Supporting Information for

Origin of stereoselectivity on isothiourea catalyzed Michael addition reaction of aryl ester with vinyl disulfone

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Part 1: Computational details.

The relevant parameters of GRI, *i.e.*, global electrophilicity index ω, which is calculated from the electronic chemical potential μ and the chemical hardness η with the equation $\omega = (\mu^2/2\eta)$. Both quantities may be approached in terms of the one-electron energies of the frontier molecular orbital HOMO and LUMO, E_H and E_L, respectively, as $\mu \approx (E_H + E_L)/2$ and $\eta \approx (E_L - E_H)$. According to the HOMO energies obtained within the Kohn−Sham scheme[1], Domingo and co-workers provided nucleophilicity index N[2], de fined as $N = E_{HOMO(SR)} - E_{HOMO(TCEN)}$, to handle a nucleophilicity scale.

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

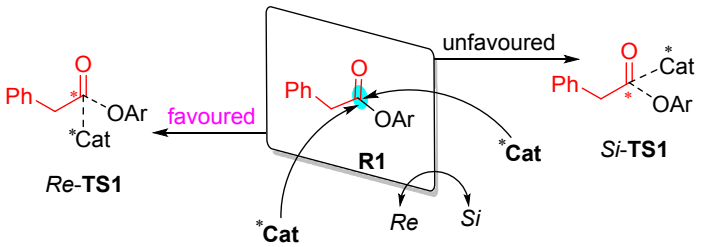


Fig. S1 Different ways for the catalyst to attack the reactant **R1**.

Part 3: Different conformations and configurations of TS3s.

The intermediate **M2** acts as a nucleophile and attacks on reactant **R2**, we considered and studied the different conformations of the key transition state **TS3**. Therefore, based on the transition states **TS3*SS*, TS3*RS*, TS3*RR*, TS3*SR***, each transition state **TS3** is rotated 90° per time based on the dihedral angle *Φ1* (C1–C2–C3–C4), and rotated four times for a total of 360°, so there should be sixteen (4 × 4) possible conformations obtained in theory. Actually, we have only obtained sixteen conformations including **TS3*SS*, TS3*RS*, TS3*RR*, TS3*SR*** & **TS3'*SS*, TS3'*RS*, TS3'*RR*, TS3'*SR*** & **TS3''*SS*, TS3''*RS*, TS3''*RR*, TS3''*SR*** & **TS3'''*RS*, TS3'''*RR*, TS3'''*SR***, which have been summarized in the **Table S1**. As summarized in **Table S1**, we found that all structures of the four transition states **TS3*SS*, TS3*RS*, TS3*RR*, TS3*SR*** should be the conformations with the lowest energies among the conformations. More importantly, the relative energies of **TS3*SR***, **TS3*SR'***, **TS3*SR''***, **TS3*SR'''*** are 16.3, 23.0, 25.5, 19.0 kcal/mol, respectively. This indicates that the transition state **TS3*SR*** is the most stable structure in the searched configurations.

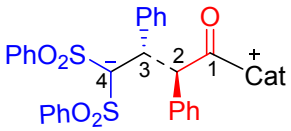


Table S1 The relative Gibbs free energies for different conformations of **TS3*SS*, TS3*RS*, TS3*RR*, TS3*SR*** & **TS3'*SS*, TS3'*RS*, TS3'*RR*, TS3'*SR*** & **TS3''*SS*, TS3''*RS*, TS3''*RR*, TS3''*SR*** & **TS3'''*RS*, TS3'''*RR*, TS3'''*SR*** with the energy of **Cat+R1+R2** as 0.0 kcal/mol (unit: kcal/mol)

SP	Φ1(Optimized)	Energy
TS3(SS)	18.08	19.8
TS3'(SS)	-128.86	21.0
TS3''(SS)	102.98	24.3
TS3'''(SS)	-178.34	21.5
TS3(RS)	48.58	20.3
TS3'(RS)	172.83	28.3
TS3''(RS)	22.00	26.4
TS3'''(RS)	168.28	28.8
TS3(RR)	147.69	24.4
TS3'(RR)	-110.38	27.2
TS3''(RR)	168.46	25.9
TS3'''(RR)	117.57	25.8
TS3(SR)	65.59	16.3
TS3'(SR)	-45.36	23.0
TS3''(SR)	-81.71	25.5
TS3'''(SR)	164.51	19.0

Part 4: NCI analysis and AIM analysis for the structures of TS3*SS*,TS3*RR*, TS3*RS*.

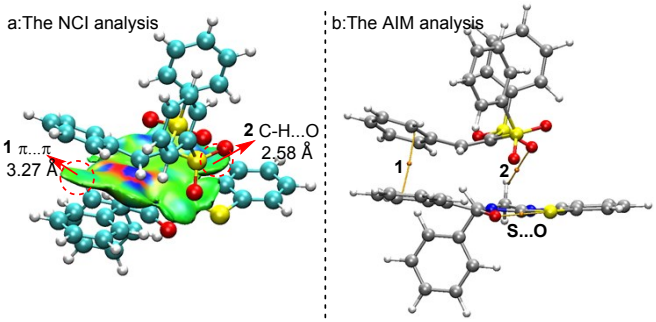


Fig. S2 (a) The NCI analysis (only the intermolecular interactions were shown) and (b) bond critical points (BCPs, color in orange) along the bond paths (color in yellow) for topological analysis of **TS3*SS***.

Table S2 The distance, type of interaction, Laplacian of electron densities (∇^2_ρ) at the bond critical points (BCPs) along the bond paths in **TS3*SS*** (The bond lengths are in Å, ∇^2_ρ is in a.u.).

BCP index (**TS3*SS***)	Type of interaction	Distance	∇^2_ρ*10^{-1}
1	π···π	3.27	0.2182
2	C-H···O	2.58	0.3656
O···S	1,5- O···S	2.74	0.6938

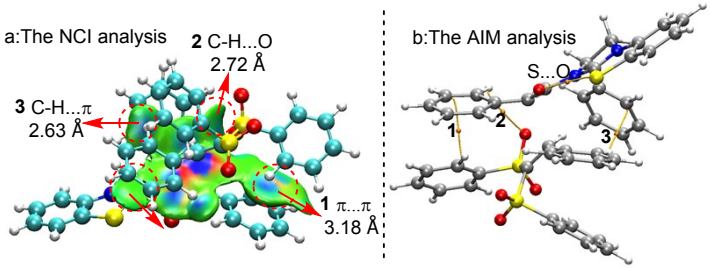


Fig. S3 (a) The NCI analysis (only the intermolecular interactions were shown) and (b) bond critical points (BCPs, color in orange) along the bond paths (color in yellow) for topological analysis of **TS3*RR***.

Table S3 The distance, type of interaction, Laplacian of electron densities (∇^2_ρ) at the bond critical points (BCPs) along the bond paths in **TS3*RR*** (The bond lengths are in Å, ∇^2_ρ is in a.u.).

BCP index (**TS3*RR***)	Type of interaction	Distance	∇^2_ρ*10^{-1}
1	π···π	3.18	0.3079
2	C-H···O	2.72	0.2500
3	C-H···π	2.63	0.2907
O···S	1,5- O···S	2.79	0.6788

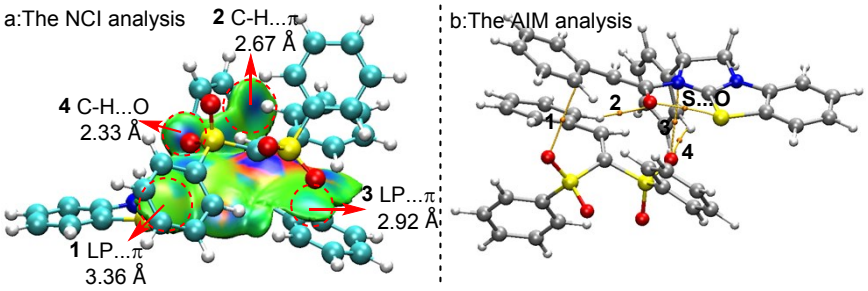


Fig. S4 (a) The NCI analysis (only the intermolecular interactions were shown) and (b) bond critical points (BCPs, color in orange) along the bond paths (color in yellow) for topological analysis of **TS3*RS***.

Table S4 The distance, type of interaction, Laplacian of electron densities (∇^2_ρ) at the bond critical points (BCPs) along the bond paths in **TS3R*S*** (The bond lengths are in Å, ∇^2_ρ is in a.u.).

BCP index (**TS3*RS***)	Type of interaction	Distance	∇^2_ρ*10^{-1}
1	LP···π	3.36	0.2846
2	C-H···π	2.67	0.3017
3	LP···π	2.92	0.4059
4	C-H···O	2.33	0.4478
O···S	1,5- O···S	2.74	0.7324

Part 5: Optimized geometries of some stationary points.

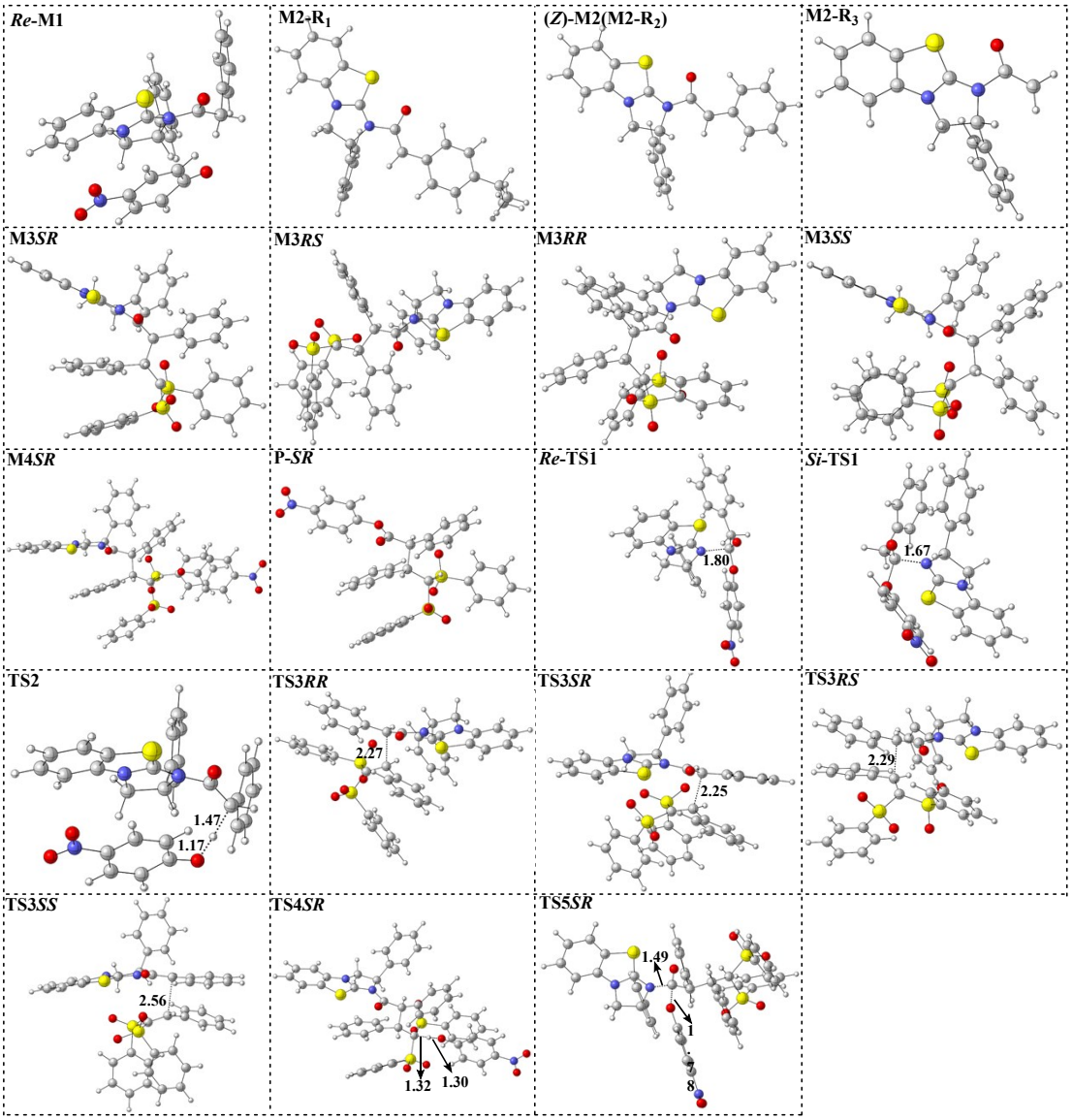


Fig. S5 Optimized geometries of some stationary points (unit: Å).

Part 6: The relative Gibbs free energy profiles of (*Z*)-M2 and (*E*)-M2.

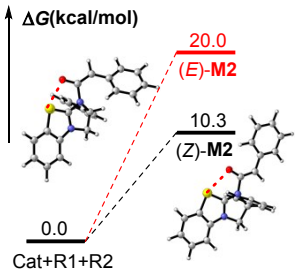
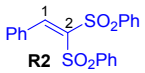


Fig. S6 The relative Gibbs free energies of (*Z*)-**M2** and (*E*)-**M2**.

Part 7: Parr function analysis on the reactant R2.

Besides, the intermediate **M2** can also react with the carbonyl carbon of the reactant **R2** to form $^{\alpha}$C-^{2}C bond through the transition state **TS3'**. Actually, we have tried but failed to locate the transition state **TS3'**, and even intermediate **M3'** cannot be located at all, indicating the ^{2}C atom cannot be nucleophilically attacked by the intermediate. Therefore, we performed Parr functions (P_k^+ and P_k^-)[3] analysis for the reactant **R2** to analyse the local electrophilicity/nucleophilicity for the two olefin carbon atoms ^{1}C and ^{2}C. As summarized in Table S5, it is obvious that the ^{1}C atom of reactant **R2** has the stronger electrophilicity. Herein, the pathway associated with the $^{\alpha}$C-^{2}C bond formation can be safely excluded here.

Table S5 Local nucleophilic (P_k^-) and electrophilic (P_k^+) Parr function analysis on the reactant **R2**.



R2

	^{1}C		^{2}C	
SP	P_k^+	P_k^-	P_k^+	P_k^-
R2	0.54	0.12	-0.14	0.26

Part 8: Cartesian coordinates and vibrational frequencies of all the optimized structures.

Cat

Zero-point correction= 0.238311

Thermal correction to Energy= 0.251870

Thermal correction to Enthalpy= 0.252814

Thermal correction to Gibbs Free Energy= 0.196207

Sum of electronic and zero-point Energies= -1085.978967

Sum of electronic and thermal Energies= -1085.965408

Sum of electronic and thermal Enthalpies= -1085.964464

Sum of electronic and thermal Free Energies= -1086.021072

Cartesian coordinates

C	3.980110	1.979297	-0.463331
C	4.747636	0.845551	-0.724041
C	4.206940	-0.431976	-0.557804
C	2.894611	-0.543808	-0.129379
C	2.125309	0.600131	0.147751
C	2.661264	1.871745	-0.021735
H	4.412283	2.964516	-0.602438
H	5.771768	0.950305	-1.064181
H	4.797038	-1.317027	-0.770508
H	2.062959	2.751295	0.191009
C	0.538698	-1.071691	0.526840
C	-1.379010	-0.142629	1.021748
C	-0.394561	1.009116	0.627290
H	-0.383872	1.820689	1.356615
S	1.964429	-2.036532	0.139102
N	0.862033	0.271434	0.606295
N	-0.677301	-1.408361	0.707242
H	-1.541752	-0.108089	2.107184
C	-2.714161	-0.010609	0.328349
C	-2.939493	-0.608660	-0.912541
C	-3.719391	0.769955	0.901800
C	-4.154102	-0.428318	-1.569175
H	-2.160266	-1.225120	-1.350349
C	-4.932170	0.956470	0.243285
H	-3.552297	1.231384	1.872221
C	-5.152221	0.356336	-0.994680
H	-4.322268	-0.902831	-2.530954
H	-5.707159	1.564007	0.699879
H	-6.099057	0.495790	-1.506417
H	-0.618112	1.412605	-0.368728

Vibrational frequencies

25.6819	35.5032	74.2058

93.0147	154.5291	188.4350
204.5191	250.5385	271.6773
279.5734	328.2344	416.9797
429.0439	434.5089	496.6898
511.0451	537.9417	551.2462
570.7405	592.2733	630.8328
658.3384	686.1450	710.0409
721.3015	729.2229	761.2107
771.9764	781.7143	848.9583
878.5545	879.8532	936.3292
948.3092	959.8106	988.9072
1002.7358	1009.9811	1019.3147
1026.3488	1040.1693	1057.9595
1062.2230	1073.8811	1088.3281
1116.0917	1121.6997	1159.2549
1181.3766	1182.6399	1205.2789
1208.4688	1238.0980	1248.6468
1303.2396	1312.7273	1337.7357
1350.7172	1363.1528	1377.7213
1387.9374	1421.6395	1508.3631
1513.3373	1519.9516	1536.3108
1558.3675	1670.9770	1679.0995
1684.1248	1704.0572	1714.1573
3059.4751	3072.6433	3155.3327
3199.4101	3207.8497	3212.4786
3217.2442	3220.2494	3227.3927
3231.8569	3233.2791	3245.3821

R1

Zero-point correction= 0.229324

Thermal correction to Energy= 0.244915

Thermal correction to Enthalpy= 0.245859

Thermal correction to Gibbs Free Energy= 0.182664

Sum of electronic and zero-point Energies= -895.104296

Sum of electronic and thermal Energies= -895.088705

Sum of electronic and thermal Enthalpies= -895.087761

Sum of electronic and thermal Free Energies= -895.150956

Cartesian coordinates

C	-1.263197	-0.585350	0.461375
C	-2.141936	-1.574289	0.028122
C	-1.670734	0.737192	0.628903
C	-3.460020	-1.240684	-0.248992
H	-1.782626	-2.590473	-0.083128
O	0.012344	-0.999145	0.790621

C	-2.986629	1.075178	0.349125
H	-0.968662	1.486957	0.970068
C	-3.855343	0.080704	-0.085215
H	-4.171941	-1.981878	-0.588770
C	1.093494	-0.303857	0.322549
H	-3.343744	2.090160	0.466616
N	-5.245185	0.439479	-0.377520
C	2.356849	-0.902008	0.898562
O	1.005436	0.633333	-0.420565
O	-5.578243	1.602697	-0.228710
O	-5.995499	-0.444742	-0.753661
C	3.614608	-0.314455	0.314682
H	2.305506	-0.738909	1.982167
H	2.310586	-1.984803	0.751521
C	3.934807	1.028044	0.534373
C	4.477843	-1.100919	-0.447220
C	5.097774	1.573009	0.000924
H	3.266568	1.647783	1.126055
C	5.645443	-0.558159	-0.981091
H	4.236781	-2.145718	-0.623495
C	5.957247	0.779752	-0.758594
H	5.335311	2.616867	0.179367
H	6.308842	-1.182227	-1.571221
H	6.866130	1.203798	-1.173033

Vibrational frequencies

20.5623	25.8657	34.9634
56.3286	62.3781	78.7260
103.7383	164.9889	202.9110
242.8305	266.8495	323.0724
334.2490	397.9673	416.6168
417.3560	425.4253	485.3692
512.2056	544.9212	569.6470
574.9456	630.5490	636.5273
674.1420	697.7692	717.2470
734.8598	769.5343	793.7786
823.2339	850.8882	873.1567
876.5755	886.9721	907.5024
934.9739	958.8423	972.3696
996.1915	1001.8581	1003.2108
1018.9694	1028.3811	1036.3559
1071.8825	1121.2852	1135.2216
1156.7254	1165.3335	1183.5599
1198.7190	1208.6931	1215.3126
1251.0932	1283.1543	1320.5642

1350.8356	1365.0076	1380.2384
1392.2760	1454.6807	1476.7353
1484.7294	1510.4671	1555.7262
1560.1688	1681.9096	1683.6876
1688.2285	1705.1814	1739.2224
1898.9441	3078.4517	3137.6077
3202.9790	3207.8042	3217.2155
3226.1977	3235.8573	3241.1908
3255.4226	3265.1217	3268.3231

R2

Zero-point correction= 0.320177

Thermal correction to Energy= 0.342084

Thermal correction to Enthalpy= 0.343028

Thermal correction to Gibbs Free Energy= 0.268642

Sum of electronic and zero-point Energies= -1868.085469

Sum of electronic and thermal Energies= -1868.063562

Sum of electronic and thermal Enthalpies= -1868.062618

Sum of electronic and thermal Free Energies= -1868.137004

Cartesian coordinates

C	-5.082506	-1.022518	-0.265453
C	-3.808033	-0.724810	0.199692
C	-3.263706	0.547758	-0.019587
C	-4.030050	1.521220	-0.675296
C	-5.294462	1.211384	-1.160396
C	-5.821294	-0.062426	-0.955910
H	-5.503592	-2.005690	-0.084903
H	-3.248683	-1.467369	0.759298
H	-3.621872	2.518257	-0.813993
H	-5.872716	1.965581	-1.683095
H	-6.814709	-0.303073	-1.320347
C	-1.948524	0.955149	0.485413
H	-1.891275	1.991636	0.820788
C	-0.803385	0.265423	0.624579
S	-0.580794	-1.446376	0.110563
S	0.521042	1.077075	1.523198
O	-0.025115	2.341013	2.016879
O	-0.905802	-2.308726	1.246606
O	1.065295	0.104569	2.468881
O	-1.309005	-1.602902	-1.147498
C	1.768995	1.453939	0.313091
C	1.413213	2.149714	-0.840837
C	3.078660	1.076742	0.581825
C	2.408972	2.463407	-1.758021

H	0.379432	2.426899	-1.025677
C	4.066544	1.410915	-0.341106
H	3.307818	0.520435	1.484349
C	3.731621	2.095999	-1.505979
H	2.154066	2.996121	-2.667472
H	5.095109	1.121221	-0.154079
H	4.504266	2.343099	-2.226581
C	1.145878	-1.625299	-0.256598
C	1.987252	-2.188633	0.697379
C	1.592964	-1.249810	-1.522734
C	3.327473	-2.372239	0.368922
H	1.593734	-2.467611	1.668171
C	2.936000	-1.429758	-1.830419
H	0.898943	-0.832086	-2.244572
C	3.796787	-1.991086	-0.886365
H	4.003823	-2.812254	1.093464
H	3.310150	-1.135509	-2.804819
H	4.844150	-2.132908	-1.132864

Vibrational frequencies

29.8341	32.2133	51.0630
60.9274	63.4655	84.3348
101.2544	114.2013	135.8340
147.6858	169.7472	178.3588
191.6637	212.1326	223.7644
239.9323	259.0315	291.0162
314.6989	325.5133	343.2559
380.5885	395.7319	414.6821
416.4186	421.1236	446.3106
480.7963	490.2993	509.9908
534.6456	554.5179	570.1853
610.0461	614.2828	621.1107
621.2688	626.6991	674.4224
697.1903	700.9236	715.1820
734.6881	752.7319	766.4277
773.5305	784.0174	844.5738
864.9078	870.5406	889.3056
949.7922	958.9139	963.9946
966.3850	998.9698	1004.3272
1007.0971	1012.4977	1013.0201
1019.4711	1020.4940	1030.3536
1033.0082	1040.0191	1061.3576
1062.5254	1070.6078	1107.2869
1112.3022	1117.3893	1120.2811
1127.9531	1163.2830	1166.2643

1177.3859	1183.6324	1184.2757
1202.6521	1203.8343	1215.9165
1256.1191	1328.1494	1330.8660
1336.3468	1337.1185	1341.3745
1366.3653	1367.0063	1369.6774
1378.0229	1499.6175	1500.8815
1501.1474	1530.1574	1532.3901
1547.9237	1661.5708	1677.3878
1679.0502	1680.4439	1681.9105
1683.2248	1693.8326	3181.8077
3210.7117	3211.4942	3213.4900
3217.4397	3218.9332	3224.0061
3227.5442	3228.1395	3232.1157
3235.2253	3236.6052	3239.1100
3245.4999	3246.1345	3250.3080

ArO^-

Zero-point correction= 0.095694

Thermal correction to Energy= 0.103290

Thermal correction to Enthalpy= 0.104234

Thermal correction to Gibbs Free Energy= 0.062661

Sum of electronic and zero-point Energies= -511.201266

Sum of electronic and thermal Energies= -511.193670

Sum of electronic and thermal Enthalpies= -511.192726

Sum of electronic and thermal Free Energies= -511.234299

Cartesian coordinates

C	2.197538	0.000000	0.000044
C	1.415241	-1.225683	-0.000259
C	1.415248	1.225673	-0.000247
C	0.047468	-1.221785	-0.000268
H	1.964980	-2.162373	-0.000413
O	3.448399	0.000007	0.000552
C	0.047473	1.221776	-0.000263
H	1.964999	2.162358	-0.000379
C	-0.658676	-0.000004	-0.000185
H	-0.516951	-2.147706	-0.000395
H	-0.516937	2.147702	-0.000384
N	-2.068348	0.000004	0.000084
O	-2.674413	1.079833	0.000214
O	-2.674413	-1.079823	0.000240

Vibrational frequencies

72.3781	100.9643	240.6198
258.6941	372.5509	425.0190
452.0984	477.9904	556.1674

631.6058	654.1871	721.0268
783.6663	810.1920	827.3858
862.0032	871.1626	989.7055
997.2360	1002.1480	1113.0738
1140.7337	1217.1631	1269.0834
1342.2393	1381.4361	1447.1048
1544.4342	1574.2169	1634.2944
1655.7908	1701.2828	3201.1555
3201.9933	3236.3862	3237.4160

ArOH

Zero-point correction= 0.109226

Thermal correction to Energy= 0.117028

Thermal correction to Enthalpy= 0.117972

Thermal correction to Gibbs Free Energy= 0.076101

Sum of electronic and zero-point Energies= -511.670647

Sum of electronic and thermal Energies= -511.662846

Sum of electronic and thermal Enthalpies= -511.661902

Sum of electronic and thermal Free Energies= -511.703773

Cartesian coordinates

C	2.068371	0.014855	-0.000032
C	1.366451	1.227469	0.000324
C	1.379819	-1.204085	-0.000380
C	-0.016317	1.222462	0.000312
H	1.925423	2.155848	0.000645
O	3.413703	0.087632	0.000075
C	-0.005534	-1.212201	-0.000406
H	1.930480	-2.139371	-0.000648
C	-0.685287	0.000682	-0.000037
H	-0.582015	2.145529	0.000574
H	-0.561049	-2.141436	-0.000643
N	-2.141784	-0.007377	-0.000031
O	-2.711560	-1.087531	0.000965
O	-2.722866	1.066617	-0.000857
H	3.800425	-0.797773	0.000127

Vibrational frequencies

63.3568	115.1781	238.4325
303.8266	371.1604	414.0712
427.4338	453.2437	510.4869
547.0554	643.7763	649.7071
701.1523	774.6872	835.2273
839.2901	870.9832	903.6367
988.6777	1001.8121	1027.2904
1129.5963	1153.7045	1201.1594

1212.1149	1329.0917	1349.3847
1408.6791	1473.6328	1506.6869
1563.0273	1677.3694	1693.6970
1731.8051	3212.6129	3240.7338
3259.5321	3264.0074	3857.5659

***Re*-TS1**

Zero-point correction= 0.469771

Thermal correction to Energy= 0.499139

Thermal correction to Enthalpy= 0.500084

Thermal correction to Gibbs Free Energy= 0.406716

Sum of electronic and zero-point Energies= -1981.083544

Sum of electronic and thermal Energies= -1981.054176

Sum of electronic and thermal Enthalpies= -1981.053232

Sum of electronic and thermal Free Energies= -1981.146599

Cartesian coordinates

C	2.357307	-0.914520	-1.065919
C	3.495419	-1.668283	-0.729922
C	2.447034	0.483563	-1.172901
C	4.706268	-1.047026	-0.491072
H	3.395791	-2.745828	-0.660149
O	1.229009	-1.639722	-1.208530
C	3.663576	1.105385	-0.929057
H	1.584377	1.062000	-1.470881
C	4.773312	0.340579	-0.589912
H	5.589920	-1.614617	-0.228261
C	-0.030139	-1.023954	-1.565874
H	3.758686	2.181653	-1.003413
N	6.041279	1.007640	-0.329841
C	-1.029130	-2.179855	-1.591332
O	-0.047275	-0.131113	-2.422585
O	6.081721	2.225022	-0.420304
O	7.003548	0.317325	-0.030435
C	-2.470168	-1.737076	-1.653209
H	-0.768917	-2.756564	-2.487902
H	-0.862827	-2.823979	-0.723779
C	-2.925847	-0.864763	-2.648787
C	-3.390834	-2.229250	-0.724217
C	-4.264907	-0.485226	-2.698348
H	-2.216781	-0.478486	-3.372464
C	-4.731364	-1.852678	-0.773690
H	-3.049976	-2.920667	0.041420
C	-5.172367	-0.975170	-1.760486
H	-4.601990	0.194130	-3.475500

H	-5.430449	-2.247802	-0.042936
H	-6.215943	-0.679333	-1.802850
C	-2.033995	4.875861	2.318260
C	-2.464474	5.311814	1.063708
C	-2.318799	4.502797	-0.062759
C	-1.739016	3.252225	0.095277
C	-1.302787	2.822574	1.357525
C	-1.444494	3.624460	2.483454
H	-2.157343	5.520322	3.181776
H	-2.919562	6.290347	0.959577
H	-2.656137	4.839175	-1.037146
H	-1.103109	3.281484	3.453986
C	-0.792508	0.972429	0.061254
C	0.199520	-0.573802	1.357043
C	-0.321712	0.572550	2.275783
H	0.457814	0.966221	2.928835
S	-1.434091	2.032106	-1.163062
N	-0.733557	1.559867	1.280274
N	-0.372505	-0.252575	0.023359
H	1.290547	-0.495423	1.272455
C	-0.152523	-1.967420	1.814667
C	-1.466706	-2.304003	2.146039
C	0.837998	-2.947526	1.864284
C	-1.783272	-3.603969	2.528907
H	-2.251917	-1.554542	2.081089
C	0.523451	-4.249582	2.247035
H	1.858897	-2.686994	1.595620
C	-0.787813	-4.579029	2.580035
H	-2.808060	-3.857309	2.781944
H	1.301383	-5.005232	2.283751
H	-1.035538	-5.592900	2.877028
H	-1.182113	0.267395	2.880369

Vibrational frequencies

-202.0122	15.4928	21.2175
30.3269	33.4023	41.0945
45.9562	49.9376	59.9074
68.1539	83.8888	99.5219
105.7214	113.0462	120.0060
150.5798	165.9003	182.2436
201.6079	203.3557	212.2894
224.7852	259.1671	269.5539
287.6961	303.2188	316.6663
324.7342	329.9698	359.5406
410.1144	419.4312	421.6246

429.4399	430.4403	431.4641
441.9496	484.2745	506.7857
510.6164	517.2419	538.3794
547.9665	549.3407	566.6632
574.3601	594.0990	601.7681
625.7418	628.8447	632.1079
656.3261	673.9575	693.3085
709.1233	715.7339	717.8875
724.5952	730.1341	745.8212
769.3880	773.5821	777.9953
781.1813	791.6341	806.9175
844.8549	857.8823	874.8135
879.4185	886.5398	890.7314
896.3228	900.8069	913.5634
949.5127	949.9464	966.7554
970.6025	981.5956	996.5218
1002.2133	1007.1695	1011.5460
1013.3784	1017.5631	1018.2227
1024.1609	1026.1292	1029.6695
1034.3391	1048.5998	1060.8894
1062.3934	1064.0854	1070.9466
1072.6085	1107.9805	1117.6462
1123.9328	1126.9775	1139.0800
1157.3699	1160.6329	1175.5956
1177.8100	1184.2019	1200.0218
1202.1366	1207.3180	1212.7934
1222.2841	1238.4224	1250.9701
1283.5965	1302.4764	1311.1659
1316.7652	1326.3672	1342.0715
1353.8336	1357.3207	1359.6734
1360.6490	1376.5780	1380.6205
1403.4876	1418.1808	1438.1388
1468.0146	1469.4439	1483.8596
1504.9066	1507.1596	1516.2207
1525.8470	1536.3062	1551.2956
1554.7824	1555.2332	1618.8396
1657.1771	1669.3947	1674.8815
1677.4781	1680.2616	1690.6698
1695.6059	1698.8446	1702.4600
1720.7457	3074.5651	3095.0700
3100.6542	3143.5246	3166.4734
3197.7887	3202.2708	3204.0846
3209.4987	3214.9735	3215.9760
3219.3766	3224.8312	3227.7790

3234.0644	3237.1867	3237.2661
3237.7257	3246.9732	3254.3282
3263.2648	3276.2445	3293.0267

M1

Zero-point correction= 0.470180

Thermal correction to Energy= 0.500053

Thermal correction to Enthalpy= 0.500997

Thermal correction to Gibbs Free Energy= 0.408974

Sum of electronic and zero-point Energies= -1981.095819

Sum of electronic and thermal Energies= -1981.065946

Sum of electronic and thermal Enthalpies= -1981.065002

Sum of electronic and thermal Free Energies= -1981.157025

Cartesian coordinates

C	4.452685	1.249639	2.298193
C	4.673030	2.370279	1.488567
C	3.743116	2.765877	0.534270
C	2.577406	2.016505	0.415215
C	2.362638	0.902150	1.235212
C	3.290040	0.498507	2.189478
H	5.207110	0.953503	3.018161
H	5.593763	2.932526	1.594788
H	3.923211	3.625207	-0.101753
H	3.118355	-0.382756	2.797672
C	0.503161	0.844821	-0.091821
C	-0.816177	-0.959932	0.543622
C	0.405779	-0.823986	1.505136
H	1.014705	-1.727723	1.521442
S	1.254420	2.243115	-0.739671
N	1.157552	0.284059	0.910749
N	-0.655962	0.214917	-0.365718
H	-0.715821	-1.854575	-0.077288
C	-2.134867	-0.961962	1.277106
C	-2.823208	-2.162630	1.435424
C	-2.650986	0.213171	1.829237
C	-4.021262	-2.192644	2.147581
H	-2.424813	-3.074180	0.997287
C	-3.852407	0.184552	2.526490
H	-2.125649	1.155288	1.691665
C	-4.537198	-1.019852	2.689451
H	-4.552848	-3.130911	2.267713
H	-4.259758	1.102742	2.936643
H	-5.476387	-1.039688	3.232830
C	-2.565459	-0.343479	-1.872928

H	-2.626599	-0.393989	-2.963351
O	-0.927171	1.369771	-2.276896
C	-1.327885	0.458698	-1.582530
H	0.098106	-0.547777	2.516528
O	-0.163759	-1.938438	-2.360470
C	1.025216	-1.819317	-1.954682
C	1.599061	-2.713631	-0.971867
C	1.887197	-0.743779	-2.389799
C	2.830630	-2.486392	-0.406657
C	3.119954	-0.524036	-1.825524
C	3.590527	-1.376145	-0.811255
H	3.228240	-3.145471	0.357604
H	3.735332	0.316553	-2.128491
H	-2.454622	-1.364258	-1.503889
C	-3.805457	0.314857	-1.288710
C	-4.827496	-0.486583	-0.778211
C	-3.951895	1.703666	-1.256998
C	-5.973799	0.087424	-0.237998
H	-4.714820	-1.566971	-0.787046
C	-5.097541	2.278776	-0.712222
H	-3.167500	2.339130	-1.658226
C	-6.111092	1.473102	-0.199417
H	-6.754061	-0.550536	0.165638
H	-5.197261	3.359414	-0.689950
H	-7.001930	1.921753	0.228266
H	1.497980	-0.071938	-3.149643
H	1.003190	-3.570344	-0.667566
N	4.813852	-1.074188	-0.149505
O	5.160891	-1.772515	0.805760
O	5.478911	-0.113105	-0.535789

Vibrational frequencies

24.9736	28.8286	36.4751
39.9797	49.8482	62.4333
68.8744	76.2875	84.0060
89.1425	105.7167	114.4554
127.3102	130.8656	139.3124
154.3686	160.9230	175.7265
205.2742	215.2098	220.6228
242.6080	251.8704	264.7664
280.4874	291.9348	303.9882
315.1121	332.7334	376.7831
379.3825	411.9386	420.9200
429.6383	431.7196	440.3241
454.4108	463.4627	475.6103

