.505835	0.873744	-1.504442
C	0.365542	1.588556	-0.442808
O	-0.900257	-1.221962	-2.596311
C	0.178196	3.103015	-0.632489
C	-0.660620	3.853498	0.189600

C	0.823336	3.728256	-1.702083
C	-0.849148	5.213626	-0.051990
H	-1.155183	3.387457	1.037185
C	0.637168	5.085831	-1.940226
H	1.480930	3.148932	-2.344903
C	-0.200778	5.834243	-1.115226
H	-1.501169	5.787421	0.598796
H	1.148927	5.559983	-2.771453
H	-0.345118	6.893589	-1.300122
C	-0.083925	1.204685	0.914892
N	-0.462904	0.872663	1.957266
H	-0.280860	1.315950	-2.479249
C	-0.476382	-1.407630	-0.321205
C	-1.616863	-2.570257	1.146213
C	-3.024449	-1.394267	-0.528414
H	-2.789140	-1.314608	-1.595857
N	-0.373007	-2.861431	1.381133
N	0.327320	-2.123501	0.464302
N	-1.730985	-1.668314	0.123416
C	-2.813476	-3.257546	1.736384
H	-2.869148	-3.069693	2.810491
H	-2.683236	-4.336396	1.576521
C	-3.966514	-2.583449	-0.242517
O	-4.011896	-2.794781	1.164105
C	-5.219734	-0.588445	-0.195011
C	-3.874643	-0.223047	-0.058171
C	-3.535274	1.040936	0.400868
C	-4.553952	1.950288	0.695296
C	-5.890136	1.596770	0.530617
C	-6.231269	0.316734	0.089100
C	-5.337911	-2.032975	-0.625982
H	-2.504000	1.320675	0.568003
H	-6.671366	2.313255	0.762928
H	-7.272993	0.027370	-0.012785
H	-5.489478	-2.122109	-1.707370
H	-6.136432	-2.576659	-0.116873
C	1.741703	-2.406746	0.359388
C	2.127029	-3.325143	-0.625132
C	2.623306	-1.875793	1.300961
C	3.473070	-3.674237	-0.678710
C	3.961699	-2.267386	1.205532
C	4.404646	-3.149162	0.221976
H	3.802161	-4.381050	-1.436406
H	4.671611	-1.870403	1.926987

C	2.185898	-0.928952	2.385603
H	1.162266	-1.122587	2.710371
H	2.222236	0.109974	2.041214
H	2.850749	-1.018482	3.246934
C	5.862037	-3.512220	0.112584
H	6.368338	-3.412601	1.075014
H	6.365716	-2.848849	-0.598610
H	5.989476	-4.536450	-0.245097
C	1.115471	-3.923533	-1.565900
H	0.619683	-3.153095	-2.166920
H	0.338957	-4.456941	-1.005880
H	1.597535	-4.635792	-2.237189
H	-3.668762	-3.498194	-0.769961
H	-4.294990	2.938799	1.060927
C	3.531612	-0.327330	-1.778430
C	2.133779	0.076047	-1.407748
H	4.025719	0.475688	-2.327383
H	4.126290	-0.514640	-0.881995
H	3.481912	-1.230194	-2.386261
C	1.812043	1.146819	-0.628045
C	2.869847	1.894918	0.066655
O	2.345348	2.627402	1.067596
O	1.236793	-0.750089	-1.943191
O	4.063016	1.870732	-0.165526
C	3.247852	3.477923	1.787335
C	2.396706	4.372276	2.661633
H	3.929554	2.853604	2.373343
H	3.844079	4.047913	1.069611
H	3.033136	5.029818	3.257918
H	1.735331	4.985228	2.044015
H	1.782707	3.771992	3.337388
H	-1.568657	1.037220	-1.312368

Vibrational frequencies

5.0212	23.3250	32.1124
33.6485	39.1113	41.9015
46.8764	53.2828	53.7490
66.4326	77.1269	90.0878
93.9585	99.0437	107.9912
112.0713	123.0147	137.2878
145.6343	156.2580	158.9669
167.1770	170.7520	174.9483
181.8187	202.1552	206.5222
210.2702	231.2168	232.9280
241.0702	251.0163	252.7117

258.8345	274.2375	279.0675
285.4715	289.5304	294.3971
303.7785	320.4016	330.4088
334.6511	339.8118	343.9785
378.6248	387.4113	396.7244
410.1947	416.7410	430.7372
438.6368	446.2122	466.7370
474.4328	485.5736	493.4686
503.5466	509.6964	515.3180
531.4782	535.4901	552.0714
559.6324	568.8729	581.0603
589.1792	608.7045	619.6111
628.2913	630.6751	641.0947
647.6399	665.5221	679.8747
694.8057	709.2118	721.0467
727.8888	743.4697	758.4280
761.1410	771.5545	788.4397
792.1212	795.5797	804.4967
819.6306	838.1142	842.5395
873.2821	876.9591	879.1849
881.4482	888.7950	898.5640
917.3800	922.7204	923.2273
936.3132	950.3970	956.7894
968.6205	979.8975	981.3022
1006.9531	1007.2254	1013.2362
1016.9531	1019.1912	1029.2963
1033.1296	1040.5815	1044.2654
1045.3284	1049.5774	1053.8794
1056.1853	1062.5814	1064.6807
1067.9775	1071.8106	1072.0301
1074.0415	1074.5782	1098.8961
1108.6734	1112.0115	1130.0501
1132.7477	1152.3213	1162.0418
1175.4734	1180.1733	1181.5355
1187.5114	1194.8798	1197.7567
1200.8767	1213.9489	1215.3340
1233.6997	1236.2206	1254.2580
1268.4147	1277.6204	1279.6943
1286.9608	1303.7715	1307.7226
1314.6167	1318.6562	1322.0663
1336.4876	1337.6957	1339.8616
1345.6678	1359.6049	1363.9507
1367.0583	1370.1738	1376.9108
1381.8439	1406.5877	1407.7676

1415.7365	1418.2968	1421.2924
1431.0458	1443.5239	1449.2383
1454.3672	1464.6690	1474.7851
1476.3094	1477.3903	1479.9510
1484.6345	1492.4803	1493.1684
1494.3149	1495.6219	1496.6294
1503.7416	1504.5191	1505.9353
1509.4318	1517.5227	1520.4934
1532.0945	1532.9364	1538.2525
1549.7012	1571.8534	1663.2756
1674.4167	1679.1011	1682.6513
1687.6506	1694.3417	1695.4727
1710.4994	1821.2375	2400.0543
3061.2086	3067.5872	3069.9856
3082.3643	3083.4945	3088.7430
3093.5834	3099.5838	3099.9378
3109.1225	3117.9160	3131.6322
3139.2765	3142.5565	3152.1237
3154.1239	3162.3741	3167.8820
3168.0751	3169.3141	3172.6708
3175.1452	3177.6678	3178.0880
3196.4961	3199.5786	3204.5228
3206.4467	3207.8600	3209.8405
3213.6468	3216.6919	3222.1651
3227.6474	3236.6411	3269.2549

TS8R

Zero-point correction= 0.670220

Thermal correction to Energy= 0.710727

Thermal correction to Enthalpy= 0.711671

Thermal correction to Gibbs Free Energy= 0.596917

Sum of electronic and zero-point Energies= -2025.275378

Sum of electronic and thermal Energies= -2025.234871

Sum of electronic and thermal Enthalpies= -2025.233927

Sum of electronic and thermal Free Energies= -2025.348681

Cartesian coordinates

C	0.423203	0.136039	-1.919496
C	-1.059502	0.158276	-1.617104
C	-1.556795	-0.777716	-0.498364
O	0.901131	0.735713	-2.879904
C	-3.089980	-0.773701	-0.595340
C	-3.831428	0.183332	0.096120
C	-3.744941	-1.669442	-1.442188
C	-5.218598	0.223848	-0.034214