502.1368	516.0379	524.5264
529.2820	540.6602	556.9223
580.8708	594.4323	616.3453
627.2354	628.3226	636.4514
650.0061	657.6000	664.4071
703.1585	714.6734	715.9237
720.2646	723.4688	727.6446
749.0292	763.2635	776.6393
786.4458	788.7690	813.1322
829.0232	838.1200	850.2437
869.6730	870.7096	872.5742
876.2061	882.6925	914.1152
933.4319	946.1855	965.3153
969.3341	986.0422	995.9034
999.4923	999.6979	1000.2042
1004.7506	1006.8036	1013.0856
1017.9794	1018.9598	1022.1455
1026.3891	1059.3288	1061.5795
1066.0316	1070.7683	1071.6152
1113.9078	1120.7913	1123.5794
1123.6713	1147.5004	1151.3016
1166.0610	1177.6907	1180.9059
1181.7531	1192.8647	1205.8102
1207.3275	1215.7358	1223.7271
1234.8812	1256.8692	1282.2495
1295.4434	1297.3615	1300.5619
1322.3415	1331.9420	1344.3073
1347.1746	1363.5855	1364.1402
1366.1954	1373.7911	1400.0967
1411.7348	1416.9530	1449.0479
1460.3398	1478.2946	1498.4274
1507.1573	1510.6837	1514.2537
1527.7021	1528.7503	1552.1666
1555.9656	1584.0618	1611.1843
1628.3794	1661.9372	1672.7071
1677.8730	1679.3629	1683.1839
1689.9502	1700.3478	1702.3891
1830.8258	3113.5312	3122.3970
3171.2621	3174.1230	3191.9888
3197.6780	3200.6028	3200.7826
3202.5680	3209.5366	3210.0583
3210.7087	3212.1378	3216.4441
3218.4189	3223.3879	3225.4070
3225.9072	3232.0847	3236.3627

3236.7465 3238.7196 3242.8783

***Si*-TS1**

Zero-point correction= 0.468665

Thermal correction to Energy= 0.498141

Thermal correction to Enthalpy= 0.499085

Thermal correction to Gibbs Free Energy= 0.404754

Sum of electronic and zero-point Energies= -1981.078535

Sum of electronic and thermal Energies= -1981.049059

Sum of electronic and thermal Enthalpies= -1981.048114

Sum of electronic and thermal Free Energies= -1981.142446

Cartesian coordinates

C	1.542260	5.059889	1.572141
C	1.438501	5.573383	0.277604
C	0.956183	4.786545	-0.767360
C	0.583763	3.481446	-0.482736
C	0.684004	2.969710	0.819480
C	1.164471	3.751830	1.863345
H	1.922459	5.689312	2.369075
H	1.736110	6.596422	0.077630
H	0.877320	5.181347	-1.774097
H	1.240955	3.348605	2.867070
C	-0.116744	1.115792	-0.309873
C	-0.320884	-0.608325	1.142794
C	0.345915	0.595319	1.883080
H	1.396942	0.412894	2.124996
S	-0.035923	2.261222	-1.617285
N	0.250914	1.652981	0.874383
N	-0.434650	-0.140849	-0.259256
H	0.328499	-1.485945	1.136424
C	-1.676086	-0.988670	1.696014
C	-1.958994	-2.317236	2.004013
C	-2.651934	-0.010894	1.903973
C	-3.197218	-2.664666	2.540142
H	-1.207210	-3.077462	1.814756
C	-3.888656	-0.356377	2.436329
H	-2.445686	1.026151	1.643544
C	-4.160364	-1.684514	2.762911
H	-3.408659	-3.701287	2.783209
H	-4.643907	0.407932	2.589290
H	-5.125352	-1.954791	3.180462
C	-1.503048	-0.842977	-2.463307
H	-1.202191	0.094520	-2.941681
O	-0.482463	-2.420323	-0.937120

C	-0.430814	-1.299797	-1.468460
H	-0.200601	0.868033	2.787623
O	0.857029	-0.914233	-2.145236
C	1.983492	-1.224902	-1.463117
C	2.827512	-0.178561	-1.064351
C	2.328249	-2.554201	-1.171125
C	4.002889	-0.445404	-0.378635
C	3.498197	-2.827310	-0.479948
C	4.315508	-1.769422	-0.091007
H	4.670114	0.348080	-0.066398
H	3.787822	-3.843773	-0.244137
H	-1.514835	-1.612242	-3.243601
C	-2.861650	-0.693797	-1.827825
C	-3.526648	0.532617	-1.870310
C	-3.476136	-1.772006	-1.180508
C	-4.787337	0.683310	-1.293268
H	-3.057605	1.376753	-2.370759
C	-4.734286	-1.623981	-0.607113
H	-2.946129	-2.716627	-1.118136
C	-5.395937	-0.397671	-0.663811
H	-5.292094	1.643524	-1.341311
H	-5.196950	-2.466457	-0.102015
H	-6.377582	-0.285822	-0.213297
H	1.665660	-3.346333	-1.490063
H	2.556257	0.841242	-1.317986
N	5.548806	-2.058671	0.633969
O	6.254142	-1.118950	0.966766
O	5.815127	-3.225575	0.874070

Vibrational frequencies

-68.3884	8.8601	21.1492
24.8434	32.1119	35.8497
43.3269	57.4292	61.8807
64.5185	79.7973	92.6063
100.7527	117.8104	119.2080
142.1672	167.5422	179.6399
191.2269	199.7919	217.8516
240.8088	246.1146	266.2732
276.1177	310.2636	318.9494
346.1612	358.4941	384.4054
408.2428	410.8166	418.6336
421.2524	429.2920	432.0189
444.5369	477.2638	485.6084
515.2772	526.4663	545.1085
546.1960	554.7453	566.7596

575.9763	584.0613	611.6137
624.3171	626.5964	632.6659
654.9075	661.0930	677.8768
700.4258	709.7647	713.8327
724.3022	725.8799	730.2884
750.3413	768.4627	786.9370
787.6222	798.5736	803.3924
841.7816	852.6745	865.5855
869.1781	872.2012	878.0142
880.4870	897.9320	906.6160
935.9205	938.1478	957.5983
965.8713	973.0900	994.8945
998.1318	999.8562	1003.5709
1005.4544	1013.4158	1016.1783
1018.3435	1021.9728	1025.3195
1029.6256	1032.5543	1041.0134
1060.9696	1065.8823	1066.9791
1071.4635	1099.9602	1111.5696
1121.5594	1124.5234	1125.6483
1152.3352	1163.2648	1175.4370
1177.0359	1183.2351	1189.6747
1194.9963	1196.7987	1207.4342
1223.5028	1235.4575	1245.3554
1289.7656	1298.5541	1299.9939
1304.7297	1327.0357	1331.7526
1335.1692	1357.6659	1358.6492
1362.9430	1367.6820	1372.0533
1396.3308	1417.8865	1443.9068
1471.1409	1472.1618	1486.5607
1505.2489	1507.8539	1515.1450
1526.3487	1538.5054	1547.9744
1550.6578	1556.6835	1615.8197
1657.1926	1662.0274	1676.5650
1677.7374	1680.5588	1688.0651
1692.4137	1697.3989	1701.8785
1721.4857	3079.7455	3105.1574
3131.6334	3154.0068	3173.0644
3189.7557	3191.9580	3201.9055
3206.0961	3211.8816	3218.0760
3220.0827	3226.3114	3228.7488
3232.2499	3232.9085	3233.1627
3235.8358	3236.9112	3241.4253
3253.6071	3261.7818	3274.5382

TS2

Zero-point correction= 0.464886

Thermal correction to Energy= 0.494109

Thermal correction to Enthalpy= 0.495053

Thermal correction to Gibbs Free Energy= 0.405588

Sum of electronic and zero-point Energies= -1981.075347

Sum of electronic and thermal Energies= -1981.046124

Sum of electronic and thermal Enthalpies= -1981.045180

Sum of electronic and thermal Free Energies= -1981.134645

Cartesian coordinates

C	4.551967	-2.139293	-1.056626
C	5.020781	-2.286574	0.253875
C	4.198580	-2.035619	1.347362
C	2.888788	-1.640050	1.099665
C	2.424349	-1.512864	-0.214282
C	3.241695	-1.755211	-1.313253
H	5.222310	-2.322510	-1.888715
H	6.048321	-2.588088	0.422820
H	4.569780	-2.133868	2.361282
H	2.868452	-1.632998	-2.324185
C	0.581486	-0.834108	0.970721
C	-1.066089	-0.228061	-0.518062
C	0.230248	-0.613297	-1.299866
H	0.704890	0.239948	-1.789947
S	1.651970	-1.157367	2.276308
N	1.097652	-1.094126	-0.225584
N	-0.645264	-0.303965	0.910037
H	-1.353630	0.803621	-0.736893
C	-2.202481	-1.169222	-0.851841
C	-3.075076	-0.813317	-1.877668
C	-2.346503	-2.401500	-0.213994
C	-4.095877	-1.678607	-2.258977
H	-2.971597	0.155680	-2.358740
C	-3.371179	-3.263917	-0.593259
H	-1.675808	-2.678306	0.595123
C	-4.247250	-2.904349	-1.615922
H	-4.782829	-1.386463	-3.046881
H	-3.487087	-4.217574	-0.088315
H	-5.048323	-3.576208	-1.906738
C	-2.085448	1.518597	1.753431
H	-2.289718	2.054515	2.683027
O	-0.471705	0.342548	3.069474
C	-1.110671	0.508342	2.033255
H	0.038598	-1.406500	-2.023709

O	-0.825137	3.119768	0.079954
C	0.418973	2.768409	-0.149626
C	0.948489	2.868915	-1.461412
C	1.259658	2.258431	0.872775
C	2.216655	2.405514	-1.755716
C	2.533268	1.805344	0.581229
C	2.991715	1.849981	-0.734940
H	2.612355	2.447970	-2.763650
H	3.176458	1.401426	1.355243
H	-1.322484	2.458848	0.911200
C	-3.343578	1.189680	0.997604
C	-3.830774	2.048080	0.005162
C	-4.100315	0.052531	1.314896
C	-5.034758	1.782173	-0.644902
H	-3.250614	2.927240	-0.260723
C	-5.296887	-0.222852	0.661141
H	-3.738340	-0.624552	2.085363
C	-5.770362	0.645208	-0.320674
H	-5.395645	2.463364	-1.409807
H	-5.858485	-1.116407	0.916290
H	-6.704096	0.433453	-0.832532
H	0.888521	2.213393	1.892679
H	0.316618	3.289793	-2.235944
N	4.293601	1.297975	-1.044214
O	4.621160	1.210502	-2.220986
O	5.000991	0.927022	-0.118370

Vibrational frequencies

-1057.0895	30.4736	37.6358
45.2640	56.0467	60.8802
65.1791	81.9726	83.7233
88.3566	101.1895	109.8458
118.3115	125.6769	131.5720
136.4065	148.9009	170.6910
201.6645	208.0917	215.3349
220.0820	244.3563	268.9684
282.0949	286.6512	311.2067
322.4888	332.7970	374.3915
388.9158	416.6781	421.8361
428.9072	436.2707	441.3899
441.8822	449.7369	469.2423
512.9625	517.9886	526.0473
542.7365	551.4427	569.2273
590.9270	593.2743	597.2686
621.0880	630.0804	630.9629

646.3188	648.9371	664.2661
676.1567	700.1067	712.5884
713.8783	717.4833	720.9093
726.7544	749.8781	764.4362
779.4673	781.1351	786.0727
808.9652	836.7399	843.8702
865.5886	868.4919	874.8170
877.6981	881.0624	898.3339
910.3464	926.5144	935.8402
963.8519	968.3325	984.2227
987.2453	993.4205	998.8860
1006.6983	1011.1911	1015.1361
1015.9813	1016.9421	1019.0726
1021.6731	1030.3940	1057.1697
1059.6425	1066.2939	1071.6478
1077.0179	1122.2503	1124.2478
1126.6416	1128.4086	1150.8438
1153.7521	1166.2134	1179.5259
1183.7644	1186.7113	1206.1667
1206.7270	1213.9602	1227.2487
1227.9713	1254.2777	1262.6237
1295.4941	1299.9289	1309.4518
1325.9608	1333.3166	1338.3972
1344.9652	1348.4753	1363.6873
1366.2292	1366.9893	1371.0752
1392.2975	1409.2411	1419.0048
1460.6394	1463.1345	1487.0123
1501.2878	1508.1070	1517.0387
1521.7701	1535.3296	1554.7488
1556.5501	1565.0190	1577.0037
1604.8086	1642.2886	1669.0476
1675.9209	1684.8216	1688.5832
1690.9432	1697.4010	1702.2472
1708.7230	1775.5762	3125.0938
3125.3455	3154.8517	3186.4525
3189.2131	3194.3960	3199.4602
3200.7938	3209.7696	3211.1486
3212.7789	3219.7518	3219.8793
3222.5984	3226.4719	3227.6017
3228.4058	3230.9099	3235.9802
3240.9832	3241.3611	3243.8130

(*Z*)-M2

Zero-point correction= 0.358542

Thermal correction to Energy= 0.379904
Thermal correction to Enthalpy= 0.380848
Thermal correction to Gibbs Free Energy= 0.305342
Sum of electronic and zero-point Energies= -1469.390446
Sum of electronic and thermal Energies= -1469.369085
Sum of electronic and thermal Enthalpies= -1469.368140
Sum of electronic and thermal Free Energies= -1469.443646
Cartesian coordinates

C	5.964328	-0.218069	0.317672
C	5.952965	-1.441620	-0.357720
C	4.752703	-2.070668	-0.681220
C	3.566107	-1.449202	-0.315023
C	3.587561	-0.220862	0.358786
C	4.780255	0.413013	0.686559
H	6.911210	0.251651	0.559725
H	6.890042	-1.911162	-0.634908
H	4.743981	-3.020735	-1.204338
H	4.781585	1.362354	1.210622
C	1.324836	-0.611244	0.205595
C	0.202173	1.165405	1.113801
C	1.734484	1.331818	1.380856
H	1.989761	1.219978	2.437473
S	1.905315	-2.030212	-0.584587
N	2.293297	0.216950	0.616581
N	0.114807	-0.176456	0.491494
H	-0.347404	1.148016	2.057822
C	-0.349176	2.250867	0.213401
C	-1.002459	3.342943	0.783128
C	-0.156452	2.204048	-1.168052
C	-1.458545	4.384920	-0.021013
H	-1.160337	3.375446	1.858180
C	-0.614215	3.244218	-1.970503
H	0.334423	1.346520	-1.621263
C	-1.263790	4.337228	-1.398683
H	-1.970358	5.228860	0.429661
H	-0.468241	3.199212	-3.044712
H	-1.622223	5.145583	-2.027419
C	-2.278340	-0.390037	0.511002
H	-2.267167	0.591300	0.969556
O	-0.795775	-2.049323	-0.415749
C	-1.084645	-0.966721	0.148650
H	2.107931	2.286034	1.006758
C	-3.580916	-0.988976	0.293153
C	-4.735021	-0.280785	0.690412

C	-3.778148	-2.255861	-0.298391
C	-6.009921	-0.800716	0.510690
H	-4.614686	0.698924	1.147437
C	-5.058331	-2.770251	-0.475433
H	-2.909376	-2.821138	-0.612781
C	-6.186097	-2.054521	-0.075494
H	-6.873411	-0.222894	0.828939
H	-5.176439	-3.748723	-0.933824
H	-7.180998	-2.464280	-0.217102

Vibrational frequencies

21.4629	25.1145	26.6223
35.2445	54.9906	69.6295
84.8922	98.2952	116.1568
164.5312	170.7133	191.1902
204.4316	225.8432	239.0963
274.4144	284.5836	308.6967
348.8467	351.2129	414.4344
420.3135	423.4461	433.3190
438.5499	508.0925	526.5581
530.0168	547.7091	564.8869
581.5011	592.3394	625.1612
628.8949	631.4215	643.3004
697.5360	699.1974	709.8313
718.8367	723.2092	732.0677
734.5357	767.0762	786.1252
790.6259	794.9626	813.0655
875.5953	877.5881	880.2756
881.9183	922.8404	931.1354
945.9460	966.1982	979.4726
999.4307	1003.7560	1006.9132
1012.9500	1017.8454	1022.0369
1029.3647	1040.9973	1052.8781
1062.5420	1067.2345	1071.2566
1073.1135	1116.4522	1124.6660
1127.7348	1159.5475	1165.9037
1173.9392	1180.9013	1181.8627
1184.0098	1208.4058	1208.6041
1220.0596	1244.9857	1263.4124
1294.7565	1298.7005	1329.0411
1335.9010	1341.6599	1364.4385
1365.4080	1367.0814	1387.3523
1419.5330	1462.7719	1474.7580
1507.3423	1512.6424	1515.2788
1528.7936	1542.3943	1552.8936

1555.5317	1644.5909	1648.5413
1676.8926	1678.9601	1685.6803
1694.1431	1701.8658	1740.8707
3112.9963	3131.6460	3184.4561
3193.0750	3194.1270	3200.4630
3203.9712	3210.5693	3210.7989
3214.2462	3218.5701	3220.1721
3223.3417	3227.3734	3229.5866
3231.2696	3235.6591	3257.0405

(*E*)-M2

Zero-point correction= 0.358934

Thermal correction to Energy= 0.379903

Thermal correction to Enthalpy= 0.380847

Thermal correction to Gibbs Free Energy= 0.307532

Sum of electronic and zero-point Energies= -1469.380466

Sum of electronic and thermal Energies= -1469.359497

Sum of electronic and thermal Enthalpies= -1469.358553

Sum of electronic and thermal Free Energies= -1469.431868

Cartesian coordinates

C	-5.187239	-0.372051	-1.731845
C	-5.707961	-0.854940	-0.527472
C	-4.880303	-1.095275	0.566659
C	-3.520704	-0.848318	0.426272
C	-3.008006	-0.357598	-0.782645
C	-3.828130	-0.113546	-1.878094
H	-5.852463	-0.193778	-2.569394
H	-6.771412	-1.046989	-0.441041
H	-5.283660	-1.470507	1.500813
H	-3.417752	0.263326	-2.808471
C	-1.094098	-0.540256	0.477406
C	0.633809	0.342863	-0.690263
C	-0.571228	0.137550	-1.650483
H	-0.427930	-0.715969	-2.319800
S	-2.248617	-1.040686	1.652954
N	-1.633112	-0.169684	-0.689382
N	0.226639	-0.465773	0.487648
H	1.541908	-0.068482	-1.131087
C	0.840027	1.802218	-0.325987
C	1.469989	2.626492	-1.261915
C	0.385960	2.347946	0.875703
C	1.635002	3.983819	-1.007452
H	1.835800	2.201627	-2.193775
C	0.555560	3.708400	1.128496

H	-0.069272	1.712793	1.631517
C	1.174627	4.528758	0.190119
H	2.128251	4.614278	-1.740140
H	0.204514	4.124028	2.067502
H	1.305809	5.586713	0.392623
C	2.325451	-0.849643	1.673041
H	2.848678	-0.738600	2.617657
O	0.238438	-0.479520	2.771507
C	0.973276	-0.623589	1.765109
H	-0.803080	1.035499	-2.223768
C	3.117984	-1.302238	0.537520
C	2.610419	-2.113887	-0.498904
C	4.492637	-0.993485	0.484266
C	3.417444	-2.542489	-1.548121
H	1.569927	-2.426709	-0.463637
C	5.302100	-1.438536	-0.553333
H	4.919908	-0.386194	1.278117
C	4.770184	-2.209307	-1.587221
H	2.988843	-3.163732	-2.329684
H	6.356315	-1.176334	-0.559029
H	5.400506	-2.552971	-2.400727

Vibrational frequencies

22.8629	29.0638	41.1488
51.1596	67.2908	73.9975
98.7052	119.7238	131.3422
147.7506	175.4187	206.1761
215.9420	236.1117	251.1093
290.1007	298.0215	323.5099
377.0898	391.7509	419.6567
424.2809	433.3116	437.2540
458.6443	491.3313	518.8397
525.7668	544.4045	552.2601
580.0330	594.6627	628.2105
629.7791	641.4462	663.6430
667.6768	694.7259	714.9992
719.6549	724.8648	733.4837
744.1402	761.4732	775.3745
778.4052	786.0678	791.9517
869.6027	881.8724	889.7032
890.7670	913.8734	930.9330
965.1443	975.4077	979.8179
995.1438	1009.2427	1010.5028
1013.3452	1017.1520	1019.4583
1034.9922	1039.9645	1050.9176

1063.0616	1066.7862	1070.9880
1072.8905	1115.9010	1125.9897
1129.7324	1143.2265	1166.1803
1175.9719	1180.3398	1185.3732
1206.1731	1214.7094	1219.1371
1221.7260	1248.9740	1265.9396
1304.4548	1306.8603	1334.0757
1335.4820	1337.4355	1361.0307
1364.0048	1366.1371	1378.0694
1418.2004	1425.4185	1463.4834
1501.5183	1505.0292	1507.4496
1525.5559	1539.7572	1550.4803
1553.4036	1614.8855	1650.3900
1674.5008	1678.6302	1681.5281
1693.1161	1699.6681	1740.9751
3106.4703	3165.7825	3187.1084
3187.7225	3190.0969	3198.4021
3200.5890	3204.2155	3206.2550
3210.7224	3211.2051	3219.9182
3221.5945	3224.6233	3232.0271
3234.0182	3246.6025	3249.5166

TS3*RR*

Zero-point correction= 0.679853

Thermal correction to Energy= 0.723217

Thermal correction to Enthalpy= 0.724161

Thermal correction to Gibbs Free Energy= 0.601435

Sum of electronic and zero-point Energies= -3337.487464

Sum of electronic and thermal Energies= -3337.444100

Sum of electronic and thermal Enthalpies= -3337.443156

Sum of electronic and thermal Free Energies= -3337.565882

Cartesian coordinates

C	-1.353254	1.369625	1.227345
O	-1.326074	0.986703	2.404946
C	-0.706855	2.426706	0.587698
H	-0.975588	2.641318	-0.438573
C	1.230835	0.884996	-0.042541
H	1.582142	1.258361	0.922000
C	0.961835	-0.459345	0.020991
C	0.134016	3.403748	1.253595
C	0.675143	3.216203	2.543421
C	0.516621	4.561091	0.547506
C	1.541583	4.157835	3.091641
H	0.409615	2.320848	3.094577

C	1.380647	5.496422	1.102015
H	0.134771	4.707070	-0.461166
C	1.898698	5.304582	2.382661
H	1.945106	3.991642	4.086783
H	1.656102	6.377273	0.529029
H	2.574970	6.033411	2.817813
C	1.615733	1.830515	-1.118636
C	2.752586	2.595470	-0.812641
C	0.962691	2.072309	-2.335525
C	3.253756	3.534496	-1.709323
H	3.247480	2.452928	0.144676
C	1.451562	3.026999	-3.219344
H	0.072361	1.515969	-2.589054
C	2.602557	3.755299	-2.917359
H	4.138501	4.105734	-1.448551
H	0.926265	3.204914	-4.152210
H	2.977949	4.497008	-3.614829
S	0.355376	-1.492643	-1.269555
S	1.532521	-1.275886	1.506430
O	-0.688080	-2.382872	-0.754798
O	-0.006916	-0.612351	-2.388381
O	1.106878	-0.521784	2.682095
O	1.228888	-2.702900	1.384330
C	3.308303	-1.088058	1.407520
C	3.899267	0.020397	2.011749
C	4.056869	-2.031306	0.710470
C	5.275222	0.193251	1.893469
H	3.290390	0.721288	2.575544
C	5.432317	-1.845648	0.600882
H	3.572835	-2.898286	0.271425
C	6.037657	-0.734843	1.185267
H	5.751684	1.048538	2.360312
H	6.027923	-2.572352	0.058157
H	7.109860	-0.594628	1.095166
C	1.738442	-2.483473	-1.777523
C	2.794004	-1.851926	-2.432329
C	1.753750	-3.839497	-1.471167
C	3.903356	-2.611278	-2.787947
H	2.746755	-0.787775	-2.648378
C	2.869625	-4.588244	-1.839117
H	0.917195	-4.276991	-0.938071
C	3.939475	-3.974413	-2.489764
H	4.739342	-2.140392	-3.293368
H	2.906068	-5.647745	-1.610406

H	4.808894	-4.561689	-2.766362
C	-4.567623	-4.796119	-0.010169
C	-4.175830	-5.085692	1.300429
C	-3.501056	-4.143487	2.072536
C	-3.223290	-2.907652	1.502493
C	-3.630674	-2.621852	0.193161
C	-4.303983	-3.556661	-0.583887
H	-5.087571	-5.549192	-0.591857
H	-4.395317	-6.059463	1.723784
H	-3.192348	-4.370621	3.087046
H	-4.607133	-3.322928	-1.598438
C	-2.573134	-0.673264	0.768396
C	-2.590705	0.742543	-1.045706
C	-3.207667	-0.633480	-1.443995
H	-2.543028	-1.194308	-2.106429
S	-2.368073	-1.538133	2.240517
N	-3.282592	-1.322405	-0.156083
N	-2.118761	0.496776	0.343981
H	-1.722115	0.941744	-1.675655
C	-3.563212	1.898004	-1.109060
C	-4.743285	1.870790	-0.361943
C	-3.293393	2.990222	-1.931185
C	-5.641520	2.929425	-0.437141
H	-4.958070	1.021468	0.283645
C	-4.194345	4.050133	-2.009698
H	-2.373313	3.012483	-2.511191
C	-5.368240	4.020220	-1.262628
H	-6.554743	2.905443	0.148112
H	-3.975862	4.897906	-2.650513
H	-6.070004	4.845748	-1.320248
H	-4.197294	-0.523401	-1.889572

Vibrational frequencies

-116.8945	-6.1336	16.8015
26.2084	27.6657	30.4165
34.2296	36.1287	39.5177
42.4825	45.2272	51.6171
63.0506	66.3778	68.0814
69.9910	78.4981	84.5463
88.0278	100.4469	109.3852
121.1172	130.3898	138.1936
166.0950	171.2875	180.1174
184.4412	192.7640	197.0414
207.2106	210.5681	220.1300
232.7618	235.6222	240.2951

251.8643	257.7215	269.6558
281.3319	290.5734	318.2291
321.8164	326.1728	335.5147
347.1075	364.5712	395.1548
405.7308	415.3190	416.1045
416.2684	419.0735	427.7919
431.3275	432.9635	436.4427
452.6786	465.4663	483.1216
505.0678	518.3976	525.5020
532.1796	535.6777	548.9938
553.0066	568.7919	578.6480
583.9594	597.6959	600.1708
619.4014	621.5202	622.2165
626.6484	629.2939	635.9388
636.8775	640.1454	682.2411
699.8838	704.7551	706.3533
711.0206	712.8571	717.7376
720.6149	730.8505	731.4293
736.9253	743.4157	753.8243
770.0499	772.7479	777.5081
785.2930	787.4315	789.9380
802.7475	818.0412	834.7610
869.5240	870.9553	872.7378
874.2926	877.2205	877.4435
878.2177	925.7198	930.7128
948.5591	951.7518	957.7237
962.0943	966.2281	973.3988
989.5487	991.2451	996.1990
1001.8642	1003.2374	1007.3413
1008.1962	1009.3832	1012.2875
1014.1002	1015.7262	1015.9559
1018.6836	1019.2421	1027.6406
1027.9595	1033.8949	1039.9854
1040.5564	1051.0597	1058.1531
1061.7153	1063.3722	1069.4495
1071.0677	1075.8627	1078.6869
1105.0718	1112.4499	1115.3743
1116.6383	1118.4987	1129.1392
1130.6689	1131.7132	1160.3200
1161.4752	1166.6122	1173.1971
1176.8242	1180.2709	1181.6115
1185.1817	1188.0144	1188.2212
1190.8916	1199.6537	1201.4443
1204.8269	1215.4559	1221.4890

1223.0857	1227.1633	1249.7665
1259.2352	1299.8146	1305.2092
1311.2541	1325.8200	1331.7093
1334.5024	1334.9943	1338.1394
1340.8499	1347.5001	1359.9766
1362.9642	1363.9779	1365.5361
1369.5761	1369.9823	1394.4336
1397.5412	1418.7301	1467.2261
1473.3242	1496.3909	1497.9558
1499.2605	1503.8944	1515.7944
1517.9493	1526.4167	1527.6497
1530.2723	1540.5470	1548.9581
1551.4972	1560.6600	1571.6846
1623.1755	1653.6128	1669.4970
1673.4082	1673.7847	1676.5256
1677.2707	1680.6626	1681.8924
1685.1236	1691.7246	1695.3657
1704.7977	1735.8104	3117.9467
3164.3416	3168.4137	3181.1248
3186.3544	3190.0434	3192.0704
3200.9953	3205.3746	3206.2595
3210.0280	3210.8853	3212.4456
3214.5517	3214.7210	3219.3206
3223.7779	3227.1022	3227.2228
3228.3151	3228.3466	3229.4062
3229.8740	3235.4687	3235.6324
3236.1819	3237.1782	3239.5111
3241.0463	3243.4400	3247.5136
3251.2939	3252.6174	3295.0818

M3*RR*

Zero-point correction= 0.684112

Thermal correction to Energy= 0.727465

Thermal correction to Enthalpy= 0.728409

Thermal correction to Gibbs Free Energy= 0.605947

Sum of electronic and zero-point Energies= -3337.521177

Sum of electronic and thermal Energies= -3337.477824

Sum of electronic and thermal Enthalpies= -3337.476879

Sum of electronic and thermal Free Energies= -3337.599342

Cartesian coordinates

C	0.345037	-1.034212	-0.996773
O	0.018295	-0.928942	-2.161349
C	1.739744	-0.783320	-0.474019
H	1.754345	-0.935845	0.604093

C	2.084896	0.699771	-0.774985
H	2.011273	0.815350	-1.860522
C	1.035881	1.666003	-0.226788
C	2.686284	-1.780045	-1.127606
C	2.961685	-1.728684	-2.497085
C	3.282699	-2.775210	-0.352063
C	3.822544	-2.657044	-3.075763
H	2.491832	-0.968982	-3.114374
C	4.141363	-3.706372	-0.931215
H	3.072664	-2.822893	0.713277
C	4.414292	-3.648781	-2.295124
H	4.031090	-2.606013	-4.139681
H	4.594583	-4.475392	-0.313119
H	5.085538	-4.371319	-2.748305
C	3.516452	1.049403	-0.387094
C	4.166980	0.478752	0.709212
C	4.189603	2.019514	-1.136469
C	5.462767	0.866777	1.044760
H	3.659355	-0.263042	1.318743
C	5.482280	2.409813	-0.801596
H	3.680857	2.472527	-1.984819
C	6.125304	1.831559	0.291765
H	5.953847	0.412241	1.899745
H	5.989269	3.164375	-1.395153
H	7.134750	2.131756	0.554559
S	1.053175	1.992768	1.458606
S	0.570163	2.978602	-1.245060
O	1.296041	0.690783	2.139099
O	1.903737	3.093355	1.941013
O	0.895382	4.299632	-0.679312
O	1.049480	2.680290	-2.609544
C	-1.225199	2.971245	-1.348583
C	-1.873629	1.872593	-1.909587
C	-1.936772	4.058153	-0.856636
C	-3.263494	1.866882	-1.965683
H	-1.292361	1.038428	-2.295240
C	-3.329594	4.040924	-0.914462
H	-1.397938	4.892830	-0.422111
C	-3.991378	2.947990	-1.465046
H	-3.784488	1.023602	-2.408915
H	-3.894457	4.880760	-0.522637
H	-5.075776	2.935352	-1.508568
C	-0.630428	2.474516	1.850075
C	-1.687858	1.654287	1.457294

C	-0.853993	3.639703	2.570702
C	-2.987196	1.996234	1.806915
H	-1.486755	0.792216	0.827717
C	-2.162597	3.981244	2.915556
H	-0.009179	4.263290	2.842136
C	-3.222449	3.160356	2.541582
H	-3.816701	1.372493	1.486815
H	-2.351613	4.892115	3.473834
H	-4.238355	3.433682	2.808228
C	-6.334405	-2.737959	0.392358
C	-6.487856	-2.657849	-0.997760
C	-5.413450	-2.356132	-1.826622
C	-4.176276	-2.137381	-1.229278
C	-4.032291	-2.218186	0.161482
C	-5.103578	-2.518767	0.996884
H	-7.192246	-2.976213	1.010672
H	-7.462514	-2.832917	-1.438667
H	-5.534106	-2.294239	-2.902013
H	-4.975825	-2.578993	2.071925
C	-1.904457	-1.688038	-0.482911
C	-0.536264	-1.661336	1.401346
C	-2.021360	-1.900785	1.820259
H	-2.421697	-1.076141	2.414816
S	-2.646151	-1.735408	-2.025165
N	-2.714979	-1.955557	0.528321
N	-0.643337	-1.446970	-0.079017
H	-0.156131	-0.740737	1.848787
C	0.388792	-2.804842	1.742405
C	1.315593	-2.630504	2.771531
C	0.323621	-4.020609	1.059469
C	2.166206	-3.676421	3.125057
H	1.381521	-1.667822	3.272182
C	1.181450	-5.059049	1.407304
H	-0.385578	-4.157125	0.246043
C	2.100761	-4.889136	2.442229
H	2.889118	-3.537596	3.921866
H	1.136227	-5.999250	0.868000
H	2.769833	-5.700208	2.710158
H	-2.148898	-2.845287	2.351829

Vibrational frequencies

4.2736	23.9538	32.1358
34.3182	38.3598	42.9416
45.9845	50.9988	58.8525
64.8879	68.9971	70.9292

76.8750	83.5247	85.0392
85.9664	89.7973	101.0975
113.2053	121.1086	137.7526
147.6537	163.8177	169.5602
183.0519	184.7591	190.9398
201.5460	204.9102	212.8741
214.2824	224.8635	227.2597
246.9235	249.6851	255.3007
261.3223	285.0549	287.7878
305.8424	313.3748	323.5315
334.3338	336.1833	350.1297
377.4077	402.1863	410.8248
413.3494	415.1013	420.0803
427.4017	429.5954	431.6676
433.4129	456.7549	474.0698
479.4114	489.2900	517.1242
519.9224	530.3636	537.6582
545.7501	547.7304	560.1899
572.7019	590.8191	591.6806
598.7931	611.8314	618.6912
623.0155	624.5761	626.2395
627.9987	629.7742	636.2588
651.4235	693.9331	701.8343
706.4654	713.4453	715.9656
718.0395	718.8178	726.3566
729.3170	730.8438	736.5786
751.8032	765.9583	769.7513
779.8552	787.1553	790.4305
797.4400	805.5569	826.2446
863.6284	865.3250	870.2808
877.0114	878.7643	885.3385
891.4393	891.9344	933.2354
939.7809	944.5121	951.4716
956.1606	969.0139	980.7969
981.6137	993.6623	994.6496
997.2784	1003.5807	1004.5481
1005.8050	1012.0884	1014.4837
1017.3344	1018.1844	1019.2324
1019.7138	1020.2302	1024.4048
1026.9722	1031.5843	1031.7380
1039.0113	1054.9480	1057.9312
1061.0523	1064.6333	1065.4924
1065.8922	1069.2576	1074.4069
1077.7049	1088.5467	1105.6645