H	-3.328506	0.897829	0.745289
C	-5.130150	-1.629959	-1.568028
H	-3.173041	-2.409533	-1.997127
C	-5.872598	-0.685812	-0.860073
H	-5.786989	0.965721	0.517601
H	-5.629210	-2.339860	-2.219728
H	-6.953056	-0.658548	-0.955527
C	-1.172411	-0.336611	0.860641
N	-0.896395	-0.117314	1.962629
H	-1.540990	-0.184153	-2.540340
C	1.264581	1.166505	-0.422971
C	3.095696	2.325125	0.090866
C	3.491130	0.017833	-0.742225
H	3.175108	-0.338702	-1.726660
N	2.118198	3.136832	0.355304
N	1.000203	2.404881	0.026760
N	2.621699	1.130831	-0.380164
C	4.571343	2.563111	0.201856
H	4.793200	3.146622	1.095995
H	4.917103	3.121879	-0.679739
C	4.970808	0.462509	-0.783287
O	5.244211	1.327622	0.310815
C	4.799029	-1.627851	0.349825
C	3.507784	-1.105275	0.268869
C	2.470746	-1.607263	1.042467
C	2.737356	-2.687764	1.884749
C	4.018305	-3.237746	1.945714
C	5.061654	-2.706696	1.184783
C	5.739727	-0.840820	-0.536174
H	1.478618	-1.162526	1.006609
H	4.210811	-4.076543	2.607102
H	6.063083	-3.120017	1.259828
H	5.916605	-1.355497	-1.487078
H	6.708962	-0.635465	-0.075768
C	-0.290255	2.976975	0.294185
C	-1.019506	3.540249	-0.760289
C	-0.741585	2.989086	1.615829
C	-2.299892	4.008939	-0.475239
C	-2.029673	3.474863	1.851114
C	-2.829475	3.960887	0.817669
H	-2.894200	4.434767	-1.280145
H	-2.411362	3.474020	2.869085
C	0.148088	2.565315	2.753097
H	0.801100	3.396364	3.039314

H	0.777805	1.716965	2.480414
H	-0.449354	2.278289	3.619598
C	-4.236250	4.432524	1.078741
H	-4.426661	5.391697	0.589979
H	-4.425953	4.545253	2.147938
H	-4.960714	3.714779	0.680475
C	-0.421549	3.681146	-2.135821
H	-0.077511	2.727290	-2.546058
H	0.450422	4.342669	-2.094811
H	-1.149113	4.118387	-2.821828
H	5.230205	0.959600	-1.726850
H	1.943002	-3.097376	2.500414
C	-0.901534	-2.141402	-0.682862
C	0.324682	-2.228828	-1.247379
C	-1.566360	-3.336262	-0.120725
C	1.132954	-3.475533	-1.437031
O	1.008235	-1.163540	-1.716998
O	-2.359299	-2.990926	0.901593
O	-1.458411	-4.477356	-0.521981
H	0.835316	-4.260295	-0.746380
H	0.993281	-3.843648	-2.458012
H	2.187421	-3.226053	-1.300235
C	-3.328748	-3.956872	1.336071
C	-4.401488	-3.188606	2.077248
H	-3.726968	-4.470633	0.456174
H	-2.832381	-4.698129	1.969349
H	-4.869174	-2.460442	1.407735
H	-5.166749	-3.875736	2.445484
H	-3.972277	-2.654782	2.928451
H	-1.386885	1.182675	-1.436644

Vibrational frequencies

-213.8255	19.6030	23.7871
29.2027	37.2738	40.9749
47.9697	54.1179	59.9593
66.7725	72.2646	73.8483
78.9086	80.3748	92.6319
96.3070	101.0084	105.2717
126.1833	126.9873	131.3738
143.2544	144.4525	159.6986
174.3031	184.8774	199.8097
202.4498	212.4666	217.7377
228.3632	237.7100	248.4329
256.9133	262.8741	279.9690
284.6882	287.2246	291.3827

300.8123	312.2047	321.8691
322.0638	331.8628	336.2846
365.8959	381.8159	387.2410
409.3716	412.5307	418.2382
426.0053	439.3849	462.7867
476.0937	478.5139	488.4327
494.7899	505.6488	506.2346
520.1482	537.7116	541.5233
546.9757	558.1768	584.2447
587.0190	591.1958	604.9256
618.7584	628.4732	630.9924
632.2288	648.2062	674.2044
698.7999	703.9719	723.1793
726.2798	739.6233	754.3525
758.5129	764.4026	779.8831
786.7747	795.8748	803.0835
813.6184	838.7349	840.5763
866.5019	877.5927	877.6308
879.8214	882.5223	897.7874
909.9043	911.1667	919.0927
925.6488	953.0488	961.5944
968.3489	980.9848	986.4904
1005.4025	1009.2086	1012.2914
1017.1171	1023.6341	1025.3759
1025.8173	1041.5766	1047.6218
1050.0543	1053.1635	1058.2455
1061.7512	1062.2624	1064.7564
1065.9321	1068.8261	1073.9777
1074.1360	1083.0943	1096.3677
1113.5306	1117.2210	1127.7594
1138.6095	1147.4084	1155.0108
1171.9324	1174.3750	1176.9761
1184.7552	1187.7225	1199.2741
1203.3233	1213.1041	1216.9141
1234.5626	1249.6335	1253.2566
1260.4990	1277.4949	1280.7245
1286.5496	1301.3800	1302.7859
1309.1187	1310.0935	1332.8585
1335.7652	1338.4011	1342.4373
1351.2713	1355.5869	1358.4310
1362.4715	1364.9765	1378.2403
1387.8326	1405.5132	1412.6858
1418.3909	1419.3178	1421.2676
1426.5491	1439.1902	1440.0268

1458.1721	1461.4793	1466.0657
1473.4995	1474.1282	1476.3078
1488.7135	1491.3776	1493.3282
1493.9235	1497.6450	1498.1455
1499.6850	1500.3151	1503.5031
1509.2362	1516.3664	1522.6785
1528.8337	1533.7360	1549.3729
1562.9882	1677.9180	1682.0825
1682.5580	1688.0434	1695.3283
1698.3780	1700.3355	1705.0082
1714.4730	1825.7755	2413.4130
3061.6215	3071.1858	3073.6420
3075.5953	3077.6418	3080.3766
3082.0468	3090.7891	3093.5535
3094.1611	3139.5552	3142.2219
3142.9700	3144.3145	3151.2595
3154.2140	3158.2792	3165.8915
3166.0222	3168.2414	3172.3889
3174.9744	3181.9568	3183.9878
3189.4935	3190.3192	3192.2240
3193.7657	3194.6818	3204.5655
3208.2242	3212.7730	3213.1276
3214.5451	3223.9561	3229.4454

TS8S

Zero-point correction= 0.670723

Thermal correction to Energy= 0.710988

Thermal correction to Enthalpy= 0.711932

Thermal correction to Gibbs Free Energy= 0.598234

Sum of electronic and zero-point Energies= -2025.277035

Sum of electronic and thermal Energies= -2025.236771

Sum of electronic and thermal Enthalpies= -2025.235826

Sum of electronic and thermal Free Energies= -2025.349524

Cartesian coordinates

C	0.324143	-0.262680	2.004965
C	0.334433	1.187425	1.580140
C	-0.692786	1.594499	0.496769
O	1.163187	-0.733524	2.758183
C	-0.926681	3.111708	0.646967
C	-0.254949	4.040689	-0.144990
C	-1.781062	3.565076	1.654684
C	-0.445072	5.406533	0.059615
H	0.409050	3.706118	-0.936542
C	-1.971517	4.928050	1.856248