1110.0426	1111.9030	1113.0850
1115.7200	1127.7975	1129.4924
1141.2602	1150.1684	1152.2422
1159.0247	1166.2589	1174.8573
1175.1895	1178.1711	1180.8528
1186.8966	1192.4133	1194.4778
1198.2721	1199.8534	1208.4654
1212.9621	1218.6518	1224.6885
1232.9096	1250.6520	1255.8740
1264.8411	1270.1153	1294.5028
1301.9785	1310.7247	1327.2567
1332.0143	1335.7974	1337.1746
1337.7128	1341.0209	1352.8362
1359.1986	1362.0982	1364.1337
1365.2440	1369.2192	1371.2370
1376.1171	1404.0090	1430.0116
1434.0350	1463.0227	1495.4632
1496.0557	1505.9022	1506.6841
1506.8093	1516.8780	1521.7350
1528.3253	1531.7437	1533.0536
1546.0117	1553.2894	1557.8082
1611.7909	1673.3011	1677.8965
1678.7022	1678.7720	1680.1888
1681.3815	1682.3312	1682.8680
1689.7890	1692.6668	1698.6490
1700.3116	1821.8991	3114.8151
3127.8149	3159.3229	3179.5355
3185.8449	3189.4395	3190.6332
3199.5717	3200.1099	3200.2556
3205.3506	3205.9883	3206.0790
3206.8102	3207.4035	3211.4586
3211.9165	3214.1074	3214.6770
3217.1403	3217.3196	3222.4588
3225.0630	3226.2194	3229.0382
3231.1037	3233.2519	3235.4834
3235.7331	3239.1120	3239.6745
3247.8724	3251.3201	3256.4461

TS3*RS*

Zero-point correction= 0.681032

Thermal correction to Energy= 0.724635

Thermal correction to Enthalpy= 0.725579

Thermal correction to Gibbs Free Energy= 0.602589

Sum of electronic and zero-point Energies= -3337.495420

Sum of electronic and thermal Energies= -3337.451817

Sum of electronic and thermal Enthalpies= -3337.450872

Sum of electronic and thermal Free Energies= -3337.573863

Cartesian coordinates

C	1.974557	1.219658	-0.386321
O	2.563393	1.314538	-1.468728
C	1.149765	2.144713	0.290103
H	0.843562	1.876123	1.293935
C	-0.846712	1.490946	-0.506010
H	-1.180906	2.243355	0.206908
C	-1.215078	0.194825	-0.097528
C	1.126626	3.575234	-0.000248
C	1.717825	4.161139	-1.133382
C	0.394108	4.405006	0.867930
C	1.586535	5.525346	-1.370215
H	2.264351	3.532937	-1.826012
C	0.259992	5.766730	0.621172
H	-0.074269	3.960484	1.744293
C	0.859468	6.337033	-0.500682
H	2.050556	5.958568	-2.251727
H	-0.311546	6.384390	1.307711
H	0.758492	7.399978	-0.695706
C	-0.732228	2.060935	-1.866537
C	0.021903	1.509457	-2.910384
C	-1.347886	3.305767	-2.070344
C	0.126882	2.173706	-4.127237
H	0.532557	0.567331	-2.771816
C	-1.256287	3.960132	-3.293324
H	-1.894488	3.768561	-1.252570
C	-0.516451	3.393648	-4.327685
H	0.718228	1.733895	-4.924043
H	-1.746191	4.918871	-3.429552
H	-0.431311	3.903931	-5.282083
S	-1.722436	0.021327	1.570214
S	-1.196025	-1.288239	-1.037319
O	-1.324819	-1.303126	2.071215
O	-1.245585	1.208621	2.302037
O	-1.235395	-0.940525	-2.460986
O	-0.127602	-2.201002	-0.597695
C	-2.746179	-2.083156	-0.657123
C	-3.916173	-1.518481	-1.163186
C	-2.754852	-3.251380	0.094396
C	-5.128334	-2.141643	-0.894851
H	-3.871584	-0.604785	-1.748731

C	-3.976151	-3.873070	0.346952
H	-1.820235	-3.649876	0.472282
C	-5.155296	-3.317698	-0.143224
H	-6.051360	-1.712645	-1.269851
H	-4.004478	-4.787500	0.929813
H	-6.104989	-3.801164	0.062783
C	-3.508197	0.071233	1.608379
C	-4.172007	1.135109	0.999801
C	-4.192241	-0.952572	2.250555
C	-5.560598	1.165342	1.036692
H	-3.615729	1.915872	0.489016
C	-5.584699	-0.908031	2.282915
H	-3.639414	-1.771889	2.696806
C	-6.264935	0.144640	1.677990
H	-6.093804	1.982089	0.562305
H	-6.134768	-1.704948	2.772394
H	-7.349452	0.170846	1.699660
C	3.207791	-5.715045	-0.799960
C	3.522304	-5.426248	-2.132024
C	3.487091	-4.119647	-2.611109
C	3.124306	-3.110931	-1.727733
C	2.821014	-3.406399	-0.392102
C	2.855873	-4.708751	0.092865
H	3.239131	-6.742067	-0.453699
H	3.794872	-6.231287	-2.805011
H	3.725825	-3.895784	-3.644923
H	2.614227	-4.923660	1.127974
C	2.493123	-1.144587	-0.431379
C	1.803499	-0.457720	1.652488
C	1.880825	-2.009637	1.610562
H	0.878800	-2.445870	1.599428
S	2.988806	-1.373283	-2.060789
N	2.517803	-2.247107	0.312331
N	2.033038	-0.088139	0.226764
H	0.801693	-0.157144	1.949201
C	2.811360	0.209035	2.560233
C	2.358732	1.023626	3.596825
C	4.182942	0.013015	2.380596
C	3.270262	1.637169	4.453881
H	1.289460	1.179047	3.724395
C	5.092192	0.626688	3.235077
H	4.542472	-0.617811	1.570161
C	4.636035	1.438641	4.273595
H	2.912883	2.272295	5.257662

H	6.156658	0.473191	3.091363
H	5.347211	1.916957	4.939165
H	2.487964	-2.413174	2.421831

Vibrational frequencies

-247.3688	14.9287	23.9939
27.1519	28.1403	30.5453
35.7794	41.4860	47.8368
50.8487	55.8524	60.8851
64.6343	77.4311	78.3963
81.6041	84.1721	98.4381
101.1141	112.2565	123.3775
133.5751	142.1405	158.3991
177.5054	182.0148	183.7196
186.5788	192.7093	202.7667
206.2677	219.6382	231.0994
233.6550	238.1921	251.3969
258.8494	263.0846	286.7993
293.5412	307.7265	317.7941
322.7287	330.9434	340.6455
347.9885	370.1108	386.1510
399.4754	407.8397	411.2147
415.3540	416.6172	431.7678
438.4206	440.5235	458.9604
464.4560	472.2005	491.7335
505.9484	522.9721	531.2070
534.7451	545.5784	548.9886
559.3174	569.3699	581.9278
583.5479	593.8956	604.2051
613.5266	620.1677	621.3191
625.7702	628.1340	633.2668
635.2196	642.3885	688.6747
697.6434	700.4780	705.3701
713.8319	719.9777	720.3658
725.7985	731.6530	734.1412
743.8295	752.6656	770.9722
775.0195	775.2569	784.1244
789.1018	791.4287	801.0307
820.8424	827.2107	868.3806
868.6936	869.8393	874.3299
878.9846	880.1652	889.3236
898.5759	931.6572	936.1463
947.6686	952.5854	955.5885
956.4108	975.8729	982.5878
996.0155	999.7029	1002.5647

1003.4442	1004.3028	1008.5952
1011.9703	1012.5363	1012.9709
1015.6327	1016.4140	1018.7565
1019.5329	1023.1182	1024.8614
1030.7458	1031.6444	1032.2464
1048.6545	1061.1035	1061.5772
1062.3588	1067.6253	1067.9249
1072.6168	1073.9379	1077.6832
1101.7811	1111.2782	1114.8579
1117.6698	1119.6250	1125.2432
1127.3312	1129.1212	1150.9808
1159.6205	1164.9792	1173.6725
1176.7186	1179.6088	1179.8346
1180.5866	1181.3156	1184.5544
1199.8765	1203.0566	1206.5579
1208.5309	1209.5385	1216.9900
1220.9377	1229.0901	1247.1363
1262.5490	1293.9925	1303.7978
1306.8088	1313.9626	1317.3403
1328.6263	1334.3362	1334.7156
1335.5868	1347.8194	1360.8426
1363.4603	1365.2983	1365.5783
1366.3160	1367.0317	1368.5321
1394.5487	1418.4203	1454.7193
1470.7314	1479.2436	1491.8150
1497.6307	1498.7547	1512.7985
1515.2009	1523.6564	1527.4982
1530.9182	1532.0753	1541.1322
1553.2439	1555.1818	1556.4434
1617.8014	1662.0167	1668.6694
1675.7002	1676.9695	1678.9312
1680.6873	1681.3918	1684.0298
1689.2727	1694.1454	1694.5495
1700.4295	1728.3491	3119.3559
3174.9034	3180.0028	3182.9793
3189.9922	3193.2844	3194.4469
3200.6693	3204.3982	3205.3213
3210.6688	3213.8355	3214.2360
3217.0430	3219.3757	3220.4964
3220.6135	3221.8278	3222.3210
3223.9185	3230.7001	3230.8381
3232.6588	3233.8268	3234.0020
3240.4812	3241.0362	3242.4319
3247.2123	3247.3721	3247.4395

3249.6589 3263.9336 3273.3249

M3*RS*

Zero-point correction= 0.683722

Thermal correction to Energy= 0.727453

Thermal correction to Enthalpy= 0.728398

Thermal correction to Gibbs Free Energy= 0.604389

Sum of electronic and zero-point Energies= -3337.521105

Sum of electronic and thermal Energies= -3337.477373

Sum of electronic and thermal Enthalpies= -3337.476429

Sum of electronic and thermal Free Energies= -3337.600438

Cartesian coordinates

C	1.170853	-0.774275	1.133892
O	1.428066	-0.430032	2.267518
C	-0.226162	-0.848632	0.558077
H	-0.207363	-1.272804	-0.444835
C	-0.690680	0.639249	0.434320
H	-0.577629	1.060329	1.442581
C	-2.153241	0.825812	0.105978
C	-1.099232	-1.730797	1.424603
C	-1.773985	-1.238053	2.543974
C	-1.231802	-3.077832	1.080332
C	-2.578762	-2.087082	3.299861
H	-1.717746	-0.183730	2.798641
C	-2.036419	-3.925974	1.838467
H	-0.722645	-3.457328	0.197400
C	-2.713459	-3.430329	2.950409
H	-3.114054	-1.693598	4.158237
H	-2.139412	-4.968298	1.553135
H	-3.348209	-4.084640	3.539845
C	0.309352	1.387279	-0.450081
C	0.278383	1.292001	-1.846286
C	1.316311	2.153904	0.144237
C	1.240532	1.935151	-2.622092
H	-0.500172	0.708177	-2.329564
C	2.282768	2.794763	-0.629813
H	1.341682	2.247840	1.228153
C	2.250540	2.682739	-2.017629
H	1.199769	1.852082	-3.703974
H	3.054075	3.387143	-0.146328
H	2.998267	3.183782	-2.624169
S	-2.879484	2.161009	0.867511
S	-2.907813	0.152201	-1.263735
O	-4.256002	2.325428	0.369627

O	-2.688370	2.082360	2.330375
O	-3.245285	1.105444	-2.342731
O	-2.062204	-0.996163	-1.677360
C	-4.478490	-0.541259	-0.744619
C	-5.655449	-0.081251	-1.321427
C	-4.480718	-1.566215	0.197695
C	-6.864716	-0.660826	-0.942746
H	-5.609523	0.723457	-2.046178
C	-5.692604	-2.138493	0.568592
H	-3.547027	-1.907541	0.632415
C	-6.883522	-1.686336	-0.000272
H	-7.792163	-0.307472	-1.381639
H	-5.704239	-2.937218	1.303841
H	-7.827873	-2.133247	0.294288
C	-1.927523	3.603599	0.374671
C	-1.297221	4.382128	1.338048
C	-1.753632	3.847002	-0.987072
C	-0.471349	5.428778	0.929360
H	-1.445022	4.150948	2.387328
C	-0.922357	4.887413	-1.384199
H	-2.232455	3.194353	-1.714688
C	-0.279793	5.675034	-0.427177
H	0.029703	6.042201	1.671377
H	-0.763090	5.078034	-2.440698
H	0.375544	6.480685	-0.743190
C	7.906626	0.286185	-0.530589
C	7.982874	0.821708	0.761485
C	6.877977	0.831336	1.604920
C	5.689961	0.291611	1.122599
C	5.622022	-0.241001	-0.170935
C	6.724743	-0.254535	-1.019371
H	8.786632	0.292083	-1.163377
H	8.920740	1.235274	1.114257
H	6.939157	1.244452	2.605288
H	6.658623	-0.671759	-2.017729
C	3.486569	-0.575864	0.568412
C	2.222077	-1.464636	-1.167679
C	3.722702	-1.382828	-1.585055
H	3.860916	-0.785459	-2.486969
S	4.139774	0.159704	1.969241
N	4.338774	-0.714693	-0.433463
N	2.253641	-1.015484	0.260375
H	1.647292	-0.726041	-1.731448
C	1.608557	-2.834170	-1.324653

C	0.567831	-3.014859	-2.235298
C	2.059958	-3.910076	-0.556727
C	-0.013153	-4.272146	-2.388341
H	0.186226	-2.166040	-2.797085
C	1.473432	-5.162616	-0.705547
H	2.855469	-3.766940	0.170933
C	0.439323	-5.344911	-1.624565
H	-0.826744	-4.406030	-3.092827
H	1.818236	-5.995559	-0.102161
H	-0.018202	-6.322240	-1.737294
H	4.170344	-2.370711	-1.716209

Vibrational frequencies

10.4463	14.3232	25.8613
31.5632	34.8141	40.1140
49.1193	49.8113	58.7301
60.5426	62.3650	64.7879
68.1571	75.1344	80.0116
88.7729	90.1739	94.3876
98.6077	109.4420	117.6775
126.9074	143.2099	164.2681
174.1937	179.5281	188.5395
191.7816	200.3701	212.3717
219.1240	223.3193	231.1410
245.9031	253.4499	261.7971
264.4337	276.9336	287.0845
301.0056	307.6703	318.4633
323.5437	324.7067	350.9731
376.5835	400.6245	410.6831
412.5835	413.2644	414.4239
414.5245	433.5831	434.6182
441.4036	457.8473	471.2339
476.0099	492.8418	504.4040
518.9675	527.7363	543.3999
545.7116	551.0906	565.5849
570.9770	581.7410	587.4637
600.2977	614.7868	622.4062
623.5053	623.8614	626.8748
629.4660	634.6818	647.0014
655.5956	684.8143	703.2999
706.3699	707.3524	715.2936
716.2685	720.4901	727.1114
729.6568	732.0903	741.9566
749.5898	765.8546	767.4031
774.0225	781.3476	787.5759

796.1293	816.8862	835.5418
860.2849	866.9500	869.5956
872.2787	878.3847	878.7147
889.9374	897.5805	924.4251
940.7186	945.6054	953.3204
957.0861	959.8198	983.6012
991.5301	992.3511	995.0574
997.4641	1002.3739	1004.4195
1007.1974	1007.7935	1014.1075
1014.7554	1015.5792	1017.5811
1018.5663	1019.8487	1021.7868
1021.9990	1025.3754	1032.3162
1037.7860	1059.8751	1061.2039
1061.6739	1063.8456	1066.2998
1067.0947	1069.2377	1070.3079
1073.2632	1089.3066	1107.8110
1112.0402	1115.2773	1117.4272
1119.9739	1125.4908	1127.6126
1147.8913	1148.5156	1151.5917
1172.3934	1172.7724	1174.0097
1174.8823	1178.5477	1186.3680
1195.0163	1199.4298	1200.9196
1201.8600	1203.7388	1209.8307
1210.1154	1223.3905	1234.4417
1238.4207	1247.5526	1251.5348
1255.5644	1274.0823	1287.4164
1303.9805	1317.6151	1323.2786
1327.4387	1337.6261	1339.6956
1341.4437	1349.5621	1357.0757
1360.3231	1361.1117	1364.7872
1367.3596	1367.5841	1373.3462
1390.1221	1403.1583	1405.8079
1420.7847	1465.3431	1497.8338
1498.8062	1502.7095	1503.9948
1507.5912	1515.9592	1521.2030
1532.1329	1533.3659	1534.0464
1545.7696	1550.9068	1553.6661
1612.3905	1670.2818	1674.7405
1678.0679	1680.5566	1682.2264
1682.8078	1683.0778	1683.2181
1690.8080	1692.0822	1692.4701
1695.7113	1831.7933	3076.1170
3127.5198	3151.4905	3187.8080
3190.7678	3192.3902	3197.9891

3198.1729	3198.3395	3200.7582
3201.1884	3202.2811	3202.7753
3204.7588	3210.2260	3212.2261
3213.6306	3213.9541	3219.2823
3223.0232	3223.2185	3224.6010
3225.7866	3226.6869	3227.9142
3230.5887	3234.2561	3235.2117
3237.0543	3243.6014	3244.3397
3247.4660	3258.9461	3264.5357

TS3*SR*

Zero-point correction= 0.680759

Thermal correction to Energy= 0.724394

Thermal correction to Enthalpy= 0.725339

Thermal correction to Gibbs Free Energy= 0.602304

Sum of electronic and zero-point Energies= -3337.489125

Sum of electronic and thermal Energies= -3337.445490

Sum of electronic and thermal Enthalpies= -3337.444546

Sum of electronic and thermal Free Energies= -3337.567581

Cartesian coordinates

C	-7.552167	0.791874	0.663830
C	-7.495170	-0.588607	0.443458
C	-6.319660	-1.200231	0.018147
C	-5.200668	-0.399922	-0.180755
C	-5.265657	0.980367	0.049118
C	-6.437062	1.599518	0.471372
H	-8.481106	1.242725	0.994794
H	-8.379686	-1.193723	0.607693
H	-6.274799	-2.270547	-0.151875
H	-6.472318	2.669224	0.644993
C	-3.075725	0.728008	-0.591420
C	-2.049653	2.796082	-0.573124
C	-3.573176	2.958946	-0.248878
H	-4.114235	3.495790	-1.030767
S	-3.592358	-0.905595	-0.728399
N	-4.030550	1.570714	-0.196817
N	-1.918159	1.336128	-0.829260
H	-1.799597	3.324382	-1.496652
C	-1.187959	3.310025	0.560827
C	-0.460274	4.487168	0.389805
C	-1.212543	2.684938	1.811260
C	0.222748	5.052957	1.465590
H	-0.434240	4.968495	-0.584617
C	-0.526573	3.249261	2.882899

H	-1.748356	1.747835	1.938714
C	0.182561	4.439798	2.714698
H	0.783127	5.971460	1.325047
H	-0.546067	2.759128	3.850717
H	0.710669	4.880715	3.553915
C	0.377631	1.325132	-1.627394
H	0.388648	2.358057	-1.293338
O	-1.082370	-0.550787	-1.759960
C	-0.832974	0.623610	-1.474090
H	-3.726356	3.449647	0.713286
C	1.340691	1.003555	-2.677151
C	2.209414	2.018486	-3.117582
C	1.486240	-0.276443	-3.237191
C	3.178427	1.773047	-4.081387
H	2.123319	3.009653	-2.677255
C	2.461651	-0.518947	-4.200152
H	0.842932	-1.077169	-2.896620
C	3.310862	0.498019	-4.631073
H	3.835687	2.576751	-4.400161
H	2.564757	-1.519888	-4.609060
H	4.069308	0.300413	-5.382071
C	4.756431	1.723911	-0.644657
C	3.646966	0.881354	-0.633759
C	2.530877	1.199675	0.150878
C	2.541148	2.399489	0.878960
C	3.645091	3.240981	0.859794
C	4.764441	2.899684	0.099941
H	5.614594	1.461188	-1.255627
H	3.639176	-0.005654	-1.257723
H	1.669470	2.664718	1.470077
H	3.630331	4.159783	1.438208
H	5.632175	3.551517	0.081624
C	1.292728	0.396768	0.250000
H	0.518758	0.914016	0.810993
C	1.165767	-0.996958	0.329658
S	2.418990	-2.196815	0.071809
S	-0.208378	-1.559452	1.293553
O	0.228936	-2.095465	2.593166
O	1.853579	-3.479236	0.510535
O	-1.152024	-0.427878	1.369257
O	2.957676	-2.133603	-1.291422
C	-1.075353	-2.880117	0.457379
C	-2.093437	-3.470106	1.203578
C	-0.849437	-3.223122	-0.868597

C	-2.920626	-4.408375	0.594270
H	-2.240510	-3.193619	2.242977
C	-1.678192	-4.169170	-1.465357
H	-0.058725	-2.738905	-1.428506
C	-2.716670	-4.752071	-0.741363
H	-3.719242	-4.873207	1.162851
H	-1.513341	-4.446049	-2.501144
H	-3.363407	-5.482981	-1.216069
C	3.759210	-1.784390	1.182784
C	5.056777	-1.771137	0.683465
C	3.481312	-1.547331	2.526660
C	6.108310	-1.506363	1.557147
H	5.227771	-1.952321	-0.372351
C	4.541392	-1.280046	3.386965
H	2.454258	-1.568999	2.883174
C	5.849892	-1.260046	2.903551
H	7.126663	-1.486128	1.183858
H	4.346154	-1.086266	4.436323
H	6.671162	-1.048025	3.580504

Vibrational frequencies

-242.4528	6.9472	22.6208
27.1232	33.2618	34.2779
46.2257	47.1635	51.2963
55.4871	58.6293	62.3284
71.0768	81.0067	83.8830
85.6785	91.1555	95.3362
106.0976	116.2198	118.5098
122.5584	129.5832	156.7185
165.6505	171.1338	178.4788
187.5068	194.0359	198.4756
206.5904	210.4632	219.3047
231.9842	238.7668	251.1895
259.6546	271.6412	281.2589
284.9249	305.5513	311.8392
317.6046	327.7055	338.6948
339.8604	350.7558	376.2466
400.3717	410.0900	413.5205
417.7890	421.0250	429.7090
430.4514	433.2792	452.2089
455.9886	491.3467	510.7948
523.8070	528.4799	528.7304
540.0657	546.6123	548.9452
554.7585	571.4362	581.1565
587.7890	599.2758	609.0742

616.5662	620.6843	623.0343
625.3954	628.5312	632.2798
636.7046	649.1059	694.8826
705.0673	707.5785	709.0463
714.8074	716.4650	720.9882
728.7139	731.3150	732.1005
741.6346	750.5551	766.1920
776.3289	777.0933	783.3461
789.1346	792.2243	799.5744
820.4585	851.2709	860.8290
870.9756	871.6506	876.6556
876.9252	881.6105	883.6777
889.3438	927.5808	934.8991
948.3649	952.8200	966.4515
967.0324	968.6973	981.9573
983.8762	991.4206	1000.5931
1004.8931	1008.8401	1010.6432
1012.0505	1013.7835	1014.2922
1014.4184	1016.0856	1016.8933
1020.6234	1026.4180	1027.5398
1028.7646	1033.3372	1034.9786
1040.2256	1056.2453	1061.7766
1062.6806	1064.5058	1067.2754
1068.6804	1069.3621	1076.6705
1104.7270	1111.1680	1115.6415
1120.0524	1121.0106	1122.1522
1128.3884	1132.7924	1148.9055
1159.7280	1163.1962	1173.6946
1174.2405	1176.6250	1178.2935
1180.0882	1184.4127	1185.0026
1200.9934	1202.9269	1204.2868
1208.0391	1210.4442	1224.3391
1229.0844	1232.7434	1244.8601
1262.1314	1275.0273	1299.6045
1307.9829	1311.2229	1315.2836
1327.3580	1338.1904	1339.6308
1342.3995	1342.7012	1357.9060
1359.1050	1363.3332	1364.0517
1368.0351	1368.8384	1376.2523
1392.6478	1419.3666	1457.0950
1469.8953	1475.4388	1494.1087
1498.3848	1504.0240	1513.3389
1517.9007	1523.9019	1525.2045
1531.4541	1535.4600	1540.0853

1550.1233	1550.6490	1558.7175
1616.5210	1660.7156	1668.9166
1674.9829	1675.8801	1678.8928
1679.7293	1681.6391	1683.5118
1685.1328	1692.0917	1694.8169
1695.4668	1740.7374	3123.6537
3128.2677	3187.1964	3188.0366
3191.0311	3202.5344	3203.6163
3208.5784	3208.8095	3209.0320
3209.5555	3210.3201	3211.8371
3213.9419	3215.0396	3215.8554
3216.4695	3217.1501	3220.7107
3223.1427	3223.6279	3223.9405
3225.5154	3228.6071	3228.9391
3232.6864	3233.6601	3233.8200
3238.4896	3239.1735	3245.8495
3258.0516	3259.3638	3261.9124

M3*SR*

Zero-point correction= 0.684046

Thermal correction to Energy= 0.727390

Thermal correction to Enthalpy= 0.728334

Thermal correction to Gibbs Free Energy= 0.607392

Sum of electronic and zero-point Energies= -3337.519302

Sum of electronic and thermal Energies= -3337.475958

Sum of electronic and thermal Enthalpies= -3337.475014

Sum of electronic and thermal Free Energies= -3337.595956

Cartesian coordinates

C	-8.608041	0.055450	0.620957
C	-8.460856	-0.392842	1.939899
C	-7.208433	-0.684287	2.468046
C	-6.101914	-0.515584	1.642565
C	-6.258453	-0.064435	0.325999
C	-7.508548	0.228397	-0.208906
H	-9.598694	0.272496	0.238005
H	-9.339277	-0.516025	2.563084
H	-7.096652	-1.032188	3.488539
H	-7.612343	0.576025	-1.230617
C	-3.990663	-0.321977	0.449914
C	-3.053155	0.408874	-1.546225
C	-4.604890	0.347844	-1.675957
H	-4.941753	-0.447693	-2.343323
S	-4.399487	-0.809144	2.038900
N	-5.019957	0.034963	-0.302949

N	-2.823125	-0.225932	-0.207872
H	-2.576519	-0.212579	-2.308026
C	-2.496664	1.814370	-1.567783
C	-1.502112	2.162182	-2.478001
C	-2.948885	2.756965	-0.637814
C	-0.946001	3.440210	-2.451562
H	-1.133270	1.426936	-3.188122
C	-2.400507	4.032940	-0.617655
H	-3.722630	2.494596	0.081275
C	-1.392999	4.373655	-1.522340
H	-0.150366	3.691421	-3.143910
H	-2.750907	4.759360	0.108131
H	-0.955120	5.366101	-1.495208
C	-0.399452	-0.626159	-0.520200
H	-0.432917	0.249466	-1.170798
O	-1.631663	-0.996880	1.537618
C	-1.602724	-0.618053	0.386388
H	-5.020969	1.305478	-1.990913
C	-0.492455	-1.858769	-1.405156
C	-0.120888	-1.757468	-2.748377
C	-0.916874	-3.089880	-0.903352
C	-0.177558	-2.872105	-3.579638
H	0.237622	-0.803693	-3.128565
C	-0.974831	-4.204752	-1.735889
H	-1.192615	-3.182591	0.144423
C	-0.608026	-4.097585	-3.074878
H	0.121190	-2.784592	-4.619182
H	-1.304646	-5.158437	-1.336412
H	-0.651378	-4.967676	-3.721997
C	0.440679	3.046824	1.615696
C	0.317666	1.905884	0.823565
C	0.953739	0.711510	1.178721
C	1.691723	0.689049	2.367918
C	1.827708	1.829546	3.153366
C	1.205525	3.019191	2.778609
H	-0.058392	3.961091	1.307095
H	-0.241792	1.978719	-0.102635
H	2.173758	-0.230925	2.683760
H	2.418830	1.784187	4.063400
H	1.309108	3.910595	3.389511
C	0.912320	-0.544367	0.302243
H	0.893907	-1.405456	0.984980
C	2.138682	-0.738350	-0.569799
S	2.598132	0.408144	-1.741079

S	3.171447	-2.043382	-0.224110
O	2.408009	-3.297905	-0.094383
O	3.052393	-0.180264	-3.009644
O	4.328925	-2.017629	-1.135186
O	1.478992	1.373512	-1.834179
C	3.837142	-1.768209	1.424333
C	3.374441	-2.530529	2.491907
C	4.747217	-0.729417	1.619632
C	3.813047	-2.232996	3.782239
H	2.673487	-3.336338	2.302390
C	5.176992	-0.438164	2.909120
H	5.108320	-0.153842	0.772602
C	4.703985	-1.182809	3.991278
H	3.455602	-2.819180	4.622759
H	5.879907	0.373287	3.069721
H	5.037129	-0.947670	4.997161
C	4.008989	1.320178	-1.110134
C	5.283519	1.009407	-1.573285
C	3.813107	2.233550	-0.074708
C	6.387066	1.619930	-0.978761
H	5.391842	0.280498	-2.367956
C	4.921355	2.835929	0.511978
H	2.807592	2.459419	0.268792
C	6.207018	2.525111	0.065749
H	7.387200	1.382294	-1.326554
H	4.780630	3.545447	1.321366
H	7.069034	2.992148	0.531580

Vibrational frequencies

20.6879	25.6650	35.9574
39.2155	40.1331	46.0121
49.6742	54.7346	55.9317
63.0579	68.9097	70.0014
78.1855	79.7801	80.7979
86.7341	94.9730	103.0292
103.7141	116.0243	123.4322
135.1972	155.3005	177.8852
180.4748	184.7406	190.9398
195.7890	205.0005	212.2670
214.7770	223.3266	226.5516
242.9282	249.6752	264.1309
271.6531	282.3061	288.6877
307.2654	315.0673	318.4474
324.9052	343.0580	352.9531
380.9238	408.9497	414.8180

416.1531	417.8614	425.8915
427.6963	432.3353	436.1459
440.8139	456.5109	461.6934
467.8709	487.2777	503.6242
516.5856	528.4668	540.3649
545.2191	554.8898	560.9149
566.2058	581.0981	586.4617
592.0072	613.1091	620.0652
624.1642	624.6728	627.4344
629.1005	633.5072	644.4671
652.5746	687.2241	705.3381
709.1947	710.4943	719.0350
721.6492	724.3930	727.9488
731.9053	732.4255	736.5567
747.0830	767.2005	771.6573
774.6747	778.5780	790.6782
797.7355	800.3707	841.2657
851.2908	872.6190	874.4233
876.4274	881.4731	882.8055
885.7611	898.1067	931.7270
944.6638	952.8012	955.1565
957.6356	961.9994	974.6607
987.7908	992.6144	998.7627
999.8579	1005.1486	1006.3530
1011.9715	1012.3666	1012.6642
1014.8817	1017.2929	1019.4467
1019.7322	1020.7144	1025.4183
1025.8915	1029.0392	1030.6392
1034.9839	1050.9722	1060.7938
1061.8754	1063.2599	1065.7251
1066.7006	1069.5440	1074.0078
1083.1744	1100.0177	1108.9870
1111.7300	1114.5215	1117.4299
1121.9956	1123.6334	1132.0850
1149.2405	1151.4828	1155.3792
1169.7402	1173.5851	1175.9879
1176.3459	1179.1636	1181.5980
1187.1034	1197.6220	1198.2318
1199.8566	1203.2820	1209.4272
1211.1496	1214.3287	1226.2891
1231.6836	1243.7191	1253.3173
1265.7951	1282.3149	1298.7645
1302.5103	1303.5157	1314.7098
1325.5679	1331.4899	1334.5944

1334.6522	1346.3747	1354.5590
1360.8800	1361.3447	1362.8821
1364.1307	1365.4892	1372.0762
1383.5160	1391.6260	1395.3342
1420.3504	1464.7645	1495.5064
1495.8310	1499.1506	1501.0934
1509.3180	1510.9288	1519.3829
1528.9327	1530.9087	1533.0731
1549.9528	1550.1597	1554.1439
1605.0657	1670.9234	1676.9243
1677.0739	1677.8163	1679.2394
1679.4853	1679.7896	1680.7623
1692.7900	1695.0047	1695.6335
1699.8405	1834.8741	3067.4935
3128.3747	3152.9210	3162.1305
3183.0735	3191.5550	3193.5395
3194.6718	3204.7037	3204.9080
3205.8442	3206.7359	3209.6411
3213.7525	3214.4317	3216.9451
3217.6243	3218.0031	3220.6327
3222.5065	3223.1184	3224.4389
3228.3913	3229.1796	3230.4818
3230.9720	3234.0190	3234.9823
3235.5617	3236.6868	3240.5324
3241.7125	3246.1369	3257.5230

TS3*SS*

Zero-point correction= 0.680250

Thermal correction to Energy= 0.723873

Thermal correction to Enthalpy= 0.724817

Thermal correction to Gibbs Free Energy= 0.602615

Sum of electronic and zero-point Energies= -3337.482476

Sum of electronic and thermal Energies= -3337.438854

Sum of electronic and thermal Enthalpies= -3337.437909

Sum of electronic and thermal Free Energies= -3337.560111

Cartesian coordinates

C	8.089302	-0.682824	0.360505
C	8.077808	-0.056598	-0.890420
C	6.896044	0.089680	-1.610947
C	5.723223	-0.400497	-1.048504
C	5.744323	-1.023009	0.206036
C	6.921280	-1.175890	0.930388
H	9.025016	-0.785503	0.898438
H	9.003805	0.321806	-1.308232

H	6.888796	0.572800	-2.581578
H	6.920990	-1.661058	1.900154
C	3.513988	-1.154915	-0.326004
C	2.395779	-2.049637	1.478456
C	3.929368	-2.239876	1.664593
H	4.248492	-3.275829	1.527596
S	4.091916	-0.383608	-1.748523
N	4.463282	-1.421907	0.572213
N	2.304221	-1.534752	0.073146
H	1.877631	-3.009233	1.522148
C	1.805921	-1.082954	2.483279
C	2.456817	0.124933	2.760125
C	0.621004	-1.388459	3.149244
C	1.921031	1.015397	3.683096
H	3.380512	0.381349	2.244662
C	0.071880	-0.486392	4.060094
H	0.102848	-2.320536	2.942617
C	0.721497	0.713481	4.329208
H	2.431862	1.950311	3.889506
H	-0.869675	-0.722958	4.542981
H	0.296659	1.415099	5.039330
C	-0.066640	-1.864173	-0.320104
H	-0.095525	-2.145143	0.725730
O	1.528207	-1.434197	-2.054138
C	1.206103	-1.632533	-0.880909
H	4.268249	-1.870177	2.632480
C	-1.141944	-2.451451	-1.120687
C	-1.997619	-3.384510	-0.509110
C	-1.358429	-2.150006	-2.475987
C	-2.997233	-4.026387	-1.229295
H	-1.862124	-3.601545	0.546515
C	-2.373708	-2.782319	-3.191214
H	-0.702928	-1.445440	-2.972704
C	-3.191214	-3.729568	-2.578015
H	-3.637784	-4.749807	-0.733658
H	-2.520898	-2.535853	-4.238502
H	-3.975367	-4.225626	-3.141576
C	1.276374	1.998172	-2.636037
C	0.376248	1.161773	-1.983208
C	0.343745	1.111172	-0.585164
C	1.251758	1.893442	0.141313
C	2.142703	2.737781	-0.512695
C	2.155836	2.793357	-1.905864
H	1.287666	2.027803	-3.721013

H	-0.316233	0.556333	-2.552255
H	1.224616	1.864114	1.225908
H	2.820958	3.356583	0.066711
H	2.851296	3.450975	-2.418369
C	-0.623879	0.281929	0.176179
H	-0.281944	0.000673	1.169343
C	-2.009820	0.453725	0.054011
S	-2.966337	-0.175693	1.388408
S	-2.768629	1.670490	-0.949362
O	-2.540506	1.429553	-2.378745
O	-2.187597	-1.295570	1.947840
O	-4.159524	1.783739	-0.490806
O	-3.344066	0.880562	2.343464
C	-1.951479	3.203765	-0.521202
C	-1.348394	3.964557	-1.513245
C	-1.972412	3.605777	0.813180
C	-0.736547	5.164808	-1.155923
H	-1.344205	3.606817	-2.536949
C	-1.363344	4.808125	1.154191
H	-2.441865	2.973136	1.563943
C	-0.746733	5.584791	0.171519
H	-0.249373	5.766821	-1.915884
H	-1.366110	5.139485	2.187327
H	-0.267716	6.519375	0.445581
C	-4.489583	-0.827723	0.720426
C	-4.561893	-1.331184	-0.572993
C	-5.583462	-0.855247	1.581518
C	-5.764628	-1.881402	-1.007887
H	-3.699282	-1.291160	-1.232808
C	-6.776982	-1.414930	1.136301
H	-5.499016	-0.428629	2.575259
C	-6.866777	-1.926682	-0.157202
H	-5.832003	-2.277436	-2.015967
H	-7.638186	-1.441610	1.795345
H	-7.800847	-2.356050	-0.505138