H	-2.304474	2.847158	2.280734
C	-1.305012	5.854845	1.057119
H	0.081135	6.118617	-0.567899
H	-2.643772	5.265424	2.638489
H	-1.455537	6.918068	1.212443
C	-0.171137	1.331562	-0.862996
N	0.226947	1.170206	-1.937488
H	0.084765	1.746411	2.489489
C	0.781110	-1.204351	0.159127
C	2.196978	-2.463809	-1.016457
C	3.277706	-0.834320	0.509297
H	2.994666	-0.682525	1.556582
N	1.026941	-2.948818	-1.294118
N	0.171564	-2.151737	-0.562920
N	2.097628	-1.401525	-0.152305
C	3.523061	-3.043694	-1.411324
H	3.606972	-3.107329	-2.497769
H	3.587674	-4.059789	-0.996990
C	4.446048	-1.839764	0.407474
O	4.584215	-2.241537	-0.949844
C	5.296680	0.349091	0.143246
C	3.913074	0.426386	-0.051773
C	3.342003	1.552015	-0.625320
C	4.170970	2.616386	-0.988805
C	5.545814	2.549698	-0.776353
C	6.119344	1.408573	-0.211287
C	5.674496	-0.991425	0.731627
H	2.279238	1.598292	-0.824700
H	6.177197	3.383641	-1.065611
H	7.193777	1.345135	-0.066070
H	5.812061	-0.928480	1.816937
H	6.576914	-1.424788	0.294563
C	-1.184535	-2.618019	-0.437520
C	-1.432266	-3.542239	0.587031
C	-2.151292	-2.254869	-1.375203
C	-2.705637	-4.100941	0.661399
C	-3.415725	-2.838074	-1.253220
C	-3.709344	-3.758604	-0.247527
H	-2.917502	-4.824266	1.445201
H	-4.184630	-2.571247	-1.974627
C	-1.861840	-1.282211	-2.485979
H	-0.814030	-1.316931	-2.790697
H	-2.067108	-0.253547	-2.170811
H	-2.490228	-1.500893	-3.351957

C	-5.091431	-4.344243	-0.120050
H	-5.583910	-4.414286	-1.092464
H	-5.715286	-3.713603	0.522401
H	-5.058448	-5.340585	0.326584
C	-0.343743	-3.929519	1.553025
H	-0.018357	-3.067704	2.145595
H	0.530699	-4.313012	1.016583
H	-0.696445	-4.705728	2.234304
H	4.308975	-2.713833	1.057347
H	3.736564	3.498992	-1.447395
C	-3.292658	-1.007707	1.906295
C	-2.047641	-0.260779	1.538874
H	-4.015831	-0.333155	2.367329
H	-3.764362	-1.422598	1.013718
H	-3.028063	-1.810763	2.593464
C	-1.975036	0.794785	0.690934
C	-3.172765	1.183834	-0.081448
O	-2.838294	2.010321	-1.085019
O	-0.980913	-0.774536	2.185276
O	-4.313988	0.813065	0.106760
C	-3.907341	2.485914	-1.915394
C	-3.290767	3.462916	-2.891514
H	-4.368469	1.630355	-2.418330
H	-4.664573	2.954185	-1.280331
H	-4.054905	3.849729	-3.569046
H	-2.838848	4.300595	-2.354731
H	-2.514354	2.970189	-3.481719
H	1.350495	1.468535	1.294853

Vibrational frequencies

-143.8004	22.0159	30.1384
32.1011	33.2771	40.8848
45.6923	49.6277	53.3620
61.5194	74.9484	79.4211
83.0344	87.0558	91.6965
108.5276	110.4050	116.6763
127.6533	147.7226	151.1471
160.8563	167.9239	173.3721
181.1562	191.2720	197.9217
203.0397	210.9226	222.1264
233.3137	239.3299	245.2971
249.3315	256.1190	258.9879
282.9277	285.7203	287.4713
299.9952	305.6502	319.0076
324.7619	337.1923	346.2574

374.4447 377.7836 391.5288
400.0537 408.8524 413.8552
430.9760 438.4354 461.2249
475.0302 490.8492 495.1933
496.3180 501.8148 505.3714
519.9340 529.8587 542.1717
557.4852 562.7229 581.3472
585.7217 589.6190 609.4942
618.8265 629.6158 635.5937
636.5187 643.8927 676.6018
695.3068 705.2796 718.0149
725.5635 729.8438 748.6332
760.8473 767.5597 784.1427
787.8275 789.4204 811.6744
836.8595 837.8774 839.6775
869.7764 871.0489 878.0547
882.0235 888.4942 904.2182
910.6267 917.2461 922.5839
924.8177 948.4219 959.2594
969.8649 980.0080 985.1778
1000.3067 1005.5317 1010.5091
1020.2945 1021.2734 1023.3221
1026.5249 1043.0593 1044.7249
1047.2617 1050.9017 1054.6936
1059.9433 1063.4420 1065.4828
1067.6217 1069.6055 1075.3367
1076.2009 1078.7000 1091.9469
1109.5073 1115.5963 1128.5577
1149.1616 1157.5374 1167.7646
1178.6402 1178.9480 1183.0988
1185.8084 1190.8872 1194.4915
1204.9451 1209.4545 1213.7068
1231.0326 1231.8448 1252.8274
1271.1822 1280.2788 1282.2077
1286.5965 1294.8248 1296.0429
1311.8665 1320.9090 1335.1599
1335.9022 1337.9773 1340.5390
1352.0876 1354.4010 1356.2208
1361.9445 1365.7252 1380.1055
1383.9093 1403.1222 1406.4834
1410.5820 1411.9760 1419.4991
1423.0705 1433.1687 1441.1783
1460.9914 1463.2984 1467.2758
1470.1104 1473.5984 1474.1773

1479.5410	1491.7585	1494.2573
1494.4372	1495.8629	1499.0346
1501.3912	1503.3774	1504.3548
1509.4030	1519.1695	1521.3706
1530.2459	1534.6508	1549.8235
1562.5748	1681.8131	1683.4799
1683.8326	1686.3761	1695.4168
1697.4576	1698.5677	1708.8442
1757.9782	1824.1917	2406.4111
3059.0069	3066.0856	3072.0202
3080.4890	3080.9058	3084.1151
3091.5380	3092.1383	3092.3199
3099.6192	3121.0718	3137.0669
3139.6638	3144.0226	3147.8841
3152.0856	3162.3190	3162.8791
3166.2951	3167.6134	3168.2472
3172.0135	3176.1184	3178.9862
3184.4189	3194.0754	3194.7459
3194.9541	3202.9150	3204.2869
3209.7191	3212.7406	3217.2093
3229.0009	3229.9398	3264.2814

PR/S

Zero-point correction= 0.285056

Thermal correction to Energy= 0.304530

Thermal correction to Enthalpy= 0.305474

Thermal correction to Gibbs Free Energy= 0.236134

Sum of electronic and zero-point Energies= -973.727965

Sum of electronic and thermal Energies= -973.708491

Sum of electronic and thermal Enthalpies= -973.707547

Sum of electronic and thermal Free Energies= -973.776887

Cartesian coordinates

C	2.344081	2.422445	-0.421645
C	0.938122	1.940073	-0.285334
H	2.433935	3.376251	0.103520
H	3.062440	1.709334	-0.030613
H	2.556867	2.605515	-1.478978
C	0.489797	0.738838	0.118514
C	1.370539	-0.336411	0.649067
O	0.085049	2.980349	-0.581635
O	1.042368	-1.026763	1.588163
O	2.513554	-0.488607	-0.022774
C	3.398391	-1.512349	0.479861
C	4.641707	-1.487511	-0.379374