Vibrational frequencies

-260.7509	12.9907	23.0838
30.6262	33.8976	37.1434
44.3803	47.9654	53.1218
57.1956	59.1997	64.6156
70.1513	73.9808	78.6686
81.3025	96.1154	100.3038
104.5846	122.9636	126.3590
130.2460	138.3498	159.6454

164.0879	172.6153	175.5066
180.5558	187.5984	195.2340
202.9590	207.8829	226.0336
233.0154	240.3221	241.8416
262.8840	269.7453	278.2058
287.2294	294.6140	314.0726
323.3877	324.5394	336.4734
345.1691	357.2866	386.3692
411.5446	414.8001	416.8771
418.7706	425.0016	428.7725
433.2778	435.5107	440.9114
454.2037	484.0101	499.9009
514.5629	521.0736	527.9471
542.8565	545.5504	546.9208
555.5836	565.3320	580.0085
583.6827	597.2356	599.4055
614.8641	621.0816	623.8985
625.1331	627.1698	628.0736
634.5047	648.6077	694.2674
706.1017	706.6096	711.0066
714.9081	718.2880	722.0279
726.6797	730.5881	733.3073
735.2562	750.4267	770.6411
771.6740	776.4513	780.5079
786.1091	787.0223	797.6066
822.3511	828.2060	865.3667
867.4697	871.7483	875.1608
879.2335	879.7464	890.7723
903.1333	927.8312	943.1872
952.0101	956.0164	957.2078
969.8476	974.9362	987.8818
991.7024	993.8012	994.4944
996.3455	1004.7574	1005.4783
1011.6113	1014.5492	1015.0545
1016.5334	1018.1900	1018.4751
1020.7236	1020.9857	1026.4304
1026.9448	1030.1842	1035.4379
1040.0183	1044.9345	1059.4740
1061.7473	1064.0244	1064.5635
1068.1247	1070.4995	1073.6794
1104.2531	1109.4115	1113.4253
1116.5429	1119.8654	1122.1943
1124.3092	1129.4207	1152.1425
1154.4998	1158.1806	1165.0029

1171.3757	1172.7926	1176.1184
1182.2114	1184.2372	1187.4932
1190.2520	1198.1890	1204.1517
1204.5322	1208.3584	1213.1526
1216.9527	1233.5431	1244.0998
1256.1946	1286.0940	1293.3320
1299.0472	1301.6756	1312.6434
1327.0136	1338.2984	1338.6431
1338.7443	1340.6692	1349.4240
1358.9633	1360.5595	1360.9888
1363.3916	1367.6753	1368.3650
1390.8601	1416.1144	1447.3512
1457.7149	1467.9648	1497.1349
1499.8572	1504.7954	1507.9026
1512.2836	1515.0052	1527.6250
1531.3341	1533.2543	1536.1938
1548.6445	1551.7214	1555.7585
1607.5084	1661.7410	1668.4669
1675.8357	1679.0938	1679.7591
1681.5979	1682.5179	1683.5187
1683.9667	1691.2816	1693.7714
1698.1497	1739.9352	3116.9544
3151.9573	3185.8892	3189.1932
3195.3447	3197.4200	3197.8095
3200.1786	3202.5778	3206.5095
3207.6045	3210.4173	3212.2423
3213.2415	3216.8128	3217.4935
3218.3128	3220.4894	3222.6555
3223.0458	3225.2431	3227.5930
3228.2145	3229.1357	3230.9427
3232.7708	3234.4868	3243.3846
3243.5413	3246.0664	3247.9939
3249.6062	3249.6726	3271.6039

M3*SS*

Zero-point correction= 0.684445

Thermal correction to Energy= 0.728082

Thermal correction to Enthalpy= 0.729026

Thermal correction to Gibbs Free Energy= 0.604675

Sum of electronic and zero-point Energies= -3337.514598

Sum of electronic and thermal Energies= -3337.470960

Sum of electronic and thermal Enthalpies= -3337.470016

Sum of electronic and thermal Free Energies= -3337.594367

Cartesian coordinates

C	-7.459243	-1.189565	-1.600998
C	-7.547110	0.207853	-1.567423
C	-6.466923	0.989108	-1.172416
C	-5.291245	0.338080	-0.813674
C	-5.214277	-1.059435	-0.846690
C	-6.290723	-1.847627	-1.240185
H	-8.318885	-1.771410	-1.913380
H	-8.473293	0.692257	-1.855068
H	-6.536029	2.070629	-1.147355
H	-6.213636	-2.928897	-1.261799
C	-3.110004	-0.509499	-0.137389
C	-1.919427	-2.462310	0.260092
C	-3.315728	-2.799668	-0.349403
H	-3.894322	-3.464778	0.291860
S	-3.771237	1.066971	-0.266915
N	-3.953964	-1.485162	-0.436065
N	-1.891765	-0.961448	0.203340
H	-1.892700	-2.740005	1.318342
C	-0.796398	-3.154788	-0.474972
C	-0.085641	-4.164536	0.173150
C	-0.492098	-2.826436	-1.797443
C	0.941268	-4.834116	-0.489263
H	-0.328149	-4.417698	1.201648
C	0.529858	-3.500454	-2.458770
H	-1.024184	-2.020637	-2.294217
C	1.250910	-4.499876	-1.804878
H	1.495188	-5.613831	0.022715
H	0.764136	-3.246547	-3.487574
H	2.051149	-5.018368	-2.322973
C	0.370588	-0.668166	1.165615
H	0.567976	-1.481799	0.470239
O	-1.248785	1.106135	0.825690
C	-0.923664	-0.053400	0.723370
H	-3.227230	-3.229003	-1.349934
C	0.192139	-1.266481	2.555695
C	0.885807	-2.431795	2.898539
C	-0.611719	-0.647667	3.517999
C	0.766435	-2.974670	4.175319
H	1.529440	-2.902642	2.160137
C	-0.734509	-1.194619	4.793156
H	-1.139235	0.270609	3.272060
C	-0.048606	-2.360716	5.123936
H	1.312768	-3.877555	4.428677
H	-1.365450	-0.706438	5.528969

H	-0.145454	-2.786648	6.117270
C	4.232665	-2.257204	0.069027
C	3.036868	-1.547713	0.140245
C	2.869865	-0.522002	1.078818
C	3.928906	-0.223192	1.937784
C	5.124994	-0.934762	1.871082
C	5.280444	-1.956794	0.937127
H	4.343767	-3.043461	-0.672306
H	2.238512	-1.786966	-0.561562
H	3.810390	0.584400	2.655625
H	5.935674	-0.691548	2.551161
H	6.211070	-2.513041	0.885015
C	1.588933	0.309277	1.140247
H	1.593023	0.829886	2.101948
C	1.589489	1.417806	0.108454
S	1.843110	3.024162	0.615755
S	1.315098	1.094388	-1.525078
O	0.423856	-0.087958	-1.625685
O	2.275841	2.971200	2.028107
O	0.893485	2.309122	-2.245919
O	2.699229	3.765041	-0.329125
C	2.843099	0.552342	-2.305315
C	2.820962	-0.567289	-3.129675
C	4.018670	1.259665	-2.068821
C	4.004324	-0.992725	-3.728778
H	1.888197	-1.103949	-3.266458
C	5.194854	0.829276	-2.675649
H	4.001640	2.120506	-1.404570
C	5.188909	-0.295624	-3.501443
H	4.002427	-1.871854	-4.365489
H	6.121166	1.365359	-2.496303
H	6.112097	-0.632088	-3.962706
C	0.296282	3.937827	0.645623
C	-0.144033	4.584029	-0.506082
C	-0.448135	3.967178	1.821438
C	-1.356119	5.268138	-0.475549
H	0.457520	4.533451	-1.406172
C	-1.658080	4.655219	1.842441
H	-0.071502	3.460952	2.704007
C	-2.112706	5.303806	0.695274
H	-1.707836	5.779126	-1.366212
H	-2.243488	4.689427	2.755739
H	-3.054471	5.843348	0.715300

Vibrational frequencies

14.6823	19.8011	23.3356
26.9589	31.2009	34.9551
37.2617	41.6287	44.6107
46.9562	50.6899	60.6498
62.1942	73.6755	77.8355
84.3320	95.2711	103.7931
112.4451	121.2761	123.9369
134.2321	157.1159	163.7959
179.4402	185.1451	193.7254
196.4845	200.9540	214.0715
221.8376	231.7278	236.4921
244.7881	248.5313	253.0188
271.0547	274.7037	298.2635
309.5739	315.7275	319.1142
327.5480	335.1048	344.1142
374.3607	402.9222	412.9323
416.7410	418.5212	422.1818
425.7706	428.3034	432.7471
434.7745	456.9426	458.8059
472.8527	507.5664	514.1515
520.3942	528.4993	544.1500
545.6848	549.6575	563.1398
565.1374	580.6579	594.0331
596.1337	613.9916	622.7430
625.0462	625.6801	629.1090
629.6578	633.5790	636.1452
655.1317	702.4907	708.2022
709.0951	712.3026	718.4248
720.3380	724.7202	727.4515
730.6701	732.5490	735.8760
751.7424	769.5130	774.5103
776.0989	780.4853	781.9523
794.5628	810.6030	829.2136
871.1651	873.7678	877.7311
881.3655	883.9867	885.2874
885.8251	887.4371	934.8537
944.9680	954.8680	958.3952
959.8710	961.5467	977.4925
984.2117	993.8776	999.3203
1006.5942	1007.4391	1008.3264
1011.0714	1013.1861	1013.9969
1016.1103	1016.8584	1017.4772
1019.2451	1024.2897	1026.6838
1028.5107	1031.1131	1032.5016

1036.5625	1057.2970	1060.9905
1064.4861	1066.2868	1066.8427
1070.0687	1073.4703	1075.3456
1077.7994	1096.6358	1106.7835
1117.5945	1118.4021	1119.0286
1127.4241	1128.6762	1134.1279
1146.5863	1151.5352	1159.4967
1170.8091	1178.9843	1180.4044
1182.6279	1184.2078	1186.9086
1188.2851	1198.1997	1203.9750
1205.6709	1206.4118	1211.0118
1213.7594	1216.1799	1225.4762
1227.7728	1241.5656	1247.3404
1258.6278	1266.7761	1284.9748
1296.2394	1301.5687	1307.6267
1327.1393	1338.9286	1340.8452
1346.8531	1347.6816	1361.1248
1361.4155	1362.8835	1367.0160
1368.6627	1370.3991	1374.8141
1376.7904	1404.4281	1411.0730
1432.2183	1461.6219	1498.4280
1499.1007	1507.9621	1508.9964
1510.2996	1517.8407	1519.7680
1533.8631	1534.9185	1535.0801
1552.2215	1553.4634	1556.1733
1614.4107	1676.6780	1676.7278
1677.1906	1677.8119	1679.6141
1681.1093	1683.4918	1684.5031
1690.9830	1695.1821	1697.0750
1697.3133	1852.7646	3118.6344
3123.3213	3128.9593	3173.3321
3185.1951	3192.3268	3193.9314
3196.2937	3200.9521	3201.5485
3204.3207	3204.4301	3211.9638
3212.5799	3212.5947	3213.8002
3217.2366	3219.8303	3220.3202
3221.4861	3223.6189	3224.3640
3224.8483	3225.6618	3230.7011
3232.8106	3233.5047	3235.8367
3236.4331	3238.6353	3241.6161
3248.2418	3252.2226	3264.8409

TS4*SR*

Zero-point correction= 0.789585

Thermal correction to Energy= 0.841791
Thermal correction to Enthalpy= 0.842735
Thermal correction to Gibbs Free Energy= 0.701063
Sum of electronic and zero-point Energies= -3849.204827
Sum of electronic and thermal Energies= -3849.152621
Sum of electronic and thermal Enthalpies= -3849.151677
Sum of electronic and thermal Free Energies= -3849.293349
Cartesian coordinates

C	-1.991885	-1.158539	-1.101849
O	-2.266053	-1.235233	-2.278767
C	-0.602564	-0.970734	-0.524516
H	-0.646736	-1.146694	0.545979
C	-0.231729	0.545372	-0.751512
H	-0.037671	0.642842	-1.827214
C	1.107965	0.984507	-0.114452
C	0.339832	-1.996112	-1.118715
C	0.612088	-2.046566	-2.486598
C	0.890824	-2.960405	-0.273867
C	1.427304	-3.048999	-2.999040
H	0.180738	-1.306816	-3.153262
C	1.713789	-3.961351	-0.785405
H	0.663772	-2.926686	0.789807
C	1.978594	-4.009127	-2.151616
H	1.635265	-3.081730	-4.063770
H	2.137271	-4.705881	-0.118474
H	2.614806	-4.790545	-2.556150
C	-1.453783	1.408630	-0.439442
C	-1.790117	1.805668	0.859176
C	-2.326655	1.737413	-1.482594
C	-2.983007	2.481972	1.108546
H	-1.119332	1.610593	1.690087
C	-3.522700	2.407584	-1.235562
H	-2.070436	1.452193	-2.500022
C	-3.862471	2.771082	0.065618
H	-3.220746	2.788880	2.122570
H	-4.185621	2.646560	-2.061379
H	-4.793559	3.292280	0.263273
S	1.359977	0.748871	1.653191
S	1.586525	2.638217	-0.640423
O	1.142890	1.988595	2.411239
O	0.555997	-0.421883	2.056073
O	2.872951	2.917087	0.010831
O	1.501304	2.596658	-2.105394
C	0.481496	3.946768	-0.118094

C	-0.509088	4.377767	-0.996423
C	0.687876	4.561771	1.113570
C	-1.347688	5.416387	-0.605962
H	-0.612855	3.906259	-1.966700
C	-0.153930	5.604219	1.489467
H	1.488620	4.221589	1.757498
C	-1.174795	6.021993	0.637891
H	-2.131075	5.755053	-1.275751
H	-0.007671	6.093151	2.446664
H	-1.829667	6.833576	0.938555
C	3.067967	0.292728	1.859543
C	3.969469	1.243443	2.327958
C	3.440654	-1.023846	1.607506
C	5.286196	0.854967	2.551406
H	3.635368	2.259524	2.503867
C	4.762638	-1.395207	1.829848
H	2.715294	-1.734643	1.224547
C	5.679901	-0.458906	2.302234
H	6.006306	1.579540	2.916368
H	5.076210	-2.412723	1.622697
H	6.712036	-0.752027	2.467433
C	-8.760815	0.038566	0.322327
C	-8.898208	0.054581	-1.071659
C	-7.815172	-0.194781	-1.906511
C	-6.586491	-0.461818	-1.311777
C	-6.458759	-0.479507	0.082996
C	-7.538701	-0.230420	0.923972
H	-9.624346	0.240358	0.945794
H	-9.866682	0.264882	-1.510894
H	-7.923018	-0.181088	-2.984876
H	-7.423307	-0.245652	2.001854
C	-4.319202	-0.931839	-0.573644
C	-3.000256	-1.241449	1.317076
C	-4.443741	-0.819445	1.733487
H	-4.467590	0.171062	2.193838
S	-5.047190	-0.807138	-2.116954
N	-5.145955	-0.768136	0.446200
N	-3.052984	-1.139687	-0.174433
H	-2.281441	-0.512413	1.695766
C	-2.600661	-2.633756	1.745534
C	-1.550067	-2.799170	2.646955
C	-3.277014	-3.750727	1.248240
C	-1.178990	-4.080404	3.053184
H	-1.007950	-1.929283	3.008515

C	-2.903043	-5.026662	1.653236
H	-4.090055	-3.628029	0.535583
C	-1.853278	-5.191911	2.557274
H	-0.358756	-4.206199	3.751984
H	-3.426286	-5.892527	1.261703
H	-1.560483	-6.188824	2.869626
H	-4.908308	-1.556165	2.390432
C	4.182488	-0.457124	-1.324728
C	4.984514	0.655691	-0.939845
C	4.855676	-1.682395	-1.614218
C	6.350285	0.536508	-0.816372
H	4.491659	1.595695	-0.718256
O	2.892767	-0.405580	-1.420248
C	6.221381	-1.799510	-1.492660
H	4.244340	-2.527922	-1.912436
C	6.971657	-0.689639	-1.083272
H	6.957499	1.377897	-0.502817
H	6.727903	-2.735367	-1.698387
N	8.389954	-0.812869	-0.928761
O	8.919697	-1.897465	-1.164399
O	9.033970	0.168221	-0.561520
H	2.085511	0.328096	-0.710901

Vibrational frequencies

-1156.7442	11.6700	17.3235
22.7838	29.0089	31.4487
34.5126	37.3394	40.9357
47.5223	50.4655	54.9497
61.9783	64.3994	66.3732
71.3906	74.9413	78.4565
80.9091	91.5509	95.4673
105.9101	110.3089	113.0914
115.2858	119.9586	126.3522
132.9385	141.0491	156.1028
157.8759	173.3912	180.9818
183.7214	191.9293	199.1785
202.1391	208.1314	213.5687
227.7263	228.8318	236.1313
240.6797	250.6388	252.8173
264.7618	277.7320	279.5274
290.2016	304.3560	308.5941
316.9934	321.9455	326.4573
334.5978	364.1383	386.6834
404.5711	409.2593	412.5214
416.0233	421.1218	422.4288

429.7034	431.3470	433.6018
435.2505	443.1249	450.5698
462.0110	465.5046	472.7564
499.0028	507.9718	518.0890
525.6574	532.3254	540.8158
543.5682	544.8236	556.9581
562.6288	571.6826	588.1724
592.9036	596.3202	616.2199
621.2353	623.9340	626.8231
627.9518	630.6159	635.5399
643.8270	652.3960	661.1058
680.8075	690.5743	705.1845
706.7559	713.9100	716.3384
718.6847	719.4279	720.7718
727.5268	731.6526	738.6617
753.8327	764.0688	766.2978
773.4254	774.8205	776.2274
784.3098	789.6687	802.1321
806.2411	825.1062	844.4956
846.2655	858.5837	859.5467
866.8773	871.6818	873.4993
874.5404	877.0832	884.2512
885.5890	897.4587	904.8719
927.2583	940.6901	944.4311
952.7988	955.7360	968.6338
977.4029	996.1078	996.3276
996.8583	999.6713	1000.4823
1003.5652	1006.6197	1007.6722
1010.7340	1012.1759	1013.9992
1015.2353	1016.4449	1017.4388
1020.1131	1021.0583	1022.0996
1025.5072	1026.4567	1028.6075
1032.7351	1033.3242	1057.7850
1060.2263	1061.7855	1066.1551
1067.5813	1070.0910	1071.6479
1072.2286	1093.8491	1102.5123
1110.3425	1113.1455	1120.3106
1121.7986	1125.5195	1126.5005
1126.7935	1138.2053	1147.2108
1149.1056	1152.2696	1158.9082
1169.3912	1177.5185	1177.6065
1177.7880	1180.0130	1186.5106
1190.8738	1196.8151	1204.5694
1211.6288	1212.1390	1218.0931

1218.8042	1221.6517	1230.9143
1237.9473	1244.2124	1256.6662
1269.3871	1286.4293	1303.9946
1305.4144	1310.0741	1321.6287
1327.8970	1331.7968	1332.3743
1337.4785	1343.8092	1347.0630
1353.9684	1360.6380	1363.3729
1363.8856	1365.0430	1368.3226
1368.4146	1372.8278	1377.6246
1382.7190	1399.5260	1408.3098
1431.4794	1433.9648	1439.0380
1466.4430	1497.0791	1501.0465
1503.9491	1506.6407	1507.8627
1513.9048	1516.0180	1520.8455
1524.5070	1529.7845	1532.9976
1536.8328	1550.0461	1553.8815
1556.1250	1593.1507	1611.3258
1613.4311	1670.2724	1675.5660
1677.1657	1678.1190	1680.2265
1680.6605	1680.8093	1684.3551
1684.8747	1687.6872	1692.1180
1693.1503	1699.3681	1701.7241
1839.0052	3092.4922	3124.3869
3164.0387	3187.0853	3189.3398
3191.5864	3199.3055	3201.9349
3207.9204	3208.8341	3209.4377
3209.4709	3213.3346	3213.5253
3215.6785	3216.4371	3221.6314
3222.9012	3223.5233	3224.7603
3226.2869	3228.5223	3230.6296
3231.0560	3231.3668	3231.6326
3233.6797	3234.8474	3235.3482
3238.5956	3242.4217	3244.3891
3244.6916	3245.7860	3248.1809
3252.0724	3256.7150	3259.3690

M4*SR*

Zero-point correction= 0.794029

Thermal correction to Energy= 0.846765

Thermal correction to Enthalpy= 0.847709

Thermal correction to Gibbs Free Energy= 0.704866

Sum of electronic and zero-point Energies= -3849.205723

Sum of electronic and thermal Energies= -3849.152987

Sum of electronic and thermal Enthalpies= -3849.152043

Sum of electronic and thermal Free Energies= -3849.294886

Cartesian coordinates

C	-2.108239	-1.113656	-1.140410
O	-2.407555	-1.147971	-2.313094
C	-0.709278	-0.924635	-0.592396
H	-0.712429	-1.165072	0.467436
C	-0.376725	0.605168	-0.751990
H	-0.229273	0.759386	-1.828307
C	1.010293	0.958096	-0.174095
C	0.271615	-1.852240	-1.275174
C	0.546693	-1.759677	-2.640175
C	0.882905	-2.850244	-0.514753
C	1.429077	-2.654614	-3.234065
H	0.063327	-0.996265	-3.241958
C	1.768342	-3.744847	-1.109896
H	0.651155	-2.927830	0.546155
C	2.039982	-3.647779	-2.472125
H	1.641314	-2.576279	-4.295366
H	2.240424	-4.518046	-0.511671
H	2.728551	-4.345349	-2.939176
C	-1.573003	1.459258	-0.347364
C	-1.864237	1.817882	0.972265
C	-2.486298	1.808737	-1.350110
C	-3.048616	2.488113	1.277938
H	-1.172385	1.597260	1.777643
C	-3.674708	2.466064	-1.044966
H	-2.266347	1.550865	-2.383245
C	-3.965101	2.800886	0.276033
H	-3.251439	2.766435	2.307470
H	-4.368343	2.719824	-1.840425
H	-4.888595	3.315420	0.520544
S	1.304693	0.729420	1.617549
S	1.610436	2.594816	-0.742194
O	1.087862	1.993233	2.326237
O	0.484538	-0.425126	2.021671
O	2.907938	2.795554	-0.097353
O	1.495347	2.529366	-2.199747
C	0.538494	3.909510	-0.196088
C	-0.494970	4.314637	-1.036818
C	0.800894	4.548336	1.012630
C	-1.325912	5.350231	-0.624283
H	-0.636156	3.827068	-1.994528
C	-0.031495	5.590923	1.407385
H	1.635361	4.227287	1.622987

C	-1.097500	5.980335	0.598316
H	-2.145053	5.667940	-1.260264
H	0.155593	6.100900	2.346014
H	-1.746195	6.790291	0.915910
C	3.008905	0.269100	1.800602
C	3.891719	1.198446	2.343153
C	3.387971	-1.035561	1.499600
C	5.196556	0.795245	2.604201
H	3.552304	2.206364	2.553113
C	4.698317	-1.419746	1.762998
H	2.683500	-1.728456	1.050476
C	5.595383	-0.509305	2.318029
H	5.903187	1.501688	3.025999
H	5.020228	-2.426102	1.520241
H	6.618350	-0.814557	2.514458
C	-8.851520	-0.058279	0.496399
C	-9.025013	0.001435	-0.892465
C	-7.960485	-0.203862	-1.762135
C	-6.713392	-0.471125	-1.206942
C	-6.549027	-0.533170	0.182918
C	-7.610946	-0.328342	1.058362
H	-9.701450	0.108953	1.148169
H	-10.007393	0.211381	-1.299821
H	-8.095898	-0.157326	-2.836615
H	-7.469412	-0.376522	2.132146
C	-4.422330	-0.933441	-0.544282
C	-3.048158	-1.286346	1.300100
C	-4.483096	-0.889671	1.767134
H	-4.503052	0.090070	2.250333
S	-5.191714	-0.766708	-2.062634
N	-5.222724	-0.814841	0.501853
N	-3.142073	-1.135238	-0.185770
H	-2.325478	-0.563504	1.683878
C	-2.625992	-2.689053	1.669771
C	-1.553378	-2.875155	2.540986
C	-3.302046	-3.795153	1.147996
C	-1.159261	-4.165727	2.891967
H	-1.014539	-2.013218	2.925422
C	-2.905351	-5.080342	1.498495
H	-4.132706	-3.657147	0.458706
C	-1.833286	-5.266204	2.371707
H	-0.322008	-4.307082	3.567235
H	-3.428418	-5.937360	1.087820
H	-1.523225	-6.270390	2.641090

H	-4.920466	-1.645966	2.420147
C	4.464536	-0.495779	-1.365707
C	5.264661	0.632714	-0.949037
C	5.177116	-1.742528	-1.541755
C	6.606309	0.514761	-0.704202
H	4.749615	1.575742	-0.798661
O	3.219929	-0.413882	-1.556688
C	6.520288	-1.854137	-1.293086
H	4.593892	-2.601716	-1.859784
C	7.250269	-0.729419	-0.862771
H	7.192233	1.364487	-0.370919
H	7.039090	-2.798641	-1.414936
N	8.632380	-0.850179	-0.588533
O	9.183113	-1.947862	-0.735359
O	9.260924	0.143261	-0.204914
H	1.781879	0.315212	-0.661488

Vibrational frequencies

13.9481	18.5144	26.8885
28.7133	31.1244	33.2026
38.5047	44.0645	46.5620
49.9637	54.6986	62.4797
64.2370	66.5449	68.8241
70.4013	75.3461	78.1049
85.3338	86.1054	92.8276
102.7408	109.3857	112.3383
115.3548	124.8749	129.0502
139.5788	141.4500	148.1334
155.6107	180.1326	183.5806
185.4754	194.7992	202.0973
207.5031	212.1992	222.3663
224.2934	232.2525	234.9886
241.7675	252.4108	255.8226
260.9212	275.1060	281.0182
290.5807	293.1059	314.6846
323.8189	324.9695	331.5469
364.6077	381.1878	399.0525
405.8423	411.5507	415.2695
416.4374	419.4024	429.2856
430.8515	432.9479	435.6856
440.5072	445.6958	459.2329
460.9848	462.0128	486.2350
488.3985	503.8672	518.7397
527.6628	532.5088	536.8670
543.5591	556.8248	558.7275

564.4772	578.1395	589.3144
592.3426	613.0471	620.6524
623.5678	624.6307	625.9378
627.8235	632.4150	636.7767
651.7216	659.0236	668.0487
692.0159	700.9677	705.6843
705.9470	715.9326	716.7456
719.0930	722.8283	728.0355
732.0139	733.4709	742.5115
754.8856	764.8322	768.5791
772.3274	772.7496	786.8795
787.6758	794.9798	801.7851
812.8026	822.0607	839.3216
844.3209	853.2542	866.4093
869.1611	872.7671	873.4400
876.1675	876.3477	877.5157
885.7564	899.6646	928.8462
942.7565	950.9018	954.2221
958.2511	969.0720	978.4813
994.9098	996.4862	996.8545
998.0171	999.0387	1000.1012
1000.9659	1004.1799	1004.6230
1009.9956	1011.0581	1014.0693
1014.3308	1016.6901	1020.5200
1022.7826	1023.6304	1024.2653
1026.8325	1029.9968	1032.8223
1033.1813	1057.4740	1060.2933
1061.7169	1065.0565	1066.7002
1068.2760	1069.1548	1071.6307
1087.1116	1099.6758	1111.8681
1113.3506	1118.1023	1120.3652
1123.1009	1126.8514	1128.2048
1129.1428	1146.0515	1148.5477
1150.6490	1155.8415	1167.9770
1174.0783	1179.7800	1180.2553
1180.4969	1189.0880	1191.6987
1201.3069	1201.9688	1211.0205
1213.4770	1221.6859	1221.9622
1222.7786	1230.1732	1237.2984
1244.2521	1254.0017	1265.0872
1280.1629	1290.5338	1293.5201
1305.5911	1307.5688	1328.8690
1329.2954	1335.2251	1338.2517
1341.9682	1343.7538	1349.8725

1350.9735	1354.3861	1357.4361
1363.7780	1365.1124	1367.9500
1371.1664	1372.1342	1372.9158
1385.1210	1395.0071	1400.9411
1408.7497	1435.7808	1448.9059
1466.1404	1497.2221	1504.1862
1506.7926	1507.4692	1512.4298
1514.7759	1519.8731	1530.8084
1532.3750	1538.7292	1544.7412
1550.0291	1553.9879	1554.9861
1575.7186	1612.5807	1634.1312
1641.9475	1671.1564	1674.4215
1674.6929	1680.1357	1681.9815
1682.2396	1683.0467	1684.7581
1686.0708	1692.4597	1695.6010
1696.2130	1698.6248	1841.3479
2836.7084	3094.9899	3123.1877
3159.9001	3181.0584	3184.6625
3189.3154	3202.7190	3203.1680
3206.8580	3209.8680	3211.9367
3212.8679	3214.5345	3215.5989
3216.9188	3217.9446	3218.7646
3220.5048	3221.8623	3224.0792
3226.0350	3227.5443	3227.8282
3228.4664	3232.2588	3232.5378
3232.8669	3233.7596	3237.5199
3237.7261	3239.5873	3241.5014
3242.2706	3245.9079	3246.3436
3249.8842	3256.1076	3269.6482

TS5*SR*

Zero-point correction= 0.793610

Thermal correction to Energy= 0.845321

Thermal correction to Enthalpy= 0.846265

Thermal correction to Gibbs Free Energy= 0.704893

Sum of electronic and zero-point Energies= -3849.192442

Sum of electronic and thermal Energies= -3849.140731

Sum of electronic and thermal Enthalpies= -3849.139787

Sum of electronic and thermal Free Energies= -3849.281158

Cartesian coordinates

C	-1.393344	0.174387	-0.635867
O	-1.407789	0.228141	-1.870694
C	-0.146902	-0.423600	0.060875
H	-0.028390	-0.047851	1.076641

C	1.093646	-0.000785	-0.798800
H	0.779613	-0.237323	-1.824183
C	2.322441	-0.930989	-0.610678
C	-0.294683	-1.936577	0.112747
C	-0.705866	-2.665279	-1.009415
C	0.043829	-2.626847	1.279436
C	-0.775613	-4.055421	-0.959776
H	-0.970274	-2.137361	-1.921360
C	-0.018541	-4.017714	1.324672
H	0.354041	-2.063803	2.155738
C	-0.427727	-4.736539	0.204722
H	-1.095279	-4.608024	-1.837666
H	0.239547	-4.537581	2.243049
H	-0.478612	-5.820082	0.239367
C	1.376716	1.497362	-0.769713
C	1.938089	2.153098	0.329048
C	1.042002	2.257368	-1.895366
C	2.235817	3.513642	0.269486
H	2.137046	1.617273	1.248624
C	1.324335	3.617326	-1.951946
H	0.555567	1.767516	-2.732965
C	1.944403	4.247255	-0.874376
H	2.680345	3.999328	1.132810
H	1.070976	4.181125	-2.844736
H	2.176519	5.307106	-0.918828
S	3.349397	-0.707980	0.889404
S	3.304867	-1.098200	-2.151678
O	4.359829	0.326487	0.669241
O	2.371413	-0.555635	1.974280
O	4.623971	-1.609139	-1.777883
O	2.442240	-1.897715	-3.024480
C	3.507964	0.495011	-2.905666
C	2.882763	0.713709	-4.128875
C	4.320360	1.450298	-2.296498
C	3.077860	1.937177	-4.764365
H	2.260965	-0.060848	-4.563993
C	4.487762	2.671846	-2.937173
H	4.786850	1.244795	-1.338767
C	3.872624	2.911490	-4.166802
H	2.604676	2.127345	-5.721570
H	5.100060	3.439215	-2.476144
H	4.014332	3.867871	-4.659811
C	4.199733	-2.249265	1.160991
C	3.502326	-3.303713	1.742015

C	5.556217	-2.331492	0.861383
C	4.181673	-4.489701	2.002079
H	2.453504	-3.193685	1.991884
C	6.224913	-3.518486	1.139580
H	6.060173	-1.484420	0.411660
C	5.538196	-4.594473	1.700868
H	3.653611	-5.324783	2.449527
H	7.282455	-3.604239	0.915494
H	6.066057	-5.518959	1.910684
C	-8.352513	-0.363623	-1.623513
C	-7.999776	-0.475432	-2.972314
C	-6.664700	-0.498136	-3.366220
C	-5.690532	-0.414651	-2.378905
C	-6.053045	-0.303385	-1.031478
C	-7.383580	-0.275667	-0.629741
H	-9.399953	-0.345884	-1.343910
H	-8.776296	-0.545909	-3.725573
H	-6.392154	-0.580076	-4.412612
H	-7.647877	-0.189031	0.418408
C	-3.757384	-0.281520	-0.877089
C	-3.174695	-0.158880	1.337489
C	-4.716091	0.051833	1.192560
H	-5.030130	1.076328	1.406116
S	-3.928137	-0.374778	-2.589752
N	-4.921019	-0.234977	-0.226056
N	-2.704038	-0.264002	-0.072036
H	-2.716654	0.725641	1.781712
C	-2.870142	-1.394487	2.151289
C	-2.282420	-1.280194	3.408026
C	-3.260120	-2.651315	1.678716
C	-2.076283	-2.417393	4.190171
H	-1.994505	-0.301516	3.784080
C	-3.061353	-3.780996	2.459541
H	-3.705556	-2.746358	0.690295
C	-2.466670	-3.665476	3.717944
H	-1.614749	-2.322127	5.167584
H	-3.357732	-4.755409	2.085020
H	-2.306934	-4.550658	4.325348
H	-5.275378	-0.647350	1.815315
C	-1.125548	2.629309	0.872386
C	-0.689258	2.197359	2.154567
C	-1.114121	4.029968	0.620242
C	-0.242599	3.101769	3.100087
H	-0.686799	1.144609	2.410574

O	-1.584480	1.859041	-0.080432
C	-0.676437	4.932088	1.560547
H	-1.448194	4.361021	-0.356388
C	-0.229941	4.461946	2.800821
H	0.097913	2.765989	4.072125
H	-0.660629	5.995884	1.355776
N	0.234989	5.400810	3.790858
O	0.233554	6.594230	3.510085
O	0.613729	4.971452	4.875028
H	1.961804	-1.963367	-0.513694

Vibrational frequencies

-117.5020	11.9242	15.0860
17.4129	21.8356	24.0214
26.4820	32.9371	44.5165
47.4879	50.7422	56.9900
62.0092	65.7594	68.0377
70.8293	76.2538	81.5897
84.4069	92.7823	102.8860
105.7025	109.7436	117.2426
119.5417	128.5950	134.3823
139.7186	156.3413	169.6062
170.1588	175.8178	181.0387
184.7995	192.4043	199.9592
202.6481	218.4359	223.4705
228.9535	230.0085	245.7481
253.0769	261.3477	268.6886
269.2493	278.8113	281.2819
289.4212	306.8219	317.8337
322.9593	328.8533	346.2785
361.9884	387.4126	401.7701
404.9744	412.3934	414.2949
415.3428	419.0642	424.2955
430.4213	431.3922	434.7368
438.3336	448.3387	451.9047
475.3810	484.0173	491.4837
505.2622	518.8056	526.9399
531.2967	533.6649	542.8085
543.6373	549.8202	561.2120
573.7699	584.1025	588.5465
592.1399	596.8515	615.4290
622.3210	622.5018	626.1331
626.7933	631.0754	647.5979
650.6176	657.0535	668.4842
693.7796	700.0776	701.1263

705.6019	709.7445	713.4950
717.2283	725.9625	727.1252
730.5994	731.2848	741.6942
746.8469	767.6410	768.5974
772.6851	778.4245	781.6916
788.8103	790.5337	805.1534
807.4467	830.4770	840.8401
856.4475	862.5881	866.2796
869.3803	871.7565	871.9928
879.4049	883.3303	883.9159
889.6504	898.6572	913.1875
941.3804	958.3710	961.5489
965.3547	966.3409	969.7919
977.4015	988.6192	989.1397
995.0931	998.3908	1005.0236
1006.4479	1007.4038	1011.6006
1012.4518	1012.6998	1013.4469
1015.2875	1016.8518	1017.5897
1018.5424	1020.9421	1025.2825
1027.0491	1030.2709	1033.8520
1035.7772	1047.8204	1060.8405
1063.6679	1066.3158	1067.1052
1069.4100	1072.2241	1074.3860
1083.8722	1095.4406	1103.6444
1115.6659	1119.5516	1122.1893
1125.1497	1128.1820	1129.2069
1132.7888	1138.6809	1141.2517
1149.6192	1153.8317	1159.6261
1166.4851	1177.8848	1178.3917
1178.8625	1184.4096	1184.5187
1189.1953	1205.0952	1206.5400
1210.8106	1211.6022	1213.3720
1214.0931	1222.5534	1225.3514
1228.9348	1234.1092	1241.2460
1245.1721	1267.3683	1288.0467
1298.2159	1298.3232	1309.8794
1322.0377	1328.4570	1333.9418
1338.5668	1339.6643	1342.1126
1350.4014	1350.7224	1358.0544
1364.2385	1366.1887	1366.4623
1367.7151	1369.5116	1372.3427
1375.6433	1387.7671	1391.7569
1398.5060	1417.4634	1444.4296
1464.6689	1499.9683	1502.8112

1505.2023	1505.3700	1505.7703
1507.2167	1513.5944	1524.4830
1532.4090	1536.4315	1537.9885
1546.6977	1549.2479	1555.1828
1556.0108	1595.7263	1621.6916
1660.4038	1673.5390	1675.8727
1676.0839	1679.5966	1679.7598
1680.3775	1682.2939	1683.0060
1688.9151	1690.9618	1693.1529
1694.9605	1697.8374	1701.9618
3087.3967	3094.4937	3116.5884
3174.0304	3176.2142	3183.5604
3194.2055	3196.1908	3197.2062
3199.2968	3205.2656	3209.8889
3212.1903	3213.6878	3217.1937
3217.3014	3222.1928	3222.2736
3222.4228	3222.7192	3225.8862
3226.0181	3226.4620	3230.0270
3230.9689	3232.9886	3234.2324
3234.6255	3236.2613	3236.4991
3240.2944	3242.2221	3248.0767
3249.1782	3250.0696	3250.7818
3255.0826	3255.7320	3255.8301

P-*SR*

Zero-point correction= 0.554113

Thermal correction to Energy= 0.592129

Thermal correction to Enthalpy= 0.593073

Thermal correction to Gibbs Free Energy= 0.480661

Sum of electronic and zero-point Energies= -2763.231864

Sum of electronic and thermal Energies= -2763.193847

Sum of electronic and thermal Enthalpies= -2763.192903

Sum of electronic and thermal Free Energies= -2763.305316

Cartesian coordinates

C	1.633842	-1.503648	0.328336
O	2.033778	-1.430053	1.459852
O	2.444904	-1.532537	-0.758989
C	3.797661	-1.301439	-0.560514
C	4.594543	-2.239158	0.087000
C	4.309121	-0.116880	-1.077980
C	5.952389	-1.983310	0.218393
H	4.155910	-3.149173	0.478484
C	5.667051	0.141396	-0.950921
H	3.636962	0.581730	-1.566299

C	6.459553	-0.798697	-0.303567
H	6.613774	-2.682426	0.713796
H	6.109013	1.050265	-1.338428
N	7.894086	-0.528735	-0.162473
O	8.578283	-1.362791	0.404647
O	8.325180	0.515990	-0.618901
C	0.174465	-1.486537	-0.089802
H	0.125862	-1.582215	-1.174651
C	-0.323664	-0.063428	0.317430
H	-0.125285	0.018285	1.395805
C	-1.861924	0.060047	0.241858
H	-2.284503	-0.841463	0.706232
C	-0.604790	-2.617420	0.547783
C	-0.760957	-2.708053	1.935236
C	-1.207458	-3.574148	-0.272052
C	-1.515853	-3.738829	2.488043
H	-0.287506	-1.976540	2.583626
C	-1.956878	-4.609736	0.283943
H	-1.098348	-3.494300	-1.350218
C	-2.115642	-4.690463	1.664883
H	-1.635676	-3.798398	3.564797
H	-2.418889	-5.347785	-0.364079
H	-2.703821	-5.491843	2.099961
C	0.522690	0.997831	-0.373905
C	0.514921	1.180699	-1.760790
C	1.409808	1.754733	0.397900
C	1.323058	2.152228	-2.346605
H	-0.115074	0.565823	-2.394149
C	2.218918	2.724088	-0.186886
H	1.452732	1.593978	1.471647
C	2.167356	2.935950	-1.562428
H	1.293777	2.292552	-3.422268
H	2.882730	3.315843	0.435373
H	2.790023	3.696627	-2.022390
S	-2.533361	1.339821	1.373656
S	-2.621860	0.074133	-1.421522
O	-3.879435	1.666280	0.906800
O	-2.343313	0.752235	2.700795
O	-2.672748	1.437583	-1.946731
O	-1.895208	-0.958388	-2.169306
C	-4.278735	-0.517495	-1.174261
C	-5.341841	0.360154	-1.352731
C	-4.459851	-1.863033	-0.864036
C	-6.634951	-0.133832	-1.211757

H	-5.147980	1.400783	-1.586354
C	-5.758451	-2.337097	-0.713150
H	-3.606450	-2.526206	-0.748716
C	-6.839630	-1.474497	-0.889408
H	-7.481485	0.529783	-1.348964
H	-5.925011	-3.379853	-0.466316
H	-7.850496	-1.851746	-0.775596
C	-1.510035	2.785756	1.271913
C	-0.781757	3.138522	2.404174
C	-1.481845	3.536674	0.097203
C	0.009864	4.282821	2.353577
H	-0.835950	2.523712	3.295807
C	-0.667986	4.662426	0.059125
H	-2.064773	3.232801	-0.765651
C	0.071269	5.034399	1.183148
H	0.582676	4.579197	3.225436
H	-0.614237	5.253601	-0.848497
H	0.699866	5.918140	1.144511

Vibrational frequencies

16.6940	18.9242	27.9693
31.1138	35.9352	44.2525
45.8056	54.0767	55.9260
59.6181	66.1535	70.8395
71.7100	80.1367	83.8631
92.8524	100.3780	120.9059
126.9419	133.5874	146.9214
171.3741	175.3698	184.7817
188.7676	201.8042	215.4884
228.0337	231.3098	247.2246
250.9383	256.4066	261.7166
281.4340	314.2379	320.6409
324.1575	336.1676	380.9118
396.7499	399.6184	408.5709
410.7019	416.2899	418.8247
423.6260	427.9879	446.7325
459.9299	476.5209	487.8976
511.7021	524.6737	531.2005
534.9915	546.7602	554.4523
569.4789	584.3050	616.5274
620.7912	621.4800	626.4179
628.9471	639.5813	655.6484
680.1724	699.3725	700.6501
702.1302	704.8485	718.9393
721.9144	735.5508	744.7193

751.4575	764.0479	772.5226
774.3672	779.4232	789.7390
813.4107	834.9873	846.7328
856.2572	865.5771	869.0006
878.5623	879.7690	882.2652
896.6019	902.6922	917.0574
948.4465	957.6152	962.9094
974.0771	990.7082	1003.9195
1005.4977	1006.6973	1007.5021
1009.9966	1011.0273	1012.6316
1015.1172	1016.2459	1017.8693
1026.0015	1029.2361	1035.5976
1039.0997	1039.3322	1042.4823
1061.9679	1065.8687	1068.4366
1072.8302	1086.7402	1106.4650
1115.9092	1118.8257	1120.2304
1127.7318	1129.0968	1130.0358
1153.1203	1155.9862	1161.5909
1178.5956	1179.5529	1180.8495
1182.9639	1191.8804	1193.1891
1202.3403	1207.9075	1215.6170
1218.7238	1226.8287	1232.3100
1243.9181	1247.9107	1276.4885
1284.2860	1313.3959	1326.5715
1333.8959	1338.0422	1338.6328
1344.0518	1352.2516	1360.9742
1365.6756	1366.3315	1373.0575
1379.3138	1383.5956	1397.9596
1408.1425	1477.4193	1485.5720
1500.5474	1503.7584	1507.0936
1508.5949	1530.8220	1537.7988
1550.9463	1551.5256	1552.8692
1672.9055	1675.8146	1676.1683
1677.7011	1679.8288	1684.2309
1684.5546	1689.9758	1696.1031
1697.6462	1738.1601	1881.1118
3066.4039	3086.4191	3169.3162
3201.3272	3206.2669	3206.9272
3206.9955	3213.8917	3216.7443
3218.5749	3220.7902	3225.2354
3225.9581	3226.7590	3230.8013
3232.9686	3233.1760	3237.0384
3237.1025	3244.6059	3248.3898
3253.9263	3256.8397	3257.4674

3261.5707 3261.6823 3268.3225

TS3*RR*'

Zero-point correction= 0.680939

Thermal correction to Energy= 0.724495

Thermal correction to Enthalpy= 0.725439

Thermal correction to Gibbs Free Energy= 0.602324

Sum of electronic and zero-point Energies= -3337.486010

Sum of electronic and thermal Energies= -3337.442453

Sum of electronic and thermal Enthalpies= -3337.441509

Sum of electronic and thermal Free Energies= -3337.564624

Cartesian coordinates

C	1.528821	1.200958	-1.114257
O	1.833946	0.858065	-2.257877
C	0.355646	1.822083	-0.621439
H	0.458911	2.306179	0.343670
C	-0.828011	0.079476	0.194158
H	-0.752994	0.608009	1.139235
C	-2.119074	0.136244	-0.338596
C	-0.552081	2.506855	-1.543771
C	-1.002598	1.905287	-2.727822
C	-1.027663	3.787537	-1.223934
C	-1.868812	2.584622	-3.580585
H	-0.670533	0.902210	-2.972552
C	-1.889311	4.464272	-2.077000
H	-0.706244	4.250199	-0.293740
C	-2.309375	3.867095	-3.264850
H	-2.205972	2.103506	-4.494121
H	-2.236100	5.459306	-1.814451
H	-2.984701	4.393655	-3.932287
C	0.094122	-1.085637	0.111474
C	0.571151	-1.630609	-1.087230
C	0.545557	-1.631484	1.323441
C	1.473042	-2.692310	-1.066153
H	0.245103	-1.213539	-2.031949
C	1.443925	-2.694828	1.341304
H	0.178031	-1.221607	2.261940
C	1.917728	-3.225775	0.141894
H	1.840713	-3.095647	-2.004604
H	1.773670	-3.107127	2.290239
H	2.626006	-4.048388	0.149760
S	-3.171784	1.389915	0.331132
S	-2.836116	-1.008227	-1.448948
O	-2.343885	2.112589	1.312282

O	-3.871578	2.156960	-0.695777
O	-4.225282	-0.586443	-1.662755
O	-1.978660	-1.234678	-2.618090
C	-2.914836	-2.568022	-0.568229
C	-1.995103	-3.573242	-0.848738
C	-3.918881	-2.745150	0.382900
C	-2.054514	-4.763972	-0.128225
H	-1.250993	-3.420944	-1.620872
C	-3.969664	-3.939172	1.094235
H	-4.658536	-1.969047	0.549682
C	-3.033255	-4.942676	0.846934
H	-1.337543	-5.551870	-0.334163
H	-4.745662	-4.084779	1.838730
H	-3.074901	-5.870958	1.407530
C	-4.416425	0.523994	1.277225
C	-4.046728	-0.069737	2.481953
C	-5.710841	0.428905	0.778689
C	-4.997922	-0.790659	3.196429
H	-3.028604	0.028768	2.846301
C	-6.656488	-0.292598	1.504345
H	-5.949356	0.894777	-0.170461
C	-6.299035	-0.905071	2.704667
H	-4.725730	-1.264672	4.133544
H	-7.669993	-0.382062	1.128161
H	-7.038136	-1.471600	3.261873
C	6.889661	-2.894388	0.946249
C	7.028226	-3.143706	-0.423375
C	6.216695	-2.504762	-1.356226
C	5.263058	-1.608533	-0.887791
C	5.131977	-1.365100	0.485737
C	5.938647	-1.999460	1.423684
H	7.534276	-3.407081	1.651315
H	7.778728	-3.846214	-0.767531
H	6.323850	-2.699892	-2.417442
H	5.824811	-1.800969	2.483632
C	3.476641	-0.028629	-0.369972
C	2.454271	1.096752	1.363744
C	3.520621	0.110393	1.937321
H	3.069027	-0.693585	2.523128
S	4.094363	-0.672646	-1.839297
N	4.117974	-0.442697	0.721159
N	2.484454	0.810074	-0.096122
H	1.465353	0.837368	1.748072
C	2.757424	2.550752	1.647986

C	1.868124	3.318182	2.397538
C	3.935491	3.126341	1.166690
C	2.153698	4.655483	2.667216
H	0.944914	2.873353	2.762193
C	4.219842	4.460485	1.434841
H	4.628166	2.533073	0.572935
C	3.328464	5.226240	2.186383
H	1.455796	5.249229	3.247867
H	5.134077	4.904106	1.054995
H	3.549622	6.268182	2.392853
H	4.274949	0.631207	2.529739

Vibrational frequencies

-260.0420	10.9601	18.1511
21.9971	28.2552	33.7151
36.7149	43.9968	52.9861
56.2364	64.4136	66.4296
67.5912	75.6843	76.8641
85.6618	92.6689	101.5407
107.5467	111.1520	119.2029
133.3771	146.4935	154.1474
164.9147	179.7291	188.2248
190.3663	195.6643	201.8130
207.0385	209.5395	224.3807
229.2872	244.4335	248.7411
256.3415	271.7443	280.9471
290.0642	309.5581	312.0318
317.3016	325.1126	335.4895
349.8376	379.2012	403.1245
410.7333	415.2306	420.3374
426.6890	427.3056	431.2613
432.6740	438.8764	449.7912
453.6290	470.1230	478.2209
505.5686	521.9601	528.3028
537.0211	545.4872	552.5396
560.0931	569.7240	581.5368
588.4993	591.3574	599.6374
611.2042	621.5848	624.8054
625.7214	626.9551	629.9201
633.3202	647.5649	692.6714
702.8100	705.7052	711.5414
712.1267	722.4759	724.8867
726.3518	729.1314	730.3818
738.6894	748.8782	767.7898
770.8786	771.1729	776.2779

789.6391	793.4949	798.3651
818.3756	832.6255	860.5408
866.6670	870.3152	880.2328
883.4742	889.5772	890.1222
908.8933	927.8448	941.3015
951.2468	957.6583	959.7952
971.6624	975.8535	986.2892
986.6817	991.3580	1001.6880
1002.6087	1006.9323	1009.3507
1012.0500	1013.9534	1016.0655
1016.5045	1017.1790	1017.5750
1018.8609	1020.5252	1028.7851
1029.7060	1034.5496	1034.9594
1042.0323	1054.5514	1059.5767
1061.4855	1065.0116	1066.9413
1067.7484	1069.5520	1070.8226
1104.8496	1109.8466	1112.9880
1114.2409	1121.1316	1124.0286
1124.4173	1126.5606	1156.5795
1161.7676	1163.1656	1166.0108
1174.4306	1175.4223	1176.0739
1183.7310	1187.0639	1187.3302
1194.5529	1199.3318	1200.8908
1206.0641	1208.9334	1215.4734
1223.5758	1231.6876	1248.0225
1263.7305	1299.9186	1301.4302
1319.9088	1320.9470	1326.4257
1329.2284	1334.2855	1336.9642
1341.2843	1341.5095	1358.8923
1360.7606	1362.1041	1363.6939
1366.4933	1367.2237	1367.7818
1391.0742	1418.1532	1452.8330
1471.1931	1472.7903	1494.7746
1499.8300	1503.0214	1509.9671
1513.8541	1517.0870	1526.5770
1528.4562	1534.3232	1539.9755
1552.9495	1553.5457	1554.0830
1617.9289	1662.3836	1665.6292
1673.8198	1677.1715	1679.4823
1679.9496	1682.4456	1684.4262
1689.5934	1691.9828	1694.3912
1697.9587	1741.0814	3119.4278
3144.4346	3182.8558	3185.5880
3189.1909	3192.9102	3195.9610

3198.7092	3203.1341	3206.8563
3207.0986	3208.7652	3211.7167
3214.3434	3215.2557	3219.9713
3220.5075	3222.9229	3223.1794
3225.1484	3227.3398	3229.2428
3229.5746	3233.2755	3233.9497
3236.0255	3236.6807	3237.1227
3240.9212	3243.4444	3245.9661
3261.4424	3268.1229	3271.8441

TS3*RR*''

Zero-point correction= 0.680938

Thermal correction to Energy= 0.722776

Thermal correction to Enthalpy= 0.723721

Thermal correction to Gibbs Free Energy= 0.605537

Sum of electronic and zero-point Energies= -3337.484179

Sum of electronic and thermal Energies= -3337.442341

Sum of electronic and thermal Enthalpies= -3337.441397

Sum of electronic and thermal Free Energies= -3337.559581

Cartesian coordinates

C	-1.231230	-1.564756	-0.910349
O	-1.413851	-1.584057	-2.131537
C	-0.150593	-2.095854	-0.158939
H	-0.213073	-1.981842	0.918488
C	1.096977	-0.236429	-0.567112
H	0.400110	0.118426	-1.325315
C	1.136414	0.618105	0.552135
C	0.569734	-3.292794	-0.597799
C	0.757367	-3.632947	-1.949032
C	1.205471	-4.086870	0.373892
C	1.588285	-4.689694	-2.303252
H	0.276146	-3.035497	-2.713658
C	2.047181	-5.132426	0.014206
H	1.064948	-3.845136	1.425376
C	2.256189	-5.432134	-1.330229
H	1.736782	-4.919508	-3.354521
H	2.542381	-5.713389	0.786797
H	2.922038	-6.239853	-1.617523
C	2.256806	-0.932602	-1.176718
C	2.516588	-0.691455	-2.530918
C	3.022120	-1.893077	-0.507435
C	3.538144	-1.371717	-3.189601
H	1.912817	0.033143	-3.071197
C	3.984215	-2.629616	-1.183960

H	2.796816	-2.110298	0.528241
C	4.261275	-2.357771	-2.522553
H	3.740575	-1.158098	-4.234301
H	4.448440	-3.469581	-0.675185
H	5.016955	-2.929686	-3.052132
S	2.365604	0.601621	1.792698
S	-0.065218	1.895395	0.653973
O	2.075351	1.714943	2.705322
O	2.495263	-0.750107	2.353420
O	-0.951182	1.737959	-0.514664
O	-0.709606	1.942966	1.973746
C	0.797695	3.436422	0.415892
C	1.196356	3.764509	-0.878826
C	1.096673	4.243370	1.508118
C	1.930006	4.928396	-1.078382
H	0.939062	3.114095	-1.709039
C	1.830610	5.408034	1.293596
H	0.781029	3.938293	2.498777
C	2.251120	5.744294	0.007813
H	2.252447	5.198525	-2.078122
H	2.080222	6.048194	2.132814
H	2.828598	6.649191	-0.151263
C	3.926796	1.002309	1.010999
C	4.107895	2.294048	0.518092
C	4.934405	0.047920	0.940154
C	5.312697	2.616991	-0.095007
H	3.326363	3.039591	0.622739
C	6.139127	0.384090	0.326094
H	4.771592	-0.937489	1.360506
C	6.323469	1.660704	-0.198032
H	5.462163	3.617091	-0.488467
H	6.930771	-0.354400	0.256698
H	7.260863	1.915975	-0.681509
C	-6.485309	3.131657	-0.692717
C	-6.411191	3.054667	-2.087786
C	-5.507589	2.201268	-2.713520
C	-4.677402	1.427308	-1.910896
C	-4.763537	1.505162	-0.514855
C	-5.664026	2.355604	0.117147
H	-7.195964	3.808630	-0.232047
H	-7.065471	3.670683	-2.694185
H	-5.448753	2.143707	-3.794661
H	-5.717020	2.409588	1.198810
C	-3.090935	-0.036054	-0.773162

C	-2.379186	-0.721769	1.308226
C	-3.402194	0.446340	1.460097
H	-2.909000	1.359060	1.800962
S	-3.436628	0.268132	-2.427854
N	-3.860029	0.631192	0.080183
N	-2.190481	-0.799848	-0.164167
H	-1.439787	-0.430519	1.784041
C	-2.873433	-2.039486	1.864427
C	-2.385189	-2.500014	3.086837
C	-3.848489	-2.775524	1.187858
C	-2.873383	-3.685096	3.633339
H	-1.617580	-1.934008	3.608102
C	-4.334492	-3.958757	1.733819
H	-4.223753	-2.431132	0.227208
C	-3.848641	-4.414439	2.958686
H	-2.485636	-4.040685	4.582214
H	-5.089970	-4.527231	1.201621
H	-4.225918	-5.339704	3.381574
H	-4.234288	0.178954	2.112567

Vibrational frequencies

-277.6490	-13.7742	-11.5840
11.0974	18.6518	24.5888
33.5912	34.5136	41.5057
48.2784	59.7361	65.7534
68.1413	71.1740	74.4172
82.4498	93.3329	100.7355
114.5566	118.7454	119.6812
130.7790	135.7399	159.1716
168.3169	172.8573	181.9779
187.7380	196.0695	204.0824
210.1573	221.6740	225.2152
243.5264	247.6175	256.4493
257.8936	274.2467	287.5663
291.5725	302.0052	310.7921
316.7983	334.6501	336.5150
358.1045	369.8286	403.7972
412.3222	413.8848	416.7004
418.5151	423.1028	427.5447
433.6930	439.9821	450.8468
455.3025	467.7023	483.2362
508.5655	521.5685	526.3041
536.8288	538.5597	545.8459
562.2325	568.8527	576.2545
586.3452	588.7374	601.2996

617.5454	620.7543	622.7530
625.5939	627.8768	633.4524
635.3643	644.4577	683.0635
705.6796	706.3036	710.8595
712.1637	719.2658	723.2238
726.3512	728.9911	731.6669
744.6488	746.7907	771.9093
773.6313	775.6997	777.5152
790.0523	791.3910	799.8665
816.5630	836.0418	863.5588
873.4417	874.7815	877.1849
878.2163	880.5074	884.4261
885.0661	928.1605	935.4388
949.8419	951.4940	960.6792
967.1814	974.8541	985.7939
992.1873	994.4947	1002.7929
1007.5042	1009.1989	1011.2092
1011.2386	1013.4958	1014.2600
1016.4769	1017.1681	1019.5897
1024.0245	1031.8064	1033.1329
1033.7160	1034.8031	1035.5292
1054.9513	1059.8269	1062.4985
1065.2164	1066.6252	1070.5494
1073.3130	1074.2480	1084.1929
1103.5112	1114.8497	1116.7372
1118.3337	1120.1630	1123.3738
1124.9622	1128.9155	1153.7037
1159.4016	1164.1626	1174.3665
1176.2078	1177.0190	1178.1247
1181.3517	1187.6572	1189.5165
1203.3219	1203.7949	1206.7705
1210.4381	1214.4375	1217.2302
1224.0457	1228.4931	1250.8192
1257.5559	1286.4838	1297.5504
1302.2553	1308.3488	1314.9122
1330.3321	1338.7676	1339.4124
1340.8210	1342.6672	1352.3595
1361.4061	1361.4951	1362.9806
1364.7116	1367.0474	1369.2200
1392.1038	1416.4833	1438.1863
1467.1991	1474.3061	1496.6177
1497.9825	1505.5290	1510.6250
1513.7144	1517.2689	1527.6394
1530.7274	1536.3199	1539.4296

1550.1468	1556.4717	1558.0752
1616.9131	1659.8324	1671.2031
1672.7225	1677.1170	1678.8953
1680.5396	1682.6590	1683.8852
1686.5651	1690.8672	1696.3003
1700.2690	1727.6408	3125.5840
3150.8562	3179.7152	3186.3123
3191.4435	3194.1420	3194.3521
3204.3110	3205.1242	3205.4163
3206.9919	3209.5759	3210.3411
3213.8074	3217.8245	3219.5912
3221.0986	3221.2423	3225.6008
3229.4935	3229.9488	3230.9334
3231.3304	3231.4964	3235.0011
3235.1613	3241.9147	3243.9636
3245.6825	3252.6376	3253.8690
3257.6079	3260.8331	3275.1796

TS3*RR*'''

Zero-point correction= 0.680963

Thermal correction to Energy= 0.724764

Thermal correction to Enthalpy= 0.725708

Thermal correction to Gibbs Free Energy= 0.601928

Sum of electronic and zero-point Energies= -3337.485429

Sum of electronic and thermal Energies= -3337.441628

Sum of electronic and thermal Enthalpies= -3337.440684

Sum of electronic and thermal Free Energies= -3337.564464

Cartesian coordinates

C	1.377910	-0.506016	1.412779
O	1.884595	0.202201	2.290345
C	0.079135	-1.023778	1.283400
H	-0.096772	-1.733243	0.483183
C	-0.669542	0.668166	-0.181253
H	0.025836	0.207089	-0.875512
C	-2.011365	0.450387	-0.487781
C	-0.898113	-1.036881	2.354569
C	-0.781600	-0.312388	3.558369
C	-2.065348	-1.795516	2.155830
C	-1.803356	-0.345163	4.501132
H	0.113570	0.271203	3.735414
C	-3.084036	-1.821903	3.101221
H	-2.155909	-2.378783	1.241780
C	-2.961410	-1.091475	4.281262
H	-1.694548	0.220312	5.422291

H	-3.973730	-2.417988	2.915257
H	-3.753477	-1.108450	5.022968
C	-0.100632	1.830963	0.519076
C	1.045395	2.416258	-0.039114
C	-0.608181	2.343467	1.720198
C	1.641743	3.519798	0.558835
H	1.454264	2.012806	-0.963229
C	0.003763	3.437320	2.324797
H	-1.478200	1.884864	2.173366
C	1.120366	4.034461	1.744804
H	2.516528	3.972726	0.103202
H	-0.397728	3.825555	3.255603
H	1.587779	4.892208	2.217586
S	-3.322843	1.575033	-0.160515
S	-2.277753	-0.704611	-1.796103
O	-4.434028	1.162337	-1.025965
O	-3.581619	1.695020	1.277952
O	-2.556953	-0.030845	-3.072485
O	-1.094895	-1.592659	-1.786940
C	-3.687243	-1.738809	-1.425850
C	-4.050374	-2.611382	-2.450290
C	-4.355321	-1.725238	-0.207072
C	-5.099239	-3.499786	-2.240140
H	-3.524711	-2.589844	-3.399811
C	-5.405479	-2.619274	-0.011205
H	-4.066569	-1.035754	0.578671
C	-5.774085	-3.505011	-1.020727
H	-5.390822	-4.183361	-3.030115
H	-5.940610	-2.614875	0.932601
H	-6.592894	-4.198303	-0.859326
C	-2.739006	3.154288	-0.750720
C	-2.688466	4.237530	0.116670
C	-2.366902	3.254231	-2.089845
C	-2.240096	5.462518	-0.373369
H	-2.980221	4.110798	1.153604
C	-1.921911	4.482724	-2.564386
H	-2.415009	2.379593	-2.734987
C	-1.857794	5.582278	-1.706815
H	-2.186046	6.319513	0.289388
H	-1.623081	4.583472	-3.602276
H	-1.504515	6.537133	-2.082314
C	7.421586	0.628749	-2.081878
C	7.718474	1.451553	-0.990251
C	6.821334	1.598115	0.063902

C	5.619290	0.903959	0.000358
C	5.331298	0.080628	-1.095908
C	6.222200	-0.071221	-2.152468
H	8.138298	0.532177	-2.889602
H	8.661591	1.985326	-0.961777
H	7.052581	2.235987	0.909703
H	5.984910	-0.710445	-2.995458
C	3.431370	-0.169461	0.168670
C	2.055164	-1.707417	-0.861132
C	3.250984	-1.360842	-1.801417
H	2.938741	-0.792312	-2.680414
S	4.299277	0.908207	1.189831
N	4.083154	-0.514764	-0.942327
N	2.233521	-0.733448	0.257943
H	1.105534	-1.511378	-1.364373
C	2.069528	-3.134346	-0.359493
C	1.023975	-3.990178	-0.703497
C	3.128814	-3.607107	0.418538
C	1.040331	-5.316290	-0.275267
H	0.193919	-3.607521	-1.293001
C	3.141625	-4.929965	0.846933
H	3.943811	-2.942366	0.698007
C	2.097499	-5.786715	0.498090
H	0.222735	-5.977923	-0.541755
H	3.964189	-5.292360	1.454577
H	2.107927	-6.818243	0.834659
H	3.796467	-2.253994	-2.109213

Vibrational frequencies

-194.6520	14.8220	22.2584
25.5764	29.3356	35.6332
38.3222	41.7963	47.9208
49.3210	57.1309	59.4410
63.7779	68.3922	73.5651
80.2627	81.2210	92.4735
100.6683	115.2453	118.2612
122.9861	146.1800	151.2772
160.6219	172.8543	176.5222
183.1090	187.6064	195.1970
202.7790	208.8518	221.5254
227.9770	236.5428	247.5453
263.7141	267.5207	281.6459
287.9191	302.7005	311.5267
317.7530	328.6820	336.2734
352.4762	355.3725	381.3681

397.7682	413.0325	414.2673
422.5898	428.3931	429.8035
433.4305	441.9010	447.1691
452.9366	480.9610	506.9544
523.4380	526.3561	528.3490
540.9681	545.0756	546.4618
555.9257	567.3589	577.3223
584.4112	596.9873	602.8779
617.3454	622.2178	624.2493
625.2150	626.7160	633.6804
636.8796	642.5967	694.0984
706.8754	709.4056	711.3346
718.3574	720.7058	722.6017
726.4403	730.7087	732.9965
736.8523	749.5323	767.6258
774.7774	775.9480	777.9915
787.8924	791.3025	798.2035
813.4332	818.6757	865.3796
874.6012	878.4252	878.6765
880.3299	880.8496	882.5967
890.8288	928.7557	941.7030
956.1432	958.1320	961.7047
968.4359	971.0750	983.1356
992.8529	997.4475	1002.6243
1008.0480	1008.6955	1010.9599
1011.8003	1012.5238	1014.1937
1015.7859	1016.5681	1017.5604
1017.7267	1019.7541	1029.5982
1033.4168	1034.5187	1035.9372
1036.6538	1054.3782	1063.1184
1063.2925	1066.5669	1068.7780
1070.3624	1072.2685	1076.6749
1098.5610	1108.3987	1116.1645
1123.2113	1123.8452	1127.0905
1128.5050	1132.4453	1149.0358
1160.5101	1166.9254	1168.6917
1176.0881	1179.3079	1181.1467
1185.4593	1190.4940	1193.7711
1203.8427	1204.3720	1207.6383
1208.4610	1213.9479	1221.4626
1228.7388	1242.9507	1256.5310
1270.4803	1276.2694	1307.6358
1316.8437	1318.7859	1327.9108
1331.3332	1344.0893	1344.7858

1344.9721	1347.2588	1360.9797
1363.9157	1364.0303	1365.7693
1367.1554	1370.4425	1376.4110
1410.2548	1422.0160	1468.6245
1472.4999	1483.3997	1496.0219
1501.3187	1507.8448	1514.7067
1524.3187	1526.1981	1531.4455
1535.2422	1535.9736	1542.0333
1552.9512	1553.8764	1562.6524
1620.0268	1656.6439	1672.8434
1677.2993	1678.7767	1680.3158
1683.3847	1684.0183	1684.0792
1684.9887	1695.6851	1698.1717
1698.6689	1730.0521	3118.8882
3154.7725	3181.6344	3182.6762
3184.4324	3191.4887	3192.2023
3197.4924	3198.4513	3206.5513
3207.7120	3208.4568	3212.5001
3213.3613	3213.7928	3218.5758
3219.2633	3219.9226	3220.0209
3221.4309	3222.1947	3224.7385
3228.1661	3231.7370	3232.1772
3232.5771	3233.4090	3233.8121
3236.9763	3239.1710	3242.6256
3244.7428	3246.8095	3256.2829

TS3*RS'*

Zero-point correction= 0.680717

Thermal correction to Energy= 0.724413

Thermal correction to Enthalpy= 0.725357

Thermal correction to Gibbs Free Energy= 0.601754

Sum of electronic and zero-point Energies= -3337.483520

Sum of electronic and thermal Energies= -3337.439824

Sum of electronic and thermal Enthalpies= -3337.438880

Sum of electronic and thermal Free Energies= -3337.562483

Cartesian coordinates

C	1.493502	0.636292	-1.108218
O	1.041149	0.039362	-2.089775
C	1.141321	1.904658	-0.607003
H	1.725909	2.283211	0.223817
C	-0.706067	1.148729	0.560661
H	-0.036804	0.573962	1.195314
C	-1.476148	0.277530	-0.213797
C	0.554906	2.930514	-1.463929

C	-0.275630	2.637847	-2.559827
C	0.773965	4.281890	-1.141708
C	-0.874150	3.665588	-3.283696
H	-0.461752	1.605136	-2.825112
C	0.182923	5.302888	-1.874801
H	1.406286	4.523459	-0.289878
C	-0.653390	5.000640	-2.949489
H	-1.527073	3.414413	-4.114835
H	0.367549	6.337722	-1.601164
H	-1.125223	5.795756	-3.518231
C	-0.986067	2.463629	1.189281
C	-1.617847	3.564099	0.594195
C	-0.510899	2.603525	2.506092
C	-1.798614	4.741738	1.315608
H	-1.954439	3.505883	-0.430935
C	-0.695914	3.777949	3.223626
H	0.003769	1.768416	2.977371
C	-1.349385	4.855507	2.627597
H	-2.286325	5.583502	0.833961
H	-0.329337	3.852015	4.242392
H	-1.496785	5.778933	3.178696
S	-1.088680	-1.435038	-0.024428
S	-2.826588	0.621228	-1.297956
O	-1.356840	-2.176711	-1.257616
O	0.243006	-1.531743	0.602005
O	-3.314846	1.974355	-1.012163
O	-2.517548	0.279859	-2.687624
C	-4.115301	-0.497453	-0.776338
C	-4.484498	-1.548295	-1.606047
C	-4.748368	-0.259466	0.442397
C	-5.523134	-2.385150	-1.201568
H	-3.956966	-1.697655	-2.541212
C	-5.773476	-1.107744	0.840510
H	-4.432493	0.572127	1.065944
C	-6.161210	-2.165670	0.016117
H	-5.828720	-3.210215	-1.836187
H	-6.269452	-0.946555	1.791693
H	-6.963844	-2.825123	0.330858
C	-2.218302	-2.072658	1.213836
C	-2.308615	-1.441338	2.453238
C	-2.946954	-3.217891	0.922239
C	-3.155160	-1.974008	3.417995
H	-1.744323	-0.534826	2.654096
C	-3.790467	-3.744599	1.898992

H	-2.860063	-3.672030	-0.058726
C	-3.894347	-3.125454	3.140473
H	-3.242760	-1.490443	4.385138
H	-4.373624	-4.633120	1.680226
H	-4.557764	-3.534994	3.895240
C	4.555505	-5.543414	0.342498
C	4.030298	-5.920441	-0.898097
C	3.320009	-5.016709	-1.682969
C	3.148626	-3.724411	-1.200640
C	3.675162	-3.357869	0.044403
C	4.386367	-4.254047	0.834552
H	5.104919	-6.267589	0.933509
H	4.177349	-6.932625	-1.257536
H	2.912500	-5.311481	-2.643767
H	4.790024	-3.952857	1.794908
C	2.683321	-1.399020	-0.620111
C	2.955746	0.177140	1.034153
C	3.668383	-1.149952	1.452975
H	3.258268	-1.567144	2.373784
S	2.281806	-2.382510	-1.970831
N	3.376624	-2.029157	0.323829
N	2.455375	-0.121445	-0.331626
H	2.088087	0.348269	1.679727
C	3.880171	1.372409	1.081210
C	3.732930	2.322950	2.090077
C	4.902487	1.512497	0.140661
C	4.605651	3.406723	2.163421
H	2.926931	2.222310	2.812721
C	5.770639	2.596553	0.212301
H	5.010852	0.780568	-0.656099
C	5.624896	3.543868	1.225382
H	4.482991	4.145605	2.948218
H	6.558348	2.706014	-0.525597
H	6.301185	4.390622	1.277596
H	4.747615	-1.014357	1.553968