H	2.876662	-2.471692	0.427544
H	3.615577	-1.300952	1.530022
H	5.339843	-2.253518	-0.035221
H	4.393807	-1.687680	-1.423923
H	5.135833	-0.515266	-0.315309
C	-1.267350	2.814859	-0.699556
C	-1.749042	1.392033	-0.738856
H	-2.825241	1.379536	-0.567630
C	-1.004461	0.468378	0.249182
O	-1.952069	3.788262	-0.824005
C	-1.384346	-0.977731	-0.089067
C	-2.373863	-1.657291	0.616416
C	-0.775806	-1.590500	-1.187319
C	-2.748530	-2.942926	0.229965
H	-2.851476	-1.191105	1.472999
C	-1.148880	-2.874747	-1.568415
H	-0.001113	-1.065954	-1.742213
C	-2.137935	-3.554753	-0.860173
H	-3.518671	-3.465488	0.787526
H	-0.664781	-3.344458	-2.418180
H	-2.428376	-4.557180	-1.156220
C	-1.412150	0.809715	1.629449
N	-1.737657	1.118380	2.694586
H	-1.554569	1.015335	-1.749704

Vibrational frequencies

31.5223	42.4453	49.3732
69.5826	77.7659	86.7019
98.8001	111.2898	128.0694
141.9818	158.2971	175.8365
197.5173	233.2772	253.3452
268.2243	305.0734	311.8437
324.8972	351.0602	396.6302
416.5252	423.6053	457.5512
474.9991	492.8747	539.3632
552.0124	572.0550	612.5217
631.2120	659.1966	686.5512
700.0183	720.5550	778.3904
789.2055	816.7912	839.1064
854.7027	877.1278	903.1416
915.0798	939.2441	952.8227
1005.8817	1014.6088	1029.3638
1029.9904	1061.7082	1065.9082
1073.5816	1081.4162	1116.0903
1130.8601	1140.5430	1155.9963

1184.2787	1188.3342	1188.9761
1218.5529	1243.2855	1249.8714
1278.3594	1300.3595	1307.0890
1345.3097	1352.4275	1369.7757
1374.5111	1417.0210	1428.5333
1449.2398	1456.4174	1482.7320
1485.6810	1494.3953	1504.9417
1510.0389	1532.1636	1554.6513
1683.9226	1700.3820	1751.8350
1839.3839	1925.8364	2421.2756
3084.0372	3090.5054	3096.4636
3106.9115	3154.4877	3157.2058
3170.5038	3177.6437	3180.1147
3198.9187	3211.6485	3217.8001
3229.1183	3237.5151	3248.5935

References

(1) (a) R. G Parr and R. G. Pearson, J. Am. Chem. Soc. 1983, 105, 7512-7516; (b) L. R. Domingo, M. T. Picher and J. A. Sáez. J. Org. Chem. 2009, 74, 2726-2735.

(2) (a) W. Kohn and L. J. Sham. Phys. Rev. 1965, 140, A1133; (b) L. J. Sham and W. Kohn. Phys. Rev. 1966, 145, 561.

(3) (a) L. R. Domingo and E. Chamorro. Eur. J. Org. Chem. 2009, 2009, 3036-3044. (b) L. R. Domingo, E. Chamorro and P. Perez. J. Phys. Chem. A 2008, 112, 4046-4053. (c) L. R. Domingo, P. Pérez and J. A. Sáez. RSC Adv. 2013, 3, 1486-1494. (d) L. R. Domingo and P. Perez. Org. Biomol. Chem. 2011, 9, 7168-7175.