Vibrational frequencies

-242.9347	11.4469	20.4843
25.7298	29.6826	32.5837
37.8271	38.5921	46.4994
52.4082	55.3935	65.4857
67.9122	70.6851	73.7656
85.5821	90.7481	101.3471
105.2997	111.5888	118.4050
125.6764	131.4019	147.5198

171.9321	175.9432	181.2022
187.9719	194.0117	196.9407
207.6430	210.9617	223.5970
230.8191	235.7153	260.6703
265.7903	270.5176	282.0293
295.3632	305.3674	312.4563
323.6343	329.7578	333.8687
353.0105	368.7750	390.8867
401.8433	408.3227	413.3119
415.6692	426.5299	431.7230
434.4214	442.6094	450.8419
466.9688	476.6374	494.8957
510.4416	520.5037	525.9118
535.5819	544.8807	550.9375
554.6649	570.5232	577.9964
585.0925	596.3441	602.9534
617.9169	623.3017	623.6787
626.7701	628.9476	632.2010
636.0262	651.5044	687.3338
693.1983	704.9570	710.0104
715.0092	720.0931	724.0185
726.9146	729.4918	730.9995
741.6617	747.4143	764.7936
771.0480	772.0474	775.7551
784.4949	785.1715	792.6062
822.6881	837.5304	849.0016
855.7324	869.0076	871.2562
878.1670	881.0340	884.4808
885.3163	929.9386	938.1588
941.3942	943.1155	952.4168
956.1473	970.6071	971.3577
984.5614	994.2819	998.0564
1003.4424	1006.5304	1007.6530
1010.6756	1012.0052	1013.9663
1016.7195	1017.7883	1018.1515
1020.6029	1020.9164	1022.1257
1026.0091	1030.0424	1030.3556
1036.3042	1059.2223	1063.7625
1064.7120	1065.0377	1070.1686
1072.3565	1075.3417	1076.7406
1107.0682	1114.5567	1119.8228
1120.5617	1121.3456	1125.8505
1129.8592	1131.3791	1149.6649
1159.1518	1164.8311	1176.4980

1178.9589	1179.6459	1184.1756
1184.3477	1186.7704	1191.6410
1202.1766	1204.0513	1206.1723
1210.0239	1214.5954	1216.2347
1217.7791	1230.3704	1242.8623
1263.9581	1296.4672	1302.5385
1311.8810	1322.4645	1325.0459
1327.0092	1339.0261	1340.2477
1342.2437	1343.7761	1364.3862
1364.6747	1365.3389	1366.6896
1369.7692	1370.6995	1385.3352
1390.4210	1420.5905	1457.4688
1472.1469	1479.7204	1500.0115
1505.4732	1510.3357	1515.8919
1518.5212	1524.2187	1527.5102
1533.8249	1536.1691	1541.3075
1550.2839	1556.1053	1561.5301
1617.5283	1659.0769	1665.6597
1673.1623	1679.8320	1681.6922
1684.2986	1685.4423	1686.0939
1686.9863	1692.9943	1694.3674
1704.7880	1728.9336	3117.5684
3120.4166	3182.4101	3183.2616
3187.0957	3199.0586	3199.5810
3201.8895	3202.6647	3203.3083
3206.7881	3207.9769	3208.4949
3216.4460	3217.1752	3217.6602
3217.8230	3218.0420	3220.1553
3223.0797	3225.0832	3226.1174
3227.2528	3229.4323	3231.5127
3234.6923	3235.4557	3237.3999
3238.7826	3240.9211	3245.0990
3252.7292	3265.6396	3278.1780

TS3*RS''*

Zero-point correction= 0.680235

Thermal correction to Energy= 0.724134

Thermal correction to Enthalpy= 0.725078

Thermal correction to Gibbs Free Energy= 0.600625

Sum of electronic and zero-point Energies= -3337.479720

Sum of electronic and thermal Energies= -3337.435821

Sum of electronic and thermal Enthalpies= -3337.434877

Sum of electronic and thermal Free Energies= -3337.559331

Cartesian coordinates

C	-1.414414	-0.462364	-1.275505
O	-1.073884	0.288064	-2.192372
C	-0.864306	-1.695546	-0.859965
H	-1.484340	-2.316454	-0.224003
C	0.378136	-0.791790	0.831742
H	-0.372156	-0.021955	0.992296
C	1.559092	-0.268014	0.317914
C	0.098201	-2.401338	-1.698365
C	0.996713	-1.736873	-2.554092
C	0.169041	-3.805258	-1.628385
C	1.912866	-2.462507	-3.312065
H	0.967112	-0.656074	-2.624096
C	1.093384	-4.519894	-2.378073
H	-0.520518	-4.332911	-0.972563
C	1.972315	-3.850187	-3.229824
H	2.589846	-1.932763	-3.977884
H	1.123042	-5.603225	-2.305926
H	2.690159	-4.406840	-3.824179
C	0.225252	-1.929038	1.778284
C	0.740918	-3.214894	1.573923
C	-0.527895	-1.682052	2.935630
C	0.485435	-4.223730	2.498252
H	1.327998	-3.421743	0.687744
C	-0.771737	-2.690483	3.863439
H	-0.913995	-0.680605	3.115983
C	-0.270961	-3.970929	3.641230
H	0.883297	-5.218256	2.322306
H	-1.350445	-2.473772	4.755587
H	-0.462994	-4.764232	4.356351
S	1.449366	1.396652	-0.255526
S	3.102332	-1.112539	0.522661
O	1.837431	1.544111	-1.661763
O	0.115351	1.885705	0.138431
O	3.401726	-1.166700	1.962810
O	3.089738	-2.386341	-0.206402
C	4.354448	-0.099076	-0.234146
C	5.318337	0.483219	0.582646
C	4.386638	0.013795	-1.621050
C	6.332809	1.226783	-0.011468
H	5.252485	0.361956	1.658426
C	5.399834	0.770403	-2.200674
H	3.622955	-0.472767	-2.220216
C	6.366338	1.375281	-1.397092
H	7.089696	1.697243	0.607220

H	5.439713	0.882849	-3.278766
H	7.155346	1.962021	-1.856836
C	2.646642	2.313630	0.701076
C	2.710528	2.133029	2.080707
C	3.470572	3.212960	0.035007
C	3.637983	2.872485	2.807441
H	2.071214	1.401654	2.567296
C	4.389887	3.951324	0.775254
H	3.406678	3.300272	-1.044238
C	4.474573	3.778551	2.154922
H	3.712819	2.736943	3.881099
H	5.050194	4.649610	0.271640
H	5.200259	4.348004	2.726577
C	-5.525041	4.914759	0.743806
C	-4.958878	5.559220	-0.361162
C	-4.039554	4.908686	-1.178645
C	-3.700981	3.597043	-0.868380
C	-4.273364	2.959614	0.240282
C	-5.190310	3.603475	1.063565
H	-6.237236	5.445444	1.365682
H	-5.237069	6.582714	-0.585736
H	-3.597437	5.409366	-2.032737
H	-5.622865	3.098555	1.920152
C	-2.900483	1.311775	-0.575610
C	-3.157473	-0.583722	0.716324
C	-3.997308	0.585643	1.326964
H	-3.628991	0.894302	2.308056
S	-2.559534	2.540910	-1.724429
N	-3.787373	1.660937	0.356319
N	-2.471262	0.064201	-0.433273
H	-2.400425	-0.916805	1.429452
C	-3.989433	-1.772317	0.293018
C	-3.826207	-2.992450	0.947939
C	-4.932493	-1.651051	-0.729339
C	-4.607172	-4.088166	0.585525
H	-3.079162	-3.085641	1.734782
C	-5.710038	-2.745924	-1.091086
H	-5.054239	-0.702913	-1.249082
C	-5.548901	-3.964830	-0.432369
H	-4.474718	-5.037441	1.093747
H	-6.439785	-2.649801	-1.888035
H	-6.154405	-4.818832	-0.717362
H	-5.057058	0.331572	1.391423

Vibrational frequencies

-249.0545	12.2473	19.2862
23.9635	26.6033	29.7662
38.2884	45.3436	48.5051
51.9397	54.1813	58.9379
60.2899	70.4246	72.4049
83.5770	84.9546	93.7753
110.3467	110.6504	116.2030
124.0176	131.0383	137.2524
168.8186	171.6390	176.0044
185.8276	191.2733	199.7740
204.9768	210.7616	216.4189
224.3890	237.7965	243.8528
255.7346	264.9160	275.7132
283.6396	304.9160	309.6027
323.6003	333.0499	340.7457
345.0725	362.6259	378.9255
400.0022	411.9335	412.8953
417.6588	424.8009	428.9586
431.2979	436.8804	453.1771
471.4521	486.1386	505.4814
508.5053	520.0729	525.8070
534.2763	543.2833	545.4548
556.6616	568.2996	576.3004
585.4863	590.4716	599.2204
616.2646	622.2547	622.4519
625.7017	627.8830	632.7612
635.0487	644.4289	685.4707
701.8835	705.0710	706.0503
713.4711	722.3518	725.3256
727.2919	730.9154	733.3881
738.5358	760.4252	770.0987
770.5049	773.0610	777.6779
789.6833	792.4951	797.9798
816.9464	826.5024	847.7468
866.3225	872.4208	878.3420
879.1747	881.2067	886.1291
890.3108	924.6501	935.8071
953.3739	956.7938	962.9269
965.4223	969.5580	988.2832
989.1616	991.2352	1004.8976
1006.7329	1007.1424	1008.9758
1011.9038	1013.4786	1014.1619
1015.8480	1017.3228	1017.7056
1018.0013	1027.9671	1030.5076

1032.9813	1033.7922	1037.5498
1041.4511	1056.4012	1060.5357
1061.3694	1061.6804	1067.0517
1070.6699	1072.5688	1074.2327
1101.9041	1107.5410	1114.0458
1116.9891	1118.4158	1124.6914
1126.8278	1127.6926	1153.7609
1156.9922	1163.1254	1173.1310
1177.6758	1178.8373	1179.3508
1182.0782	1185.9634	1187.1421
1196.0548	1197.7260	1201.8814
1203.5000	1212.8169	1218.3635
1223.3457	1228.4999	1250.3878
1262.0657	1297.9100	1300.0798
1302.0960	1307.0664	1322.1882
1330.5924	1330.8013	1334.3740
1337.4173	1341.0977	1360.8669
1362.3843	1363.1929	1364.8471
1365.9015	1366.6956	1372.0444
1401.6954	1417.2566	1455.7578
1473.1761	1482.1833	1498.9398
1499.9282	1508.9354	1514.3803
1517.8732	1526.0152	1527.4705
1528.7741	1529.3625	1541.3017
1551.1085	1556.0845	1559.1889
1619.6003	1659.1775	1668.4966
1672.8740	1679.7277	1679.9417
1680.7186	1681.6834	1684.7381
1687.9590	1692.7821	1692.8686
1698.5098	1735.9918	3113.1092
3155.1161	3174.2951	3177.7836
3181.6198	3184.2172	3187.3645
3188.9313	3200.1578	3206.8022
3209.2634	3209.8887	3210.0714
3212.2225	3215.3949	3218.3766
3220.8243	3220.8937	3220.9355
3222.0834	3226.6897	3227.6964
3228.0901	3231.3572	3231.6962
3232.1895	3235.7660	3244.2861
3245.4362	3245.6227	3246.0443
3246.4640	3249.7331	3269.1986

TS3*RS*'''

Zero-point correction= 0.680364

Thermal correction to Energy= 0.724195
Thermal correction to Enthalpy= 0.725139
Thermal correction to Gibbs Free Energy= 0.601065
Sum of electronic and zero-point Energies= -3337.488902
Sum of electronic and thermal Energies= -3337.445070
Sum of electronic and thermal Enthalpies= -3337.444126
Sum of electronic and thermal Free Energies= -3337.568201
Cartesian coordinates

C	-1.454195	0.558924	1.762461
O	-2.006252	0.169984	2.802124
C	-0.097558	0.820009	1.494204
H	0.115056	1.361038	0.578818
C	0.763487	-1.141788	0.450826
H	0.899191	-1.512365	1.466984
C	1.956398	-0.683427	-0.096173
C	0.904202	0.934393	2.550745
C	2.103350	1.609741	2.269831
C	0.768590	0.341240	3.822079
C	3.122733	1.700788	3.213180
H	2.230973	2.083636	1.301970
C	1.786837	0.441048	4.760813
H	-0.143154	-0.191135	4.062828
C	2.971075	1.118565	4.466327
H	4.037832	2.226579	2.957221
H	1.657553	-0.021048	5.735544
H	3.762505	1.188282	5.205914
C	-0.381281	-1.786348	-0.240400
C	-0.328569	-2.181585	-1.585940
C	-1.493421	-2.180854	0.522667
C	-1.388275	-2.875452	-2.163640
H	0.552663	-1.970226	-2.178823
C	-2.553912	-2.870344	-0.056378
H	-1.528797	-1.932212	1.580690
C	-2.513251	-3.206381	-1.409309
H	-1.326344	-3.170660	-3.206016
H	-3.407124	-3.156878	0.552249
H	-3.339556	-3.742708	-1.864863
S	3.441591	-1.147858	0.732917
S	2.117364	0.206502	-1.604624
O	4.475092	-0.123464	0.561563
O	3.085018	-1.607970	2.077545
O	3.092559	-0.467197	-2.469595
O	0.753797	0.441757	-2.107266
C	2.766863	1.838953	-1.267152

C	4.142477	2.052409	-1.264826
C	1.864140	2.884772	-1.080994
C	4.619899	3.336597	-1.023640
H	4.817364	1.223890	-1.439349
C	2.355441	4.165122	-0.841415
H	0.795614	2.705457	-1.135888
C	3.730278	4.387471	-0.802829
H	5.689286	3.517550	-1.012476
H	1.657364	4.982317	-0.692194
H	4.111966	5.385482	-0.612988
C	3.996403	-2.592151	-0.164240
C	5.099435	-2.496653	-1.003598
C	3.303321	-3.788440	0.007440
C	5.522491	-3.634771	-1.686271
H	5.607879	-1.545161	-1.112111
C	3.732784	-4.916816	-0.681804
H	2.448069	-3.833597	0.675343
C	4.840223	-4.838468	-1.527023
H	6.384186	-3.580097	-2.342922
H	3.207354	-5.857671	-0.557989
H	5.171657	-5.721927	-2.062994
C	-7.407686	-1.506821	-1.352325
C	-7.797759	-1.835985	-0.049521
C	-6.983892	-1.541543	1.040433
C	-5.770857	-0.908277	0.796690
C	-5.391414	-0.576644	-0.509985
C	-6.198600	-0.868709	-1.604268
H	-8.059081	-1.751545	-2.183747
H	-8.748526	-2.329653	0.116275
H	-7.284260	-1.801268	2.049415
H	-5.890920	-0.608242	-2.610923
C	-3.574498	0.156862	0.681377
C	-2.017155	0.998818	-0.782832
C	-3.210023	0.393529	-1.583772
H	-2.928498	-0.518257	-2.119146
S	-4.522549	-0.459489	1.976747
N	-4.149569	0.050351	-0.514298
N	-2.346950	0.665632	0.623342
H	-1.096293	0.478642	-1.056562
C	-1.813886	2.481192	-1.019345
C	-1.482767	2.885329	-2.317147
C	-1.876505	3.428482	0.000222
C	-1.215908	4.222136	-2.590165
H	-1.399666	2.143708	-3.107792

C	-1.603738	4.768665	-0.274636
H	-2.127006	3.125081	1.011784
C	-1.272882	5.167843	-1.566257
H	-0.951340	4.523891	-3.598163
H	-1.650454	5.499032	0.526487
H	-1.057270	6.210527	-1.775960
H	-3.651226	1.117734	-2.269999

Vibrational frequencies

-220.5047	16.1011	18.6385
21.5492	26.8631	32.5338
34.6123	38.8257	45.4422
48.0462	54.9849	63.0619
69.7016	73.6152	76.9499
78.8247	85.7623	92.5950
106.0084	111.1335	118.9731
129.2360	139.7611	147.5113
155.3367	173.4936	181.8804
183.9562	195.4293	201.1276
210.8493	212.4067	220.9716
229.7447	236.1162	248.2974
262.4434	273.5343	278.5377
286.3809	308.0996	321.2669
327.8927	332.4844	340.7160
354.8379	369.1513	399.4894
409.8541	410.5600	417.1385
419.5117	426.5017	428.5317
430.8727	433.6786	444.5183
450.8879	465.2972	476.9728
499.8081	509.8482	517.7024
530.7431	545.5940	546.4548
553.1675	562.4214	572.3143
594.8497	600.7015	605.1863
621.9604	623.1571	623.5704
626.0457	628.2959	630.1896
634.8522	645.1148	686.5307
702.0774	705.0456	705.6741
710.2673	712.0242	715.3139
723.1800	729.2071	735.2967
737.7979	750.9829	764.5792
769.3605	774.5647	775.1241
776.9102	778.5672	811.5095
817.1225	835.9665	858.2998
864.9108	867.7733	871.8381
878.6041	879.8181	881.8406

882.3876	922.7055	931.5042
939.1612	947.4641	949.1109
956.7085	964.3804	973.2527
980.4830	997.4848	999.5086
1000.9893	1001.2873	1010.5532
1011.1548	1012.1841	1013.7488
1014.8439	1015.9811	1017.2709
1018.9465	1022.6378	1028.9702
1030.2132	1032.9898	1034.1630
1042.4092	1058.0088	1060.8580
1064.0053	1064.5007	1067.6547
1070.4328	1072.5124	1073.1444
1106.1716	1110.8453	1117.2840
1119.1986	1120.2471	1123.1579
1126.4333	1127.4007	1152.4493
1159.3269	1163.2851	1176.0454
1178.9251	1179.7682	1180.1831
1180.5735	1184.6349	1186.0841
1196.6650	1204.2203	1204.7379
1207.6852	1208.7308	1217.2537
1226.0450	1228.5516	1255.7608
1264.3707	1293.3517	1299.7091
1313.3938	1325.7343	1326.1162
1336.7103	1338.7376	1340.4251
1343.0601	1347.3346	1353.4124
1360.7757	1363.0276	1364.4899
1365.3784	1365.6740	1366.2160
1386.4250	1416.7819	1458.1197
1471.7476	1480.0468	1495.5062
1501.4849	1502.4864	1511.8972
1515.8224	1517.2878	1526.5426
1528.9833	1534.7480	1540.4114
1550.5332	1552.3467	1554.4900
1614.3250	1660.5259	1661.2477
1675.6064	1676.2129	1678.3160
1678.8195	1680.8456	1683.4246
1685.7351	1687.0664	1688.5906
1697.6864	1711.9133	3109.4727
3172.2503	3181.4981	3181.9233
3198.3056	3201.6019	3209.1311
3210.0224	3210.8971	3210.9631
3212.2359	3215.3331	3218.5826
3220.7751	3223.1797	3223.6610
3223.9614	3225.4466	3226.4526

3228.1311	3228.2577	3230.2675
3232.9261	3233.4539	3233.6831
3238.9266	3239.0002	3244.7693
3246.0253	3246.7544	3247.1064
3248.2547	3251.8038	3259.2896

TS3*SR*'

Zero-point correction= 0.679315

Thermal correction to Energy= 0.723294

Thermal correction to Enthalpy= 0.724238

Thermal correction to Gibbs Free Energy= 0.600748

Sum of electronic and zero-point Energies= -3337.470910

Sum of electronic and thermal Energies= -3337.426931

Sum of electronic and thermal Enthalpies= -3337.425986

Sum of electronic and thermal Free Energies= -3337.549476

Cartesian coordinates

C	7.599330	-1.975972	0.327484
C	6.980048	-3.059897	0.957669
C	5.643898	-2.997665	1.344563
C	4.940455	-1.829096	1.081364
C	5.567743	-0.748116	0.446765
C	6.902154	-0.802317	0.060818
H	8.642201	-2.048009	0.039753
H	7.546719	-3.963198	1.153065
H	5.165504	-3.835487	1.839438
H	7.375315	0.041758	-0.428334
C	3.449308	0.083564	0.769073
C	3.338009	2.182283	-0.157775
C	4.822429	1.714127	-0.096651
H	5.397027	2.232182	0.675113
S	3.256399	-1.460123	1.501994
N	4.673760	0.304359	0.277482
N	2.624466	1.101342	0.598395
H	3.194533	3.113384	0.393911
C	2.833277	2.339361	-1.577602
C	2.031290	3.427865	-1.920793
C	3.157838	1.395439	-2.555640
C	1.524752	3.551784	-3.212915
H	1.791679	4.176422	-1.169846
C	2.656906	1.519509	-3.847415
H	3.788330	0.545133	-2.304152
C	1.830925	2.594335	-4.175270
H	0.893314	4.396896	-3.465069
H	2.907118	0.775849	-4.597500

H	1.433544	2.687343	-5.180378
C	0.454272	2.109198	0.890605
H	0.618334	2.480074	-0.113161
O	1.356170	0.470583	2.393781
C	1.390740	1.221746	1.403133
H	5.319974	1.817491	-1.060967
C	-0.583070	2.769429	1.663361
C	-1.541701	3.541763	0.982577
C	-0.651326	2.724922	3.068166
C	-2.503202	4.270005	1.674295
H	-1.507025	3.582296	-0.104565
C	-1.609905	3.460155	3.753570
H	0.068386	2.119331	3.609128
C	-2.538331	4.241855	3.065902
H	-3.226027	4.863469	1.121689
H	-1.633107	3.424724	4.839450
H	-3.284958	4.813108	3.608589
C	1.524835	-1.496154	-1.984126
C	0.761300	-0.512809	-1.357810
C	-0.068658	-0.854294	-0.290503
C	-0.098744	-2.184355	0.158794
C	0.652722	-3.164914	-0.481395
C	1.466303	-2.822346	-1.558462
H	2.155012	-1.224178	-2.824932
H	0.787490	0.512265	-1.705497
H	-0.736466	-2.453495	0.998891
H	0.604469	-4.191697	-0.133242
H	2.054613	-3.582683	-2.062182
C	-1.024550	0.028443	0.434314
H	-0.919828	-0.067272	1.519010
C	-2.244604	0.467274	0.017586
S	-2.667024	0.785111	-1.672866
S	-3.577963	0.360020	1.204829
O	-3.336767	1.191583	2.377547
O	-3.655026	1.859040	-1.730556
O	-4.836506	0.474040	0.465417
O	-1.404039	0.955212	-2.394312
C	-3.418180	-1.343880	1.735126
C	-2.801120	-1.614449	2.952133
C	-3.842795	-2.359637	0.881492
C	-2.597119	-2.943454	3.319250
H	-2.488110	-0.793687	3.589679
C	-3.628425	-3.681432	1.258091
H	-4.337752	-2.121715	-0.055825

C	-3.003062	-3.972054	2.471078
H	-2.118609	-3.172174	4.265439
H	-3.951212	-4.484284	0.603446
H	-2.835840	-5.005177	2.757662
C	-3.425926	-0.722690	-2.236690
C	-4.812330	-0.793943	-2.326775
C	-2.604887	-1.820590	-2.492464
C	-5.393490	-2.010586	-2.677158
H	-5.407544	0.082639	-2.097903
C	-3.201178	-3.030743	-2.831020
H	-1.524286	-1.724267	-2.427553
C	-4.590736	-3.124897	-2.918233
H	-6.472555	-2.089994	-2.753376
H	-2.581896	-3.898988	-3.029790
H	-5.050350	-4.072358	-3.180556

Vibrational frequencies

-122.4378	15.3985	19.7921
29.2255	31.1036	35.6587
38.5395	42.9865	52.8882
59.3228	59.7253	67.4301
69.4366	74.1213	79.2426
82.4388	88.1278	91.8253
104.2951	106.9472	115.0091
115.9155	127.8572	133.2502
164.9281	166.7830	174.9041
189.3012	193.3129	197.7217
206.1067	212.8293	216.8391
230.9855	243.5196	244.2686
246.3119	262.9630	265.8357
280.6674	285.0561	313.6570
315.2231	317.6345	338.0693
347.5051	365.3427	396.2942
413.1480	414.5704	418.7354
420.9471	425.9485	429.4459
435.8479	439.0738	443.0077
456.9605	464.5941	486.0791
499.3220	511.1847	520.9562
526.8345	537.1448	546.3979
555.6353	561.3210	578.7940
584.6985	593.2525	597.0755
618.8272	621.3455	622.0594
623.1492	627.8928	628.5171
634.3929	651.1189	676.8212
702.6505	705.0905	709.6087

713.8544	717.9299	721.6129
724.1051	729.8793	730.7197
734.3307	744.0209	752.8695
772.3734	773.4476	776.9511
781.2105	786.4785	788.2334
797.5062	822.9677	829.7730
864.5943	874.5105	876.5231
876.8089	877.8895	887.3263
888.9848	917.9769	924.5873
942.5955	954.9678	955.5341
957.9759	966.2830	974.8780
983.7399	986.0669	994.6382
1004.2593	1005.1763	1006.4318
1007.6605	1010.6560	1010.7317
1013.5094	1016.3883	1017.4242
1017.7374	1018.3953	1027.4919
1028.4285	1030.8013	1033.8544
1035.5580	1043.9003	1058.9434
1060.4923	1062.3775	1063.7788
1070.5939	1071.9211	1072.7864
1108.8500	1112.5574	1114.2054
1116.1158	1116.9340	1121.3460
1125.9695	1126.7252	1134.5483
1165.3283	1166.1332	1171.6254
1174.9125	1176.7909	1176.9511
1178.3524	1180.4860	1183.4431
1187.5130	1193.6406	1200.8212
1201.9117	1208.3076	1212.0966
1213.7554	1222.5335	1241.3496
1257.8952	1287.3674	1302.7211
1313.2086	1325.7072	1326.2691
1335.4521	1335.4621	1341.1865
1342.4177	1353.3274	1354.6495
1361.3943	1363.1735	1364.4388
1365.1530	1365.3105	1368.2916
1391.6531	1415.3752	1460.5016
1472.6454	1488.6233	1496.6505
1498.4593	1507.9616	1512.7069
1518.0611	1524.7285	1527.2129
1527.8367	1537.7350	1539.7701
1553.5072	1554.4299	1577.4343
1622.5904	1660.8333	1665.8743
1675.9934	1676.1055	1677.1264
1678.1916	1679.4397	1680.8553

1685.7789	1690.6239	1691.5755
1698.8413	1726.7103	3121.4150
3147.6870	3163.9957	3175.9453
3187.4508	3191.1265	3191.8204
3194.8294	3196.7785	3197.3993
3208.4773	3208.7792	3210.5957
3211.1834	3213.0601	3217.1923
3219.4040	3221.5261	3222.3537
3222.8381	3223.7368	3226.4808
3227.9120	3231.2032	3231.8079
3234.0147	3234.1060	3236.1994
3240.1201	3243.6011	3247.3294
3252.1235	3260.9426	3266.3181

TS3*SR*''

Zero-point correction= 0.680733

Thermal correction to Energy= 0.724075

Thermal correction to Enthalpy= 0.725019

Thermal correction to Gibbs Free Energy= 0.605058

Sum of electronic and zero-point Energies= -3337.482852

Sum of electronic and thermal Energies= -3337.439511

Sum of electronic and thermal Enthalpies= -3337.438567

Sum of electronic and thermal Free Energies= -3337.558528

Cartesian coordinates

C	7.432090	1.700377	-0.360334
C	6.959436	2.583801	-1.337609
C	5.666865	2.474917	-1.841328
C	4.853193	1.462009	-1.345105
C	5.336733	0.584073	-0.367316
C	6.627326	0.684310	0.140852
H	8.442772	1.809305	0.016666
H	7.609153	3.368383	-1.708579
H	5.301583	3.161985	-2.596537
H	6.984493	-0.003625	0.899264
C	3.192845	-0.189797	-0.648546
C	2.949361	-2.119094	0.591174
C	4.317643	-1.452015	0.923226
H	5.157155	-2.130040	0.765799
S	3.181961	1.086283	-1.798949
N	4.360410	-0.344657	-0.026925
N	2.285745	-1.098202	-0.281916
H	3.100096	-3.017058	-0.016903
C	2.177146	-2.470943	1.840303
C	1.917334	-3.805490	2.154467

C	1.734419	-1.458553	2.688772
C	1.212972	-4.124251	3.313145
H	2.254228	-4.593172	1.485213
C	1.013455	-1.775627	3.836660
H	1.912468	-0.417275	2.436330
C	0.758601	-3.109247	4.154046
H	1.011513	-5.163061	3.553090
H	0.643360	-0.975401	4.468676
H	0.198748	-3.357800	5.049863
C	0.212378	-2.305079	-0.681564
H	0.536224	-2.904527	0.160008
O	0.920574	-0.427074	-1.965483
C	1.081040	-1.268089	-1.081531
H	4.340921	-1.065112	1.945060
C	-0.646072	-3.028731	-1.620651
C	-1.093883	-4.305374	-1.236399
C	-1.071650	-2.526716	-2.861255
C	-1.946144	-5.047168	-2.043204
H	-0.774364	-4.705975	-0.276828
C	-1.917724	-3.278967	-3.671498
H	-0.759603	-1.535200	-3.161888
C	-2.365300	-4.536859	-3.270924
H	-2.284624	-6.024868	-1.712712
H	-2.239284	-2.870910	-4.625704
H	-3.031442	-5.111912	-3.906616
C	-4.292742	-2.901576	-0.329283
C	-3.301241	-1.931725	-0.455589
C	-2.270464	-1.850564	0.491201
C	-2.252022	-2.785692	1.538442
C	-3.242000	-3.752774	1.660268
C	-4.273538	-3.810435	0.725753
H	-5.080430	-2.954011	-1.074666
H	-3.307175	-1.259631	-1.304190
H	-1.440131	-2.750648	2.263355
H	-3.207397	-4.458621	2.484323
H	-5.050118	-4.563697	0.814248
C	-1.148385	-0.883115	0.499292
H	-0.553367	-1.029854	1.400961
C	-1.060783	0.456820	0.098162
S	-1.707598	1.239842	-1.319639
S	-0.035411	1.481455	1.120338
O	-0.061677	0.890290	2.470735
O	-0.766145	2.272348	-1.767899
O	1.294530	1.750066	0.553213

O	-2.155858	0.228422	-2.282610
C	-0.883486	3.044495	1.248788
C	-2.009436	3.113157	2.067061
C	-0.399499	4.153044	0.565440
C	-2.674093	4.327270	2.190319
H	-2.354866	2.225979	2.588960
C	-1.067206	5.367289	0.707269
H	0.472475	4.049415	-0.070107
C	-2.200587	5.451074	1.512563
H	-3.560304	4.396267	2.812136
H	-0.705077	6.245699	0.183555
H	-2.722096	6.397945	1.611030
C	-3.172926	2.124984	-0.778608
C	-3.316508	3.454828	-1.154172
C	-4.138322	1.473381	-0.013891
C	-4.460028	4.146658	-0.759805
H	-2.528428	3.937927	-1.721360
C	-5.274957	2.174018	0.373910
H	-3.993688	0.440731	0.291063
C	-5.436414	3.508483	-0.000477
H	-4.578857	5.189301	-1.036516
H	-6.033233	1.680276	0.972541
H	-6.322982	4.052862	0.308570

Vibrational frequencies

-250.1967	23.8065	29.1620
33.1826	36.3435	41.0323
48.7464	55.1432	57.9777
59.8308	66.6252	70.3798
78.5787	79.9310	86.1645
95.2462	99.5627	104.3195
112.6131	118.0822	121.6907
125.3789	133.6046	162.0991
172.3802	178.8121	182.1950
185.7559	194.8718	198.8222
210.4303	213.3840	232.2837
233.7113	238.8026	252.0866
258.0547	259.6241	276.6228
292.4861	305.8179	311.6437
322.5594	331.0707	334.2017
342.1375	360.2988	388.9137
403.4230	410.0463	415.9412
419.6353	422.7784	426.3165
434.8189	436.9412	450.1682
466.0921	476.6660	499.1982

512.3646	524.3309	528.4191
537.8955	542.2132	547.1278
557.3845	570.3353	575.9753
578.1979	596.5308	611.6262
615.7161	621.9273	622.7540
625.8617	628.6484	631.4155
634.2932	651.4847	692.5969
702.1821	705.1632	709.2690
710.1394	713.4999	723.7418
728.4242	730.6103	731.8306
744.0200	751.6595	764.1310
767.6847	770.2593	773.8740
780.7288	783.8009	794.4896
836.0906	839.2613	852.8122
864.5241	867.0176	870.0810
871.7181	882.5302	887.8659
890.9078	927.0271	935.0023
947.5010	954.0630	956.6543
960.8335	961.8590	971.1587
988.5503	990.2571	992.7580
1000.5623	1001.8105	1002.8979
1011.5100	1013.0168	1013.6462
1014.6884	1015.3620	1015.5394
1016.1231	1016.3285	1017.7085
1020.1161	1024.0299	1026.9839
1033.5284	1060.3748	1061.4882
1064.6838	1066.8729	1068.3758
1070.8286	1074.5249	1076.0270
1105.0661	1112.7991	1115.1476
1119.1076	1120.5221	1122.8135
1127.7997	1134.8557	1154.8466
1159.3277	1165.6578	1176.9546
1177.4948	1177.7210	1178.0494
1179.6607	1183.5363	1191.5713
1196.8205	1199.8876	1201.0788
1203.4945	1209.4097	1218.2869
1222.1048	1227.9422	1245.5286
1264.6994	1291.1742	1296.6993
1311.4180	1314.0544	1323.5526
1324.1147	1333.6322	1337.2060
1345.1088	1347.7578	1362.0152
1362.3916	1365.7802	1365.8758
1369.2859	1372.2062	1380.8939
1399.5301	1420.7828	1459.9802

1470.1880	1482.3104	1497.2864
1500.2069	1505.8534	1513.6128
1520.8555	1526.9872	1530.4177
1531.1789	1534.3581	1541.4363
1549.8960	1552.3954	1557.5982
1605.6253	1664.5707	1668.6264
1678.5063	1679.8036	1680.8989
1681.7249	1682.1002	1682.9468
1688.7342	1689.4240	1695.2607
1697.3335	1752.3717	3111.7428
3122.2442	3171.0100	3178.1349
3182.1225	3186.6010	3195.7168
3198.2744	3203.3716	3204.9332
3206.7105	3207.9003	3208.7401
3208.9019	3214.6741	3217.7521
3218.5080	3221.4912	3222.4839
3222.6177	3223.3436	3228.3568
3229.1613	3231.2573	3231.4450
3234.3250	3239.5143	3239.9858
3243.1497	3243.8223	3246.9157
3248.5028	3258.8869	3260.0774

TS3*SR*'''

Zero-point correction= 0.679201

Thermal correction to Energy= 0.723132

Thermal correction to Enthalpy= 0.724076

Thermal correction to Gibbs Free Energy= 0.600446

Sum of electronic and zero-point Energies= -3337.470532

Sum of electronic and thermal Energies= -3337.426602

Sum of electronic and thermal Enthalpies= -3337.425657

Sum of electronic and thermal Free Energies= -3337.549287

Cartesian coordinates

C	-7.568933	-2.021997	-0.194056
C	-6.931267	-3.149917	-0.723602
C	-5.594156	-3.100933	-1.112603
C	-4.911620	-1.905894	-0.948875
C	-5.556576	-0.780243	-0.411224
C	-6.889706	-0.821555	-0.028655
H	-8.612408	-2.083551	0.094550
H	-7.483472	-4.073662	-0.839895
H	-5.104154	-3.973611	-1.529831
H	-7.378310	0.057015	0.381120
C	-3.446434	0.048796	-0.795740
C	-3.354608	2.210212	-0.015846

C	-4.836638	1.724576	-0.049270
H	-5.411918	2.191030	-0.852485
S	-3.227893	-1.551722	-1.383782
N	-4.678660	0.297280	-0.336987
N	-2.629470	1.081010	-0.694386
H	-3.219130	3.100246	-0.632460
C	-2.853111	2.471025	1.389147
C	-2.031692	3.568392	1.644037
C	-3.190586	1.608667	2.435648
C	-1.515240	3.779951	2.921864
H	-1.778996	4.251603	0.837228
C	-2.680926	1.821693	3.713500
H	-3.834403	0.751050	2.250320
C	-1.834516	2.902427	3.954075
H	-0.866981	4.629384	3.108550
H	-2.942141	1.142251	4.518647
H	-1.431529	3.062916	4.948405
C	-0.421226	2.012135	-0.969332
H	-0.581884	2.371376	0.039815
O	-1.379448	0.417999	-2.487427
C	-1.393801	1.159971	-1.496363
H	-5.337011	1.881983	0.905874
C	0.633829	2.658485	-1.728343
C	1.655382	3.322515	-1.021933
C	0.673919	2.682722	-3.134911
C	2.667499	4.000996	-1.695128
H	1.633236	3.318219	0.066921
C	1.681041	3.370740	-3.801571
H	-0.098399	2.159748	-3.692252
C	2.681845	4.035326	-3.088557
H	3.447237	4.501703	-1.124865
H	1.686182	3.388411	-4.889089
H	3.469062	4.565317	-3.614137
C	-1.545290	-1.311509	2.133203
C	-0.791890	-0.394028	1.408657
C	0.021643	-0.832590	0.362581
C	0.052232	-2.198548	0.046984
C	-0.688542	-3.115943	0.784555
C	-1.492932	-2.673030	1.833582
H	-2.165246	-0.962717	2.954181
H	-0.810328	0.660559	1.658561
H	0.682702	-2.547119	-0.771126
H	-0.641736	-4.172988	0.538318
H	-2.077839	-3.381791	2.412937

C	0.942523	-0.007663	-0.478277
H	0.802905	-0.214111	-1.541697
C	2.195150	0.432062	-0.145426
S	2.668420	0.941891	1.474635
S	3.471495	0.175034	-1.354449
O	3.146455	0.813167	-2.627206
O	3.637300	2.029624	1.386699
O	4.762421	0.427205	-0.709719
O	1.421734	1.170564	2.214238
C	3.339627	-1.590122	-1.630952
C	2.677291	-2.043954	-2.765879
C	3.834400	-2.467982	-0.668142
C	2.491016	-3.415108	-2.932126
H	2.313096	-1.328426	-3.496232
C	3.636475	-3.833627	-0.843103
H	4.367605	-2.091263	0.200966
C	2.963440	-4.305392	-1.969051
H	1.975346	-3.784806	-3.814775
H	4.014849	-4.529622	-0.100984
H	2.810720	-5.372510	-2.102557
C	3.473987	-0.478930	2.187982
C	4.862078	-0.504340	2.259442
C	2.685062	-1.559813	2.575172
C	5.482129	-1.659289	2.731495
H	5.429991	0.358466	1.928013
C	3.319257	-2.712161	3.035030
H	1.601871	-1.498529	2.514478
C	4.711474	-2.760005	3.110270
H	6.563464	-1.703878	2.797379
H	2.725971	-3.566756	3.334909
H	5.198858	-3.662389	3.466142

Vibrational frequencies

-170.6220	12.7732	20.1092
25.3357	30.6097	32.7476
38.3689	43.0880	49.1531
58.6629	69.1976	70.5231
71.5663	75.7350	79.4886
83.1748	88.7639	94.0865
103.4147	111.6424	113.9722
115.7022	123.8860	131.1323
154.9817	167.7807	182.2915
188.8241	196.2266	198.5352
205.8142	212.9565	219.1432
229.6251	244.2147	246.3634

248.7101	261.3059	272.6625
281.0644	286.6862	307.7917
315.9548	319.8379	338.0055
343.1124	369.2819	395.8804
414.4414	416.7142	417.4402
421.4467	424.2817	425.9255
433.6821	440.4835	444.8367
458.3990	466.7035	487.3885
498.6484	515.2436	521.9904
530.5961	537.3440	546.3175
556.3391	561.6379	580.4898
583.0974	593.7154	596.2216
618.7941	621.6072	623.3184
623.7040	626.0303	627.5982
634.0155	652.9330	676.3504
706.0357	708.3557	710.5134
717.6891	719.4290	723.1295
727.1116	728.7657	733.0739
734.6355	745.3400	758.1168
765.7877	775.5662	782.2497
783.7114	787.0430	790.7136
796.6767	822.4460	829.5528
872.3323	874.7944	876.8496
881.5267	883.3355	886.9971
889.1855	919.7640	934.9346
950.1389	954.4801	964.9971
967.0452	967.8027	976.2362
979.5765	992.4599	998.8115
1002.1211	1008.9697	1009.8857
1010.4521	1010.7431	1013.6827
1015.3082	1016.0435	1017.5859
1017.8230	1018.8261	1026.7587
1030.4344	1033.3390	1033.5789
1038.6095	1042.5584	1060.1965
1060.3649	1061.0807	1061.8607
1063.4855	1071.6711	1072.1025
1109.3913	1111.0109	1113.8730
1114.1793	1117.7013	1120.1002
1125.9615	1126.5455	1133.6182
1163.3991	1165.5675	1168.4590
1171.2637	1172.3677	1177.7353
1178.1300	1182.0919	1182.1461
1184.4949	1192.3345	1199.3416
1201.7644	1207.4065	1210.8315

1218.8659	1220.3488	1236.9919
1255.7488	1284.3883	1300.8860
1304.7167	1326.7618	1332.6684
1334.5764	1335.6826	1336.8662
1338.5757	1347.7758	1350.4706
1356.3861	1360.8018	1363.0787
1363.5486	1364.3683	1365.5130
1387.5785	1416.6178	1462.9974
1470.5282	1490.5574	1496.6989
1497.6478	1508.7995	1510.6312
1517.5075	1525.8407	1528.5160
1530.3668	1532.2578	1538.8921
1548.4063	1553.3477	1562.5239
1620.3699	1654.8264	1664.6502
1672.3698	1674.8214	1675.5328
1679.4276	1679.8308	1682.2362
1686.1698	1693.6456	1694.6964
1696.5398	1734.3854	3120.7763
3157.9458	3162.1739	3173.4200
3174.6788	3180.9598	3186.3674
3191.6264	3193.9338	3195.1907
3197.4422	3198.8186	3209.2384
3209.5328	3211.8063	3214.0764
3215.0809	3216.5060	3218.8767
3220.7704	3221.5054	3222.0830
3223.6703	3232.9924	3233.8023
3234.2464	3235.7129	3235.9925
3237.5905	3242.8741	3246.4521
3251.0917	3260.2064	3266.8010

TS3*SS*'

Zero-point correction= 0.680820

Thermal correction to Energy= 0.724428

Thermal correction to Enthalpy= 0.725373

Thermal correction to Gibbs Free Energy= 0.603535

Sum of electronic and zero-point Energies= -3337.477461

Sum of electronic and thermal Energies= -3337.433853

Sum of electronic and thermal Enthalpies= -3337.432909

Sum of electronic and thermal Free Energies= -3337.554746

Cartesian coordinates

C	7.272467	-0.456786	-1.060806
C	6.958866	-0.724176	-2.397997
C	5.675238	-1.109069	-2.772685
C	4.707854	-1.208553	-1.779357

C	5.029951	-0.940730	-0.441909
C	6.313958	-0.565203	-0.059440
H	8.281322	-0.160396	-0.796774
H	7.726407	-0.628573	-3.157428
H	5.433033	-1.317262	-3.808785
H	6.550345	-0.362162	0.979522
C	2.794161	-1.429946	-0.275690
C	2.195315	-1.392458	1.934718
C	3.640972	-0.847084	1.785811
H	4.345724	-1.377260	2.426485
S	3.012711	-1.701714	-1.959279
N	3.914423	-1.110996	0.372393
N	1.716514	-1.440521	0.503882
H	2.227178	-2.430848	2.281192
C	1.337664	-0.577630	2.865972
C	1.131227	0.780006	2.620710
C	0.704394	-1.190457	3.945088
C	0.274752	1.516197	3.429761
H	1.619490	1.252598	1.775355
C	-0.139678	-0.448760	4.769964
H	0.853036	-2.251147	4.127976
C	-0.361613	0.900726	4.507992
H	0.086243	2.559933	3.198801
H	-0.634121	-0.930845	5.606843
H	-1.035228	1.472598	5.137738
C	-0.655581	-1.785946	0.762984
H	-0.559794	-0.996204	1.495019
O	0.651529	-2.887687	-0.924249
C	0.500083	-2.143127	0.052591
H	3.696298	0.229124	1.976056
C	-1.802921	-2.664673	0.940832
C	-2.715957	-2.347153	1.963508
C	-2.059979	-3.799375	0.150657
C	-3.843366	-3.127096	2.186985
H	-2.528087	-1.464419	2.569898
C	-3.190409	-4.575967	0.380299
H	-1.373649	-4.048119	-0.650567
C	-4.089445	-4.247641	1.394643
H	-4.533160	-2.860019	2.982449
H	-3.376448	-5.444454	-0.245528
H	-4.971146	-4.857646	1.565383
C	-4.662814	-1.631670	-1.298908
C	-3.579088	-0.925381	-0.794162
C	-2.323819	-1.010076	-1.416844

C	-2.181499	-1.872360	-2.515406
C	-3.268283	-2.581353	-3.016412
C	-4.516968	-2.454224	-2.415312
H	-5.625778	-1.550635	-0.804242
H	-3.698254	-0.347591	0.111676
H	-1.205542	-1.978336	-2.980079
H	-3.136765	-3.232629	-3.874606
H	-5.369162	-3.002961	-2.804115
C	-1.109795	-0.274422	-1.026113
H	-0.263968	-0.583602	-1.636968
C	-0.952287	1.047463	-0.589660
S	0.291028	2.005057	-1.400357
S	-2.055805	1.850637	0.496236
O	-2.447718	0.893105	1.539119
O	0.925553	1.108961	-2.379027
O	-1.452993	3.118255	0.929279
O	-0.330215	3.245686	-1.881767
C	-3.550972	2.242369	-0.410019
C	-4.762284	2.145729	0.270782
C	-3.484342	2.656432	-1.736316
C	-5.937636	2.468738	-0.399900
H	-4.777487	1.799640	1.299054
C	-4.669197	2.973972	-2.395675
H	-2.524383	2.725806	-2.238597
C	-5.890169	2.879237	-1.731347
H	-6.889810	2.391594	0.114178
H	-4.637094	3.290750	-3.432672
H	-6.809374	3.122072	-2.254358
C	1.626708	2.522172	-0.323462
C	1.448814	3.569849	0.578402
C	2.864049	1.902689	-0.485191
C	2.519347	3.950653	1.382490
H	0.485087	4.056308	0.655626
C	3.933607	2.311136	0.309307
H	2.984444	1.143198	-1.251350
C	3.755558	3.317596	1.257051
H	2.389598	4.752129	2.101804
H	4.909046	1.852537	0.175797
H	4.587967	3.625309	1.881254

Vibrational frequencies

-217.1147	15.8380	25.7255
30.7551	31.9879	37.3044
43.3446	44.9205	51.8280
58.2339	60.8543	68.0586

71.0089	77.3361	81.8100
84.2480	88.1452	95.6461
112.0225	117.4293	120.6087
132.8593	143.9230	148.0758
156.8927	173.3885	178.9753
189.7354	195.6204	204.6611
212.0563	221.9341	226.3921
229.1018	232.8115	248.4891
261.4556	275.8696	281.0542
284.6510	306.4227	312.7267
314.7072	320.6298	335.6001
343.2505	361.8734	374.3142
408.6814	409.3503	415.1888
416.7373	423.6982	427.4095
432.2725	432.7928	437.2689
459.6945	474.1583	502.2605
511.7476	519.8663	525.2324
535.3128	542.2514	544.9806
550.8455	562.4673	575.0002
575.6131	601.6982	604.6073
618.5674	623.6081	624.2452
625.8299	626.7457	628.3733
634.7048	655.5790	692.2056
704.3522	707.1619	708.6667
710.9162	711.3993	717.7856
721.3794	726.9037	728.2999
732.9362	744.1310	764.1511
775.6672	778.3432	778.4549
783.4972	788.6530	793.6783
836.3120	843.9932	859.3392
863.1584	873.7835	879.9039
881.2564	887.7677	899.8870
901.2769	918.1506	931.0516
935.4796	953.5660	968.0129
974.4061	977.5970	977.8315
985.0287	989.6836	990.4723
1001.2174	1005.9911	1007.6486
1009.8576	1011.7020	1013.7924
1015.8549	1016.1676	1020.0518
1021.2745	1023.9252	1024.9340
1026.5904	1036.0564	1036.6723
1046.9700	1051.6377	1062.0696
1063.8619	1064.7987	1066.5643
1069.1658	1073.6453	1075.9807

1104.3014	1108.7744	1110.7490
1121.4444	1123.3360	1125.3522
1125.5638	1130.6254	1141.6945
1152.6197	1158.0903	1167.4055
1169.2440	1177.4937	1180.2671
1181.6854	1183.8237	1187.2599
1187.7441	1196.2664	1207.8579
1208.3958	1213.4651	1222.6239
1226.5213	1228.6553	1253.6987
1261.3154	1294.1413	1300.4995
1306.5849	1310.9310	1319.7517
1325.1699	1338.9066	1341.0345
1346.0240	1352.8836	1358.1251
1363.3612	1363.4078	1364.7483
1365.3710	1366.3553	1372.5295
1411.2522	1413.4159	1455.0653
1463.3012	1475.3501	1498.0488
1498.5157	1503.8629	1514.5893
1515.4920	1520.7225	1524.8258
1534.3239	1534.7754	1535.6440
1546.5902	1553.2302	1557.5003
1608.6680	1657.0101	1665.7796
1671.3510	1674.6976	1677.4961
1679.0362	1681.1849	1682.0060
1684.7096	1690.0269	1691.2567
1700.4115	1719.5889	3106.3653
3113.8649	3185.4799	3185.8182
3193.9616	3196.4044	3202.0575
3203.6518	3203.9366	3208.3573
3211.7076	3212.8242	3217.8301
3218.9396	3220.3519	3223.6100
3227.6836	3230.0132	3230.0436
3230.8704	3231.5055	3231.6325
3237.0815	3238.7949	3238.8828
3239.7079	3241.2694	3246.2136
3248.4640	3252.1898	3254.2268
3269.9168	3275.4561	3276.3325

TS3*SS*''

Zero-point correction= 0.681178

Thermal correction to Energy= 0.724713

Thermal correction to Enthalpy= 0.725657

Thermal correction to Gibbs Free Energy= 0.603708

Sum of electronic and zero-point Energies= -3337.479939

Sum of electronic and thermal Energies= -3337.436404

Sum of electronic and thermal Enthalpies= -3337.435460

Sum of electronic and thermal Free Energies= -3337.557410

Cartesian coordinates

C	8.200025	-0.397460	-0.625012
C	8.038583	-1.779257	-0.472223
C	6.806785	-2.325935	-0.127358
C	5.736721	-1.457617	0.056112
C	5.906802	-0.076298	-0.100230
C	7.135812	0.477400	-0.441960
H	9.172324	0.001070	-0.891926
H	8.886352	-2.437779	-0.623542
H	6.683313	-3.396174	-0.005327
H	7.252828	1.549023	-0.559159
C	3.684795	-0.195113	0.459185
C	2.801032	1.929568	0.450649
C	4.354883	2.003316	0.274215
H	4.864793	2.420347	1.145737
S	4.081682	-1.864471	0.542842
N	4.708191	0.590282	0.134697
N	2.547617	0.477305	0.655404
H	2.495093	2.458301	1.356667
C	2.105707	2.518047	-0.756057
C	1.760346	1.739857	-1.858574
C	1.935557	3.904798	-0.803376
C	1.237609	2.343534	-3.000995
H	1.898150	0.662128	-1.822378
C	1.429034	4.507149	-1.950831
H	2.205753	4.511083	0.057803
C	1.077568	3.725151	-3.051460
H	0.942849	1.729746	-3.844649
H	1.296787	5.583839	-1.981895
H	0.669050	4.191678	-3.941442
C	0.216897	0.523077	1.406654
H	0.198205	1.489379	0.905521
O	1.781884	-1.195597	1.976494
C	1.473618	-0.132569	1.442516
H	4.627853	2.561527	-0.621710
C	-0.744060	0.374571	2.505685
C	-1.822600	1.271091	2.567607
C	-0.658808	-0.616835	3.501520
C	-2.785743	1.178408	3.568214
H	-1.891726	2.066083	1.831941
C	-1.617586	-0.698970	4.502852

H	0.164964	-1.318851	3.482763
C	-2.691646	0.190030	4.542447
H	-3.611699	1.884170	3.577373
H	-1.526203	-1.470570	5.262128
H	-3.441234	0.112193	5.323679
C	0.352978	-4.037803	0.737020
C	-0.288888	-2.803834	0.803844
C	-0.131194	-1.871733	-0.229752
C	0.722753	-2.193494	-1.295919
C	1.359737	-3.428552	-1.361841
C	1.171638	-4.359809	-0.343461
H	0.217660	-4.750997	1.544163
H	-0.906741	-2.553242	1.654583
H	0.855707	-1.477639	-2.103866
H	1.998383	-3.661395	-2.208121
H	1.664609	-5.325906	-0.388370
C	-0.759683	-0.525322	-0.307490
H	-0.215505	0.101688	-1.011899
C	-2.123184	-0.200247	-0.344837
S	-2.590968	1.080496	-1.458671
S	-3.452755	-1.036805	0.428679
O	-2.926966	-1.857074	1.521992
O	-1.495168	1.248710	-2.424116
O	-4.524484	-0.080481	0.724843
O	-3.936213	0.801763	-1.971302
C	-4.098930	-2.180416	-0.785897
C	-5.269534	-1.863749	-1.466432
C	-3.416326	-3.373595	-1.013776
C	-5.766530	-2.766878	-2.402627
H	-5.760192	-0.919006	-1.263375
C	-3.919872	-4.264041	-1.957177
H	-2.512055	-3.600626	-0.456491
C	-5.092060	-3.961042	-2.649148
H	-6.679823	-2.536308	-2.940902
H	-3.400747	-5.197544	-2.147212
H	-5.482459	-4.660653	-3.381204
C	-2.664465	2.602743	-0.538609
C	-3.817561	2.935378	0.166536
C	-1.515157	3.385328	-0.492411
C	-3.806336	4.089204	0.946158
H	-4.683628	2.284433	0.120487
C	-1.517334	4.534747	0.293684
H	-0.643352	3.090854	-1.068330
C	-2.659671	4.882073	1.013742

H	-4.692645	4.368584	1.506101
H	-0.627864	5.155701	0.337590
H	-2.659480	5.776275	1.628535

Vibrational frequencies

-285.4390	15.5679	21.8927
25.7562	33.7435	37.6357
42.7350	49.3113	53.9339
60.9588	62.4084	68.0393
74.8885	78.1423	84.6703
89.6083	91.6994	96.8007
106.3960	108.5817	115.1726
118.8189	135.2327	156.1070
162.1078	181.6922	189.8692
195.9549	197.1040	198.2863
206.6776	211.9643	213.5898
234.2634	235.4264	251.1353
255.0337	270.0943	274.9473
282.6389	310.6828	317.6142
322.9146	323.8802	335.3710
352.9065	366.8557	395.0972
411.3229	415.8616	418.7906
420.6172	423.1572	428.5017
430.4359	434.5995	443.7399
452.4254	471.6120	475.0638
511.2149	518.6589	526.2383
543.7936	546.2287	550.0983
556.3773	569.9416	578.2331
592.5882	597.4709	599.9934
616.7388	624.6007	624.9971
625.6354	628.5565	631.6587
639.1571	654.7443	695.2128
703.9366	707.4994	713.0991
714.2973	720.0990	727.2620
729.0201	732.4803	736.8944
740.3386	746.3462	766.1384
771.4155	781.0199	782.1992
784.7251	790.1141	799.4396
812.3340	825.9101	862.3105
867.4003	868.5150	879.5164
879.9018	883.5847	887.6411
907.7987	928.1461	935.3955
954.8086	956.1912	957.9917
967.2548	969.9537	974.1329
981.5674	986.7842	1001.4148

1004.4936	1008.3644	1011.0101
1012.1566	1013.9597	1014.4692
1014.8164	1016.8656	1018.4702
1019.5606	1027.2330	1028.1492
1030.2904	1032.2652	1038.1818
1047.1662	1056.9472	1060.9263
1062.8098	1067.1590	1067.3040
1070.9965	1075.6578	1076.7778
1111.3105	1116.2418	1120.0832
1121.1808	1123.4015	1124.0317
1125.5650	1127.9974	1159.1311
1164.0165	1166.4723	1168.7904
1172.0353	1174.6598	1181.4131
1183.1204	1184.4585	1186.7164
1188.6693	1203.5745	1207.3355
1208.7425	1212.8141	1218.9900
1219.8869	1224.7923	1247.2498
1252.4999	1297.2859	1300.1281
1312.4498	1319.1896	1334.0218
1335.6107	1340.6367	1340.8803
1341.3604	1345.1049	1362.5727
1365.2840	1366.0302	1366.2089
1367.6307	1369.0605	1371.9523
1386.5111	1413.1575	1444.1593
1465.9877	1474.6070	1500.8131
1505.1809	1505.4760	1510.2365
1514.1765	1521.5255	1523.7017
1531.0758	1536.2053	1538.7705
1552.8103	1553.6706	1554.6558
1605.5174	1662.8921	1668.8064
1674.0197	1675.7752	1679.3330
1679.4008	1681.2839	1686.2891
1691.4657	1692.7729	1693.4018
1698.2840	1739.6134	3118.2717
3139.8908	3169.1615	3186.5865
3186.9716	3190.9041	3192.1279
3200.2204	3202.0369	3204.8935
3207.8400	3212.2948	3215.9698
3216.9074	3217.9228	3219.5612
3222.3104	3222.9572	3225.2644
3226.1833	3228.2937	3228.6663
3231.4666	3237.5315	3237.9020
3240.4830	3241.2720	3243.9796
3246.4642	3246.9295	3252.2870

3254.2711 3260.0876 3299.2653

TS3*SS*'''

Zero-point correction= 0.680522

Thermal correction to Energy= 0.723974

Thermal correction to Enthalpy= 0.724918

Thermal correction to Gibbs Free Energy= 0.603455

Sum of electronic and zero-point Energies= -3337.479780

Sum of electronic and thermal Energies= -3337.436328

Sum of electronic and thermal Enthalpies= -3337.435384

Sum of electronic and thermal Free Energies= -3337.556847

Cartesian coordinates

C	-8.254707	-0.746937	-0.098124
C	-8.120987	-0.798765	-1.490020
C	-6.925792	-0.449389	-2.110983
C	-5.864999	-0.051515	-1.305821
C	-6.006544	-0.005674	0.086863
C	-7.198903	-0.349754	0.714106
H	-9.198788	-1.021286	0.359036
H	-8.961925	-1.113328	-2.097418
H	-6.823621	-0.485329	-3.189721
H	-7.296256	-0.306265	1.793160
C	-3.836397	0.696600	-0.169199
C	-2.912593	0.998611	1.921214
C	-4.452471	0.791796	2.049481
H	-4.981429	1.707584	2.322943
S	-4.255753	0.487571	-1.822579
N	-4.820157	0.412237	0.682874
N	-2.722024	1.091352	0.440697
H	-2.620274	1.954228	2.359709
C	-2.123876	-0.130105	2.550401
C	-1.077959	0.149665	3.428327
C	-2.492362	-1.459110	2.319380
C	-0.405321	-0.887845	4.074167
H	-0.795118	1.181072	3.625945
C	-1.838364	-2.490423	2.980657
H	-3.295965	-1.692026	1.623241
C	-0.793547	-2.206353	3.859965
H	0.408237	-0.659439	4.754875
H	-2.132319	-3.518600	2.797238
H	-0.280848	-3.014156	4.372161
C	-0.466530	2.010433	0.426593
H	-0.593548	2.000054	1.503993
O	-1.876947	1.848709	-1.511512

C	-1.642497	1.700967	-0.310932
H	-4.694467	-0.003992	2.754205
C	0.380398	3.109638	-0.061566
C	0.828741	4.090632	0.835894
C	0.771282	3.208522	-1.404426
C	1.599174	5.161163	0.400631
H	0.557768	4.009973	1.885691
C	1.540998	4.285293	-1.838379
H	0.458471	2.442069	-2.103054
C	1.951405	5.268486	-0.944045
H	1.926229	5.914122	1.111692
H	1.826880	4.348932	-2.884285
H	2.552055	6.105856	-1.285915
C	-1.484314	-2.351448	-1.246623
C	-0.880387	-1.120745	-0.987796
C	0.085543	-1.007148	0.012831
C	0.476415	-2.160936	0.704342
C	-0.095575	-3.393898	0.417372
C	-1.095307	-3.490646	-0.548497
H	-2.242793	-2.419688	-2.021238
H	-1.140164	-0.259424	-1.589742
H	1.246794	-2.085352	1.468000
H	0.228806	-4.276898	0.960035
H	-1.555422	-4.449930	-0.764908
C	0.839351	0.238894	0.382184
H	0.895439	0.378290	1.458186
C	2.035896	0.562321	-0.267007
S	3.236584	1.453664	0.665705
S	2.439562	0.042210	-1.882216
O	1.315519	0.294892	-2.793477
O	3.806935	2.596556	-0.044019
O	3.762602	0.593369	-2.204933
O	2.624167	1.675987	1.986581
C	2.636616	-1.741296	-1.842068
C	1.692797	-2.543847	-2.471695
C	3.747089	-2.287910	-1.201371
C	1.847801	-3.927370	-2.430364
H	0.848032	-2.082162	-2.969142
C	3.889606	-3.670585	-1.163652
H	4.497426	-1.645321	-0.754504
C	2.938540	-4.489755	-1.772349
H	1.110193	-4.563916	-2.908316
H	4.749431	-4.106235	-0.664687
H	3.053658	-5.568471	-1.738768

C	4.567519	0.291844	0.935053
C	5.739992	0.397740	0.195880
C	4.370585	-0.731094	1.860695
C	6.736932	-0.559251	0.382552
H	5.843984	1.202218	-0.523024
C	5.369975	-1.681910	2.036155
H	3.447791	-0.771267	2.431974
C	6.548976	-1.597537	1.293381
H	7.657226	-0.497164	-0.188441
H	5.232383	-2.485702	2.751546
H	7.325718	-2.342959	1.429633

Vibrational frequencies

-303.7532	13.0973	23.0777
28.8308	31.5004	41.5887
45.8996	51.7040	56.8630
62.3446	66.4735	68.1498
69.8851	78.3910	80.9922
88.2129	92.6580	96.3794
105.1969	117.9191	121.4169
124.9695	140.8218	160.9586
167.3197	175.4871	187.0472
190.4384	197.4435	206.4378
209.7527	218.6408	226.9872
236.0340	239.6796	246.6818
263.3966	266.6061	271.6092
284.8053	305.3995	319.2997
325.7123	326.4272	339.6402
347.7253	376.5655	401.8463
410.5431	412.3738	417.6579
419.6862	422.1305	426.8495
430.9991	434.2397	451.5192
453.1609	472.5182	480.6820
504.4817	517.5715	525.4605
534.3642	542.8395	547.6666
561.0264	570.1061	585.0654
587.3665	593.8145	601.4074
612.2221	623.2709	623.8884
625.2919	627.9773	629.6160
632.8014	648.7719	686.8247
704.3281	705.4334	707.0241
712.1003	716.9703	718.3210
727.5393	730.4665	732.7078
741.8471	746.7844	769.8407
772.9817	774.5008	776.9933

785.8817	787.1835	803.9582
818.6973	836.1786	861.1724
867.7249	869.2188	870.2407
874.9661	877.9570	884.1116
912.0715	931.8226	941.4970
950.8801	952.2636	953.2312
959.6702	973.0907	987.5613
988.3233	990.7124	996.2688
998.7972	1004.0417	1005.8055
1008.2838	1010.6599	1014.5306
1015.8236	1016.3591	1017.6590
1019.5919	1021.6063	1024.0804
1026.3730	1027.1707	1034.2457
1050.8848	1058.7179	1060.4460
1062.3868	1063.1281	1064.8276
1071.3797	1072.2808	1073.6389
1105.2363	1111.2796	1115.1337
1116.8614	1118.2615	1123.7914
1125.5361	1127.6756	1154.5049
1158.7938	1160.6166	1167.2742
1173.2547	1174.6414	1175.4953
1183.4979	1186.1877	1186.4425
1193.7174	1197.9913	1202.7203
1206.8410	1208.3221	1212.9988
1216.4115	1220.8066	1243.9885
1257.8952	1284.2769	1298.9135
1300.3557	1315.2880	1325.7921
1326.9866	1334.7704	1338.4037
1339.1740	1343.6372	1346.9002
1362.4053	1363.3139	1364.2049
1364.9716	1365.2247	1367.5451
1392.6342	1414.8530	1437.8204
1461.9209	1470.2035	1495.5212
1498.7377	1500.8800	1507.5617
1510.8417	1516.6277	1525.8996
1528.5661	1534.5326	1537.9509
1551.4637	1552.9735	1554.4173
1608.2928	1668.2580	1668.9167
1675.0549	1677.5128	1679.8752
1681.6417	1682.0807	1682.2489
1692.3307	1692.8731	1693.8179
1695.8329	1734.7015	3116.4465
3157.2934	3184.1890	3184.3284
3185.2094	3194.7506	3196.1362

3197.6812	3201.2801	3203.0364
3205.3539	3206.6721	3211.3489
3214.4663	3214.5793	3216.6514
3219.5257	3219.9966	3220.6980
3220.7840	3222.5547	3222.8990
3227.6842	3228.1541	3234.6632
3239.2010	3242.3826	3243.7261
3247.8009	3248.5810	3254.5895
3255.2642	3256.9431	3277.0174

TCNE

Zero-point correction= 0.047687

Thermal correction to Energy= 0.056886

Thermal correction to Enthalpy= 0.057830

Thermal correction to Gibbs Free Energy= 0.012559

Sum of electronic and zero-point Energies= -447.316515

Sum of electronic and thermal Energies= -447.307317

Sum of electronic and thermal Enthalpies= -447.306373

Sum of electronic and thermal Free Energies= -447.351644

Cartesian coordinates

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

Vibrational frequencies

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

R1-R_1

Zero-point correction= 0.313900

Thermal correction to Energy= 0.333905

Thermal correction to Enthalpy= 0.334849

Thermal correction to Gibbs Free Energy= 0.261623
Sum of electronic and zero-point Energies= -1012.909632
Sum of electronic and thermal Energies= -1012.889628
Sum of electronic and thermal Enthalpies= -1012.888684
Sum of electronic and thermal Free Energies= -1012.961909
Cartesian coordinates

C	-2.537668	0.757936	-0.254393
C	-3.443139	1.465112	0.531690
C	-2.874968	-0.456514	-0.850477
C	-4.716577	0.952525	0.733669
H	-3.139418	2.408266	0.970519
O	-1.317437	1.363410	-0.478275
C	-4.146173	-0.973470	-0.648340
H	-2.153577	-0.986414	-1.458888
C	-5.041864	-0.260273	0.139778
H	-5.447898	1.474311	1.337362
C	-0.163361	0.642776	-0.333091
H	-4.448676	-1.912483	-1.093996
N	-6.384677	-0.807456	0.348715
C	1.013946	1.507046	-0.723488
O	-0.139273	-0.496862	0.039862
O	-6.661864	-1.862373	-0.195761
O	-7.153993	-0.177974	1.054536
C	2.346304	0.852299	-0.473600
H	0.877558	1.745691	-1.785597
H	0.923480	2.455720	-0.186454
C	2.709051	-0.304410	-1.165078
C	3.246962	1.390745	0.445745
C	3.942239	-0.906665	-0.938552
H	2.018835	-0.739127	-1.883173
C	4.481970	0.788371	0.667101
H	2.980655	2.291156	0.992969
C	4.849547	-0.371867	-0.019986
H	4.208032	-1.807605	-1.485405
H	5.166880	1.231296	1.385825
C	6.198153	-1.025106	0.215077
C	6.375067	-1.442784	1.678804
C	7.341617	-0.105418	-0.228221
H	6.231803	-1.930929	-0.402594
H	5.570559	-2.109498	2.000234
H	7.329466	-1.959499	1.816250
H	6.372538	-0.567354	2.336507
H	7.235031	0.179276	-1.278466
H	7.353750	0.810826	0.371431

H	8.307604	-0.602852	-0.100255

Vibrational frequencies

16.9960	27.2838	30.3768
42.2536	51.7261	55.8920
67.0593	88.9616	113.4471
166.8065	172.5089	204.4389
227.9105	240.8734	256.5147
265.3923	302.1336	330.6172
339.2809	393.1311	404.8442
413.6949	420.2607	424.6056
473.6186	509.1023	542.6827
546.1164	563.1704	574.6476
634.8884	648.6721	659.1692
697.8583	730.2067	737.8492
767.4367	787.9503	828.2689
846.8752	852.2951	874.7792
885.8111	886.4689	908.8897
919.8704	932.3735	948.8917
965.3697	973.2470	992.4248
994.0324	1000.8625	1001.3524
1032.0893	1040.0996	1079.4650
1122.2482	1143.0426	1144.9793
1148.2698	1163.3218	1180.4575
1191.3924	1209.7606	1215.5182
1250.7503	1256.8014	1282.2462
1309.3370	1328.5114	1349.6345
1351.9023	1377.6408	1387.9220
1393.2074	1408.0050	1425.4151
1450.4170	1474.8022	1479.8021
1483.9522	1491.7808	1498.0128
1508.2352	1513.5744	1550.0927
1581.1638	1669.2757	1681.1373
1688.2993	1711.6024	1739.2459
1895.6870	3060.9523	3062.9271
3074.3840	3078.0739	3134.1012
3140.1856	3144.0620	3146.6897
3148.4926	3199.7128	3201.2926
3214.8709	3219.5869	3241.1042
3249.7035	3257.9180	3260.8561

R1-R_3

Zero-point correction= 0.146649

Thermal correction to Energy= 0.158107

Thermal correction to Enthalpy= 0.159051

Thermal correction to Gibbs Free Energy= 0.106846

Sum of electronic and zero-point Energies= -664.227280

Sum of electronic and thermal Energies= -664.215822

Sum of electronic and thermal Enthalpies= -664.214878

Sum of electronic and thermal Free Energies= -664.267083

Cartesian coordinates

C	0.905086	0.337177	-0.264322
C	0.115752	1.450473	0.011620
C	0.349518	-0.930121	-0.438886
C	-1.259021	1.302449	0.121916
H	0.588426	2.417709	0.134727
O	2.254351	0.572074	-0.431528
C	-1.024487	-1.082833	-0.325660
H	0.983723	-1.779326	-0.657659
C	-1.802261	0.034871	-0.046210
H	-1.903697	2.144712	0.337548
C	3.169695	-0.218448	0.211818
H	-1.494664	-2.049357	-0.454387
N	-3.252435	-0.130444	0.074432
C	4.559112	0.213490	-0.147889
O	2.860795	-1.111881	0.951821
O	-3.713649	-1.249350	-0.072791
O	-3.921642	0.859466	0.316874
H	4.704130	0.104211	-1.224963
H	4.692018	1.268062	0.101357
H	5.277911	-0.397725	0.393025

Vibrational frequencies

27.2145	55.5950	61.5426
72.7037	95.0872	166.7287
246.8394	286.0966	325.9884
403.3374	423.1971	438.7246
512.0327	545.9118	591.9159
603.2707	638.5134	691.0795
721.5984	774.6053	829.9417
849.9643	886.1968	901.5502
957.2553	998.1857	1005.2947
1025.9916	1037.0436	1065.4708
1133.7115	1158.5337	1193.4228
1249.2277	1285.0430	1318.5915
1377.2121	1409.8907	1470.6562
1476.4588	1478.5024	1481.0008
1554.1215	1677.3938	1689.8121
1734.3206	1899.1188	3093.7391
3173.9468	3214.3665	3255.7553

3259.7657 3267.5977 3280.3713

M2-R_1

Zero-point correction= 0.443387

Thermal correction to Energy= 0.469078

Thermal correction to Enthalpy= 0.470023

Thermal correction to Gibbs Free Energy= 0.384825

Sum of electronic and zero-point Energies= -1587.194848

Sum of electronic and thermal Energies= -1587.169157

Sum of electronic and thermal Enthalpies= -1587.168212

Sum of electronic and thermal Free Energies= -1587.253410

Cartesian coordinates

C	0.282982	-0.658321	-0.168896
O	0.163706	-1.753928	0.432089
C	1.373758	0.076246	-0.565662
H	1.214068	1.025621	-1.062767
C	2.752416	-0.314567	-0.336813
C	3.139868	-1.497838	0.323974
C	3.791901	0.523330	-0.793324
C	4.484033	-1.806515	0.509579
C	5.128273	0.203404	-0.603444
C	5.507522	-0.972388	0.056015
H	4.746747	-2.727630	1.026854
H	5.891934	0.883248	-0.976780
C	-6.798130	-0.992050	-0.272740
C	-6.594158	-2.189338	0.418529
C	-5.309118	-2.623367	0.736811
C	-4.234711	-1.833735	0.348569
C	-4.449195	-0.632903	-0.341281
C	-5.727671	-0.192842	-0.663484
H	-7.807864	-0.676237	-0.510551
H	-7.446512	-2.791977	0.711158
H	-5.150316	-3.554495	1.269844
H	-5.879015	0.739295	-1.196636
C	-2.151998	-0.674705	-0.209695
C	-1.320427	1.239131	-1.149151
C	-2.859846	1.161232	-1.412750
H	-3.094848	0.982691	-2.464807
S	-2.503023	-2.150776	0.610405
N	-3.238946	-0.006498	-0.617589
N	-1.024587	-0.069567	-0.520632
H	-0.778001	1.304197	-2.095060
C	-0.942313	2.398950	-0.251748
C	-0.455326	3.574206	-0.822168

C	-1.135889	2.328619	1.128758
C	-0.164339	4.674718	-0.019062
H	-0.297049	3.626222	-1.896278
C	-0.843349	3.427599	1.930196
H	-1.499138	1.409621	1.581911
C	-0.358432	4.602587	1.357588
H	0.220853	5.584093	-0.468512
H	-0.988348	3.364779	3.003647
H	-0.125565	5.456987	1.984549
H	-3.376067	2.056175	-1.062621
H	2.369332	-2.165481	0.689521
H	3.532049	1.445501	-1.308625
C	6.966627	-1.326741	0.265938
C	7.693824	-0.266045	1.100022
C	7.689661	-1.549908	-1.067441
H	6.993414	-2.271079	0.824967
H	7.197522	-0.113183	2.062251
H	8.730526	-0.562961	1.288183
H	7.712225	0.694517	0.573982
H	7.196931	-2.328850	-1.655730
H	7.694591	-0.630434	-1.662720
H	8.730189	-1.846889	-0.901347

Vibrational frequencies

19.3849	24.3345	24.4667
31.3053	43.0325	48.8790
64.5889	66.8492	97.4182
106.6235	134.3795	138.1707
158.0181	166.7391	203.5362
204.7647	234.5378	244.1262
250.0092	268.8653	282.4026
286.6462	296.6878	321.4088
351.5135	358.6388	412.5141
422.0064	422.7971	433.1834
437.3504	441.7853	463.3850
513.9628	527.2971	547.6297
557.2840	566.2992	579.3613
586.9545	614.5755	628.7813
638.3599	651.4235	696.7862
707.7340	716.4205	719.5583
720.4705	732.6708	752.7099
762.0538	776.2631	788.2717
795.6778	818.0881	863.8824
871.8344	873.1481	883.9984
884.2881	917.3227	922.8348

927.1552	946.7800	968.0850
969.7485	981.3274	984.6765
995.7073	1001.8886	1017.6652
1020.1747	1031.6331	1032.7860
1042.2501	1048.7560	1060.3475
1067.4426	1072.3364	1075.7498
1125.2598	1127.1615	1141.1699
1143.7387	1157.4280	1163.5806
1176.7164	1180.0975	1184.0564
1185.4048	1206.3646	1211.6642
1216.8143	1246.7808	1249.6219
1268.6712	1292.2832	1298.5278
1322.7011	1330.5025	1334.3403
1341.3167	1347.2832	1363.2407
1364.6584	1386.6717	1393.4604
1404.4293	1418.3578	1421.5045
1456.0595	1466.5585	1493.3676
1498.7181	1501.8811	1507.6300
1509.2220	1513.5749	1514.6956
1527.9529	1541.7128	1554.9067
1568.9795	1636.6481	1646.9427
1676.2945	1684.9165	1689.3596
1691.8617	1698.1926	1738.9516
3055.1436	3055.5568	3058.2121
3114.8306	3131.9298	3135.1491
3136.5451	3146.0667	3147.7287
3172.0265	3173.6701	3180.9019
3190.2014	3196.5674	3201.2365
3217.2014	3220.8753	3223.6947
3224.0471	3230.6811	3234.0838
3236.7636	3247.3744	3250.7310

M2-R_2

Zero-point correction= 0.358542

Thermal correction to Energy= 0.379904

Thermal correction to Enthalpy= 0.380848

Thermal correction to Gibbs Free Energy= 0.305342

Sum of electronic and zero-point Energies= -1469.390446

Sum of electronic and thermal Energies= -1469.369085

Sum of electronic and thermal Enthalpies= -1469.368140

Sum of electronic and thermal Free Energies= -1469.443646

Cartesian coordinates

C	5.964328	-0.218069	0.317672
C	5.952965	-1.441620	-0.357720

C	4.752703	-2.070668	-0.681220
C	3.566107	-1.449202	-0.315023
C	3.587561	-0.220862	0.358786
C	4.780255	0.413013	0.686559
H	6.911210	0.251651	0.559725
H	6.890042	-1.911162	-0.634908
H	4.743981	-3.020735	-1.204338
H	4.781585	1.362354	1.210622
C	1.324836	-0.611244	0.205595
C	0.202173	1.165405	1.113801
C	1.734484	1.331818	1.380856
H	1.989761	1.219978	2.437473
S	1.905315	-2.030212	-0.584587
N	2.293297	0.216950	0.616581
N	0.114807	-0.176456	0.491494
H	-0.347404	1.148016	2.057822
C	-0.349176	2.250867	0.213401
C	-1.002459	3.342943	0.783128
C	-0.156452	2.204048	-1.168052
C	-1.458545	4.384920	-0.021013
H	-1.160337	3.375446	1.858180
C	-0.614215	3.244218	-1.970503
H	0.334423	1.346520	-1.621263
C	-1.263790	4.337228	-1.398683
H	-1.970358	5.228860	0.429661
H	-0.468241	3.199212	-3.044712
H	-1.622223	5.145583	-2.027419
C	-2.278340	-0.390037	0.511002
H	-2.267167	0.591300	0.969556
O	-0.795775	-2.049323	-0.415749
C	-1.084645	-0.966721	0.148650
H	2.107931	2.286034	1.006758
C	-3.580916	-0.988976	0.293153
C	-4.735021	-0.280785	0.690412
C	-3.778148	-2.255861	-0.298391
C	-6.009921	-0.800716	0.510690
H	-4.614686	0.698924	1.147437
C	-5.058331	-2.770251	-0.475433
H	-2.909376	-2.821138	-0.612781
C	-6.186097	-2.054521	-0.075494
H	-6.873411	-0.222894	0.828939
H	-5.176439	-3.748723	-0.933824
H	-7.180998	-2.464280	-0.217102

Vibrational frequencies

21.4629	25.1145	26.6223
35.2445	54.9906	69.6295
84.8922	98.2952	116.1568
164.5312	170.7133	191.1902
204.4316	225.8432	239.0963
274.4144	284.5836	308.6967
348.8467	351.2129	414.4344
420.3135	423.4461	433.3190
438.5499	508.0925	526.5581
530.0168	547.7091	564.8869
581.5011	592.3394	625.1612
628.8949	631.4215	643.3004
697.5360	699.1974	709.8313
718.8367	723.2092	732.0677
734.5357	767.0762	786.1252
790.6259	794.9626	813.0655
875.5953	877.5881	880.2756
881.9183	922.8404	931.1354
945.9460	966.1982	979.4726
999.4307	1003.7560	1006.9132
1012.9500	1017.8454	1022.0369
1029.3647	1040.9973	1052.8781
1062.5420	1067.2345	1071.2566
1073.1135	1116.4522	1124.6660
1127.7348	1159.5475	1165.9037
1173.9392	1180.9013	1181.8627
1184.0098	1208.4058	1208.6041
1220.0596	1244.9857	1263.4124
1294.7565	1298.7005	1329.0411
1335.9010	1341.6599	1364.4385
1365.4080	1367.0814	1387.3523
1419.5330	1462.7719	1474.7580
1507.3423	1512.6424	1515.2788
1528.7936	1542.3943	1552.8936
1555.5317	1644.5909	1648.5413
1676.8926	1678.9601	1685.6803
1694.1431	1701.8658	1740.8707
3112.9963	3131.6460	3184.4561
3193.0750	3194.1270	3200.4630
3203.9712	3210.5693	3210.7989
3214.2462	3218.5701	3220.1721
3223.3417	3227.3734	3229.5866
3231.2696	3235.6591	3257.0405

M2-R_3

Zero-point correction= 0.276091

Thermal correction to Energy= 0.292881

Thermal correction to Enthalpy= 0.293825

Thermal correction to Gibbs Free Energy= 0.229799

Sum of electronic and zero-point Energies= -1238.495320

Sum of electronic and thermal Energies= -1238.478530

Sum of electronic and thermal Enthalpies= -1238.477586

Sum of electronic and thermal Free Energies= -1238.541612

Cartesian coordinates

C	-1.176408	2.486024	-0.244839
O	-0.331105	3.209655	0.344862
C	-2.455696	2.686383	-0.657092
H	-3.042866	1.913298	-1.131396
C	4.202982	-2.149021	-0.193220
C	4.869747	-1.123467	0.482262
C	4.229832	0.081787	0.765705
C	2.911226	0.237694	0.360914
C	2.249397	-0.798594	-0.312623
C	2.880292	-2.002691	-0.601624
H	4.721727	-3.077510	-0.404591
H	5.899648	-1.263902	0.790548
H	4.748264	0.879099	1.287158
H	2.356181	-2.794960	-1.124866
C	0.604605	0.810936	-0.231276
C	-1.301091	-0.021033	-1.176429
C	-0.132754	-1.039784	-1.393705
H	0.169162	-1.114090	-2.441272
S	1.866923	1.665243	0.579569
N	0.941929	-0.430498	-0.609887
N	-0.624439	1.137789	-0.554869
H	-1.718068	0.292666	-2.136465
C	-2.396896	-0.581403	-0.294081
C	-3.547357	-1.107756	-0.879448
C	-2.238583	-0.638480	1.091481
C	-4.533577	-1.690913	-0.086847
H	-3.675363	-1.055910	-1.957661
C	-3.224274	-1.219666	1.882517
H	-1.352321	-0.212678	1.555012
C	-4.372656	-1.748478	1.294785
H	-5.429025	-2.093704	-0.548755
H	-3.098460	-1.255377	2.959677
H	-5.142067	-2.198112	1.913897
H	-0.382648	-2.029266	-1.007759

H	-2.911268	3.649070	-0.471114

Vibrational frequencies

23.1128	23.5700	56.1438
71.8386	84.8562	115.6717
147.4139	170.9960	201.2917
224.0948	241.9103	281.3687
292.1245	313.7307	373.1323
412.2440	416.4282	433.5802
436.1232	517.5932	533.2671
547.2580	568.3967	580.1197
596.1889	602.0495	626.7113
627.4136	657.6113	669.2688
709.5606	717.3644	720.5228
731.2794	750.4309	771.7940
786.8604	796.6583	874.0732
889.1307	903.3281	944.8866
972.2386	974.7596	1001.8626
1014.4470	1017.6760	1029.5064
1031.9714	1041.5147	1058.8708
1063.8447	1068.3865	1072.1238
1122.9255	1129.8760	1158.1565
1168.4746	1175.8968	1184.6033
1208.6258	1216.3992	1243.5378
1254.4122	1292.3376	1304.0758
1329.5039	1331.7102	1363.1254
1364.3792	1391.6185	1423.8959
1465.7822	1481.7004	1506.7688
1515.5950	1529.6026	1544.4276
1555.0585	1649.7551	1678.2044
1685.5311	1694.9554	1700.1931
1772.5480	3113.5541	3139.9357
3176.5319	3196.6430	3198.8753
3209.0726	3216.6702	3217.3860
3220.9252	3229.2754	3229.3532
3247.9738	3250.0151	3311.6043

TS3*SR*-R_1

Zero-point correction= 0.765473

Thermal correction to Energy= 0.813444

Thermal correction to Enthalpy= 0.814389

Thermal correction to Gibbs Free Energy= 0.680844

Sum of electronic and zero-point Energies= -3455.300895

Sum of electronic and thermal Energies= -3455.252923

Sum of electronic and thermal Enthalpies= -3455.251979

Sum of electronic and thermal Free Energies= -3455.385524

Cartesian coordinates

C	0.758325	-1.951837	-0.356726
O	0.901367	-2.456914	-1.477555
C	1.657343	-1.203208	0.430310
H	1.337286	-0.956026	1.435871
C	1.041587	0.866452	-0.280056
H	1.700958	1.139131	0.542240
C	-0.295964	1.184744	0.011079
C	3.098267	-1.162792	0.206089
C	3.734508	-1.671328	-0.941028
C	3.895935	-0.494421	1.148090
C	5.100388	-1.504853	-1.118006
C	5.264558	-0.326921	0.955680
C	5.894533	-0.825931	-0.186085
H	5.569930	-1.904439	-2.015464
H	5.840222	0.197437	1.712934
C	1.775242	0.877902	-1.565553
C	1.398322	0.190216	-2.726278
C	3.000882	1.561436	-1.559005
C	2.216188	0.217160	-3.851388
H	0.479530	-0.377270	-2.744669
C	3.806212	1.604452	-2.691052
H	3.328943	2.056754	-0.648868
C	3.414220	0.928821	-3.843642
H	1.914331	-0.326463	-4.741028
H	4.744452	2.149503	-2.664963
H	4.043198	0.946664	-4.728299
S	-0.636338	1.629641	1.672661
S	-1.674072	1.203535	-1.075922
O	-2.006724	1.229241	2.022748
O	0.468004	1.115379	2.502336
O	-1.176622	1.242595	-2.454354
O	-2.645860	0.151305	-0.740529
C	-2.477155	2.762091	-0.756535
C	-1.843242	3.931014	-1.175110
C	-3.708878	2.778494	-0.114266
C	-2.463986	5.150081	-0.932810
H	-0.877604	3.879049	-1.670225
C	-4.327020	4.006943	0.110774
H	-4.156474	1.844159	0.205343
C	-3.704722	5.184768	-0.294164
H	-1.981543	6.072185	-1.238869
H	-5.290523	4.042722	0.608050

H	-4.185207	6.139942	-0.107408
C	-0.576219	3.413215	1.776051
C	0.554665	4.084580	1.314013
C	-1.660150	4.088923	2.321011
C	0.592901	5.470579	1.402496
H	1.384401	3.537515	0.875730
C	-1.607979	5.479043	2.405330
H	-2.528913	3.531522	2.653393
C	-0.487852	6.165900	1.947349
H	1.463699	6.009149	1.044369
H	-2.450747	6.022588	2.819747
H	-0.454771	7.248682	2.009660
C	-6.153410	-3.091098	-1.207658
C	-5.796644	-3.334219	-2.538131
C	-4.466238	-3.285804	-2.945133
C	-3.502468	-2.983088	-1.991662
C	-3.866427	-2.750935	-0.659048
C	-5.192782	-2.798945	-0.245693
H	-7.197588	-3.130148	-0.917952
H	-6.566659	-3.559515	-3.267331
H	-4.190874	-3.469874	-3.977661
H	-5.459505	-2.610837	0.788486
C	-1.603606	-2.444547	-0.560029
C	-1.024982	-1.898399	1.596046
C	-2.572862	-1.924186	1.458230
H	-2.977870	-0.908617	1.460036
S	-1.747570	-2.847745	-2.223720
N	-2.744546	-2.501658	0.122378
N	-0.581137	-2.034833	0.180611
H	-0.709167	-0.933605	1.987901
C	-0.447197	-2.995476	2.461161
C	0.265599	-2.653007	3.609290
C	-0.635834	-4.341875	2.139270
C	0.782537	-3.648372	4.436168
H	0.417789	-1.602873	3.848508
C	-0.118426	-5.334780	2.963577
H	-1.186840	-4.617758	1.242731
C	0.590119	-4.988724	4.114462
H	1.339156	-3.375417	5.326557
H	-0.267047	-6.379142	2.709587
H	0.994136	-5.764730	4.756330
H	-3.042632	-2.549423	2.218381
H	3.141819	-2.180346	-1.691015
H	3.425989	-0.094558	2.045162

C	7.367521	-0.609408	-0.482388
C	8.213624	-0.328056	0.758657
C	7.531863	0.522937	-1.506741
H	7.742535	-1.532491	-0.944532
H	8.070631	-1.094356	1.525830
H	9.274025	-0.300550	0.492862
H	7.961027	0.643565	1.196247
H	6.965539	0.314112	-2.419078
H	7.158141	1.463719	-1.086934
H	8.584555	0.660481	-1.773722

Vibrational frequencies

-231.2952	6.3795	21.7530
23.2323	25.0746	28.0472
31.1469	33.4294	39.5220
42.8008	51.7860	54.1635
57.5662	65.6888	72.5811
77.6049	82.2439	93.9258
96.3698	97.3948	102.2073
118.7287	126.3321	131.4067
138.7049	144.7905	156.9742
165.5575	178.3624	183.0179
188.6745	192.4035	201.9188
208.0875	226.4268	231.0087
233.6745	241.7412	253.8602
256.6315	261.8032	276.2715
284.0795	294.7065	302.5695
305.1717	312.5606	319.4546
328.8268	332.3011	345.0690
356.7345	370.7264	386.3495
398.8046	408.2463	411.8053
414.5681	420.1676	429.4363
430.1879	434.1582	444.3731
456.5186	464.5545	466.5460
473.3468	492.2555	510.3344
523.7861	533.5084	542.9136
546.6086	552.1468	556.8162
572.7644	579.9154	584.3727
593.7784	597.2352	613.7926
618.0230	620.7355	621.0958
628.1322	634.9106	640.8520
649.6899	686.8800	700.1973
701.4928	702.2563	712.1262
720.9044	723.2146	730.6797
732.2400	734.0139	748.1637

752.0056	763.6803	764.4867
771.1818	771.9975	788.2635
793.2282	799.4410	822.0693
830.5209	857.0735	860.7898
864.0955	865.4150	869.4765
879.9637	881.8983	884.4123
893.0723	918.4313	929.2955
931.4335	944.3861	949.5870
953.9657	955.6050	970.7056
974.5959	978.6881	983.2509
990.7891	998.0295	998.0900
999.6832	1000.2693	1007.2361
1011.9264	1012.8500	1014.8281
1017.7372	1018.0712	1021.1555
1021.8508	1026.8966	1030.1964
1033.6244	1035.5492	1049.4784
1056.9659	1059.3511	1059.5522
1061.5500	1067.7559	1072.2453
1077.7901	1084.0515	1101.5121
1106.8502	1112.1959	1115.8041
1122.0522	1127.0915	1130.3055
1135.6952	1150.2715	1153.4687
1159.7878	1160.6274	1170.3273
1175.3370	1179.0242	1179.6898
1179.8480	1185.0465	1185.7900
1195.5691	1197.7731	1205.3233
1207.2931	1211.1354	1219.6076
1221.9617	1231.3696	1247.8005
1257.0717	1271.9866	1296.9953
1300.5697	1311.3280	1317.8648
1318.9727	1328.3944	1331.0107
1332.2013	1333.9357	1337.1229
1340.3529	1345.2407	1362.0120
1363.4651	1364.7982	1366.3298
1369.9169	1372.4218	1379.6647
1401.1050	1404.7065	1417.3238
1421.9374	1450.8516	1467.4847
1471.7438	1489.8796	1495.2482
1497.5821	1498.2372	1501.1228
1508.1721	1510.0593	1513.5684
1518.6859	1521.3366	1527.9439
1528.7098	1530.0082	1539.4012
1555.0254	1558.1434	1571.6918
1617.1611	1648.4704	1671.4058

1675.5339	1677.7210	1678.5333
1681.5824	1682.4974	1683.3348
1692.2072	1692.9392	1699.7167
1701.7271	1728.6950	3052.4687
3054.7703	3064.5545	3118.8995
3133.4495	3139.6262	3143.0905
3156.9054	3170.2274	3172.6535
3175.9660	3190.4836	3192.8628
3193.2095	3198.5850	3206.5922
3208.7912	3208.9548	3209.6083
3210.1937	3210.4546	3213.3059
3213.7940	3216.1241	3222.1861
3222.3356	3222.7925	3223.2193
3230.9465	3233.0112	3233.3395
3234.4764	3234.5237	3236.4748
3237.1279	3245.4030	3245.8015
3246.0139	3249.0630	3282.6845

TS3*SR*-R_2

Zero-point correction= 0.680759

Thermal correction to Energy= 0.724394

Thermal correction to Enthalpy= 0.725339

Thermal correction to Gibbs Free Energy= 0.602304

Sum of electronic and zero-point Energies= -3337.489125

Sum of electronic and thermal Energies= -3337.445490

Sum of electronic and thermal Enthalpies= -3337.444546

Sum of electronic and thermal Free Energies= -3337.567581

Cartesian coordinates

C	-7.552167	0.791874	0.663830
C	-7.495170	-0.588607	0.443458
C	-6.319660	-1.200231	0.018147
C	-5.200668	-0.399922	-0.180755
C	-5.265657	0.980367	0.049118
C	-6.437062	1.599518	0.471372
H	-8.481106	1.242725	0.994794
H	-8.379686	-1.193723	0.607693
H	-6.274799	-2.270547	-0.151875
H	-6.472318	2.669224	0.644993
C	-3.075725	0.728008	-0.591420
C	-2.049653	2.796082	-0.573124
C	-3.573176	2.958946	-0.248878
H	-4.114235	3.495790	-1.030767
S	-3.592358	-0.905595	-0.728399
N	-4.030550	1.570714	-0.196817

N	-1.918159	1.336128	-0.829260
H	-1.799597	3.324382	-1.496652
C	-1.187959	3.310025	0.560827
C	-0.460274	4.487168	0.389805
C	-1.212543	2.684938	1.811260
C	0.222748	5.052957	1.465590
H	-0.434240	4.968495	-0.584617
C	-0.526573	3.249261	2.882899
H	-1.748356	1.747835	1.938714
C	0.182561	4.439798	2.714698
H	0.783127	5.971460	1.325047
H	-0.546067	2.759128	3.850717
H	0.710669	4.880715	3.553915
C	0.377631	1.325132	-1.627394
H	0.388648	2.358057	-1.293338
O	-1.082370	-0.550787	-1.759960
C	-0.832974	0.623610	-1.474090
H	-3.726356	3.449647	0.713286
C	1.340691	1.003555	-2.677151
C	2.209414	2.018486	-3.117582
C	1.486240	-0.276443	-3.237191
C	3.178427	1.773047	-4.081387
H	2.123319	3.009653	-2.677255
C	2.461651	-0.518947	-4.200152
H	0.842932	-1.077169	-2.896620
C	3.310862	0.498019	-4.631073
H	3.835687	2.576751	-4.400161
H	2.564757	-1.519888	-4.609060
H	4.069308	0.300413	-5.382071
C	4.756431	1.723911	-0.644657
C	3.646966	0.881354	-0.633759
C	2.530877	1.199675	0.150878
C	2.541148	2.399489	0.878960
C	3.645091	3.240981	0.859794
C	4.764441	2.899684	0.099941
H	5.614594	1.461188	-1.255627
H	3.639176	-0.005654	-1.257723
H	1.669470	2.664718	1.470077
H	3.630331	4.159783	1.438208
H	5.632175	3.551517	0.081624
C	1.292728	0.396768	0.250000
H	0.518758	0.914016	0.810993
C	1.165767	-0.996958	0.329658
S	2.418990	-2.196815	0.071809

S	-0.208378	-1.559452	1.293553
O	0.228936	-2.095465	2.593166
O	1.853579	-3.479236	0.510535
O	-1.152024	-0.427878	1.369257
O	2.957676	-2.133603	-1.291422
C	-1.075353	-2.880117	0.457379
C	-2.093437	-3.470106	1.203578
C	-0.849437	-3.223122	-0.868597
C	-2.920626	-4.408375	0.594270
H	-2.240510	-3.193619	2.242977
C	-1.678192	-4.169170	-1.465357
H	-0.058725	-2.738905	-1.428506
C	-2.716670	-4.752071	-0.741363
H	-3.719242	-4.873207	1.162851
H	-1.513341	-4.446049	-2.501144
H	-3.363407	-5.482981	-1.216069
C	3.759210	-1.784390	1.182784
C	5.056777	-1.771137	0.683465
C	3.481312	-1.547331	2.526660
C	6.108310	-1.506363	1.557147
H	5.227771	-1.952321	-0.372351
C	4.541392	-1.280046	3.386965
H	2.454258	-1.568999	2.883174
C	5.849892	-1.260046	2.903551
H	7.126663	-1.486128	1.183858
H	4.346154	-1.086266	4.436323
H	6.671162	-1.048025	3.580504

Vibrational frequencies

-242.4528	6.9472	22.6208
27.1232	33.2618	34.2779
46.2257	47.1635	51.2963
55.4871	58.6293	62.3284
71.0768	81.0067	83.8830
85.6785	91.1555	95.3362
106.0976	116.2198	118.5098
122.5584	129.5832	156.7185
165.6505	171.1338	178.4788
187.5068	194.0359	198.4756
206.5904	210.4632	219.3047
231.9842	238.7668	251.1895
259.6546	271.6412	281.2589
284.9249	305.5513	311.8392
317.6046	327.7055	338.6948
339.8604	350.7558	376.2466

400.3717	410.0900	413.5205
417.7890	421.0250	429.7090
430.4514	433.2792	452.2089
455.9886	491.3467	510.7948
523.8070	528.4799	528.7304
540.0657	546.6123	548.9452
554.7585	571.4362	581.1565
587.7890	599.2758	609.0742
616.5662	620.6843	623.0343
625.3954	628.5312	632.2798
636.7046	649.1059	694.8826
705.0673	707.5785	709.0463
714.8074	716.4650	720.9882
728.7139	731.3150	732.1005
741.6346	750.5551	766.1920
776.3289	777.0933	783.3461
789.1346	792.2243	799.5744
820.4585	851.2709	860.8290
870.9756	871.6506	876.6556
876.9252	881.6105	883.6777
889.3438	927.5808	934.8991
948.3649	952.8200	966.4515
967.0324	968.6973	981.9573
983.8762	991.4206	1000.5931
1004.8931	1008.8401	1010.6432
1012.0505	1013.7835	1014.2922
1014.4184	1016.0856	1016.8933
1020.6234	1026.4180	1027.5398
1028.7646	1033.3372	1034.9786
1040.2256	1056.2453	1061.7766
1062.6806	1064.5058	1067.2754
1068.6804	1069.3621	1076.6705
1104.7270	1111.1680	1115.6415
1120.0524	1121.0106	1122.1522
1128.3884	1132.7924	1148.9055
1159.7280	1163.1962	1173.6946
1174.2405	1176.6250	1178.2935
1180.0882	1184.4127	1185.0026
1200.9934	1202.9269	1204.2868
1208.0391	1210.4442	1224.3391
1229.0844	1232.7434	1244.8601
1262.1314	1275.0273	1299.6045
1307.9829	1311.2229	1315.2836
1327.3580	1338.1904	1339.6308

1342.3995	1342.7012	1357.9060
1359.1050	1363.3332	1364.0517
1368.0351	1368.8384	1376.2523
1392.6478	1419.3666	1457.0950
1469.8953	1475.4388	1494.1087
1498.3848	1504.0240	1513.3389
1517.9007	1523.9019	1525.2045
1531.4541	1535.4600	1540.0853
1550.1233	1550.6490	1558.7175
1616.5210	1660.7156	1668.9166
1674.9829	1675.8801	1678.8928
1679.7293	1681.6391	1683.5118
1685.1328	1692.0917	1694.8169
1695.4668	1740.7374	3123.6537
3128.2677	3187.1964	3188.0366
3191.0311	3202.5344	3203.6163
3208.5784	3208.8095	3209.0320
3209.5555	3210.3201	3211.8371
3213.9419	3215.0396	3215.8554
3216.4695	3217.1501	3220.7107
3223.1427	3223.6279	3223.9405
3225.5154	3228.6071	3228.9391
3232.6864	3233.6601	3233.8200
3238.4896	3239.1735	3245.8495
3258.0516	3259.3638	3261.9124

TS3*SR*-R_3

Zero-point correction= 0.598412

Thermal correction to Energy= 0.637494

Thermal correction to Enthalpy= 0.638438

Thermal correction to Gibbs Free Energy= 0.525746

Sum of electronic and zero-point Energies= -3106.597627

Sum of electronic and thermal Energies= -3106.558545

Sum of electronic and thermal Enthalpies= -3106.557601

Sum of electronic and thermal Free Energies= -3106.670292

Cartesian coordinates

C	1.911906	-1.945383	0.837828
O	2.411520	-1.842269	1.975331
C	1.102015	-2.921341	0.287537
H	0.848145	-2.924751	-0.763708
C	-1.040539	-1.870848	0.870755
H	-1.339715	-2.707826	0.245773
C	-1.241942	-0.649956	0.252258
C	-0.945502	-2.232430	2.298160

C	-0.178173	-1.555807	3.253810
C	-1.655730	-3.379358	2.687519
C	-0.154360	-2.002892	4.570846
H	0.413027	-0.697877	2.967713
C	-1.643406	-3.812812	4.006957
H	-2.228735	-3.927909	1.944002
C	-0.890458	-3.121215	4.954555
H	0.448982	-1.473771	5.301294
H	-2.212354	-4.691492	4.292425
H	-0.869298	-3.459421	5.985715
S	-1.643398	-0.699682	-1.467569
S	-1.084422	0.965894	0.955977
O	-1.045518	0.464029	-2.135503
O	-1.291895	-2.039395	-1.960299
O	-1.285599	0.860539	2.402355
O	0.137418	1.624866	0.474335
C	-2.471602	1.876968	0.310019
C	-3.736365	1.600660	0.826677
C	-2.260561	2.857728	-0.651408
C	-4.822524	2.322665	0.348444
H	-3.861135	0.832650	1.583929
C	-3.356356	3.584772	-1.110706
H	-1.258352	3.029180	-1.028061
C	-4.629698	3.313722	-0.615453
H	-5.817612	2.115788	0.727253
H	-3.215138	4.357498	-1.858618
H	-5.481553	3.876674	-0.983636
C	-3.415353	-0.530623	-1.596141
C	-4.236595	-1.381490	-0.858432
C	-3.929516	0.435837	-2.450745
C	-5.614223	-1.251254	-0.983919
H	-3.809165	-2.118197	-0.184094
C	-5.312826	0.552326	-2.569070
H	-3.255313	1.089666	-2.993174
C	-6.149795	-0.285967	-1.838636
H	-6.270165	-1.899242	-0.412842
H	-5.733064	1.306653	-3.225879
H	-7.226487	-0.186393	-1.929518
C	3.646177	4.861870	0.039078
C	3.901967	4.800108	1.411969
C	3.764427	3.604691	2.113590
C	3.361503	2.475927	1.412468
C	3.117973	2.543291	0.034263
C	3.253772	3.732209	-0.672394

H	3.756015	5.805469	-0.483856
H	4.207675	5.694860	1.942503
H	3.956723	3.558036	3.179817
H	3.057599	3.770151	-1.738244
C	2.631017	0.348118	0.465183
C	1.956188	-0.657318	-1.479383
C	2.127888	0.871182	-1.715537
H	1.155447	1.362020	-1.808644
S	3.092325	0.839225	2.049480
N	2.762777	1.296259	-0.465533
N	2.124625	-0.773756	-0.009229
H	0.946982	-0.961830	-1.752870
C	2.953797	-1.521433	-2.217670
C	2.503190	-2.398914	-3.202395
C	4.320532	-1.433832	-1.942514
C	3.411120	-3.181380	-3.913222
H	1.436813	-2.471783	-3.403687
C	5.226419	-2.215646	-2.650719
H	4.679426	-0.758198	-1.169137
C	4.772621	-3.089649	-3.638720
H	3.052829	-3.865692	-4.675263
H	6.286799	-2.145859	-2.431280
H	5.480481	-3.700781	-4.189151
H	2.767483	1.085127	-2.572819
H	0.970405	-3.834594	0.852336

Vibrational frequencies

-235.0873	21.1596	24.3512
29.3203	31.1197	33.7382
37.6857	41.5035	53.0461
56.0148	65.4429	72.0456
76.5410	87.2837	92.7949
93.6077	106.0170	128.8416
133.3157	139.9951	156.7858
166.0650	182.2363	184.6867
189.1003	193.3176	203.9672
222.3494	229.5787	232.2034
239.9503	250.5137	256.5277
287.5902	290.2336	302.5962
306.0026	318.2299	325.8896
330.5484	346.2899	384.2497
388.2220	402.3408	411.3566
413.5258	414.4117	427.3473
433.4545	434.6579	447.2959
466.2599	475.6219	493.5291

518.0336	524.0173	532.9624
540.9212	549.9938	553.9077
570.8380	573.9462	583.0596
600.2008	607.2198	610.6675
620.7135	620.9993	627.3414
631.4752	636.0929	674.3589
682.3712	693.7143	699.9327
705.2423	711.6011	713.4625
718.6827	722.4981	732.6602
734.1331	739.5143	753.3229
757.4558	768.4887	772.4894
773.9215	785.6922	792.4870
802.1299	852.4279	869.9754
870.7147	873.1543	874.9314
882.6896	912.9820	948.2095
950.2857	955.7226	959.7674
962.8564	968.9480	979.6125
994.5375	999.7971	1002.9308
1005.9382	1009.8273	1012.3595
1012.7109	1016.7668	1018.6293
1018.8990	1023.5509	1029.7282
1030.0285	1032.6201	1038.6798
1043.4582	1060.0980	1061.2269
1063.0751	1064.0045	1069.0464
1072.5692	1073.5252	1106.2490
1111.7395	1119.8511	1121.6765
1123.2228	1129.1041	1130.2668
1158.4692	1160.6519	1165.2165
1171.1852	1177.6892	1180.5499
1183.4260	1183.6268	1184.2601
1203.2757	1207.5393	1209.3130
1218.1279	1224.6215	1230.5009
1262.1424	1275.3737	1296.6875
1299.0183	1311.4744	1323.1892
1327.2039	1330.6799	1339.5665
1340.3840	1341.1364	1363.5646
1364.5753	1365.8973	1366.7418
1368.7324	1378.6422	1405.1247
1417.5279	1469.1342	1488.1058
1494.8045	1498.1774	1500.0782
1500.2732	1513.3488	1528.3428
1532.0387	1533.3046	1535.2412
1540.0920	1556.6176	1565.8660
1626.7276	1669.3312	1675.3774

1677.3486	1678.3484	1680.7150
1681.5062	1684.1511	1693.3572
1693.6831	1702.5226	1732.0891
3119.5850	3188.2186	3191.2508
3192.0795	3193.2974	3195.9817
3207.0805	3208.5633	3208.9495
3211.4359	3216.2022	3216.7835
3218.0466	3220.7074	3221.1207
3221.9938	3223.1792	3226.2927
3229.8545	3230.1937	3231.2217
3237.1604	3238.3458	3238.5456
3240.1047	3242.1522	3242.3511
3248.9240	3289.9662	3310.5678

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