Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Deaminative Radical Reactions via Relayed Proton-Coupled Electron Transfer

Authors: Qianqian Shi, Kuohong Chen, Limin Guo, Lili Han, Donghui Wei*, and Yu Lan*

I Supplementary Methods

1. Computational Details

All calculations were carried out by using the Gaussian16 program[1]. All the structures were optimized at M06-2X[2] functional with 6-31G(d,p) basis set in dimethyl sulfoxide (DMSO) solvent using the IEF-PCM[3] solvation model. All reactants, products, and intermediates have no imaginary frequency, and each transition state has only one imaginary frequency. The free energies used in discussion were obtained at the M06-2X/6-311++G(d,p)/IEF-PCM$_{DMSO}$//M06-2X/6-31G(d,p)/IEF-PCM$_{DMSO}$ level (denoted as L1 level). Diagrams of FMO overlap/interaction changes were drawn by Chemcraft[4].

To ensure that the selected L1 level can be applied to obtain reliable results, we have additionally performed calculations for the relayed-PCET process involving stationary points **M3** and **^{os}TS3** by employing other different methods and basis sets, *i.e.*, M06-2X/6-311+G(d,p)/SMD[5]$_{DMSO}$//M06-2X/6-31G(d,p)/IEF-PCM$_{DMSO}$ (L2), ωB97X-D[6]/6-311+G(d,p)/IEF-PCM$_{DMSO}$//M06-2X/6-31G(d,p)/IEF-PCM$_{DMSO}$ (L3), and M06-2X/6-311+G(d,p)/IEF-PCM$_{DMSO}$//M06-2X/6-31G(d,p)/IEF-PCM$_{DMSO}$ (L4). As summarized in **Table S1**, there are small differences between the relative Gibbs free energies for the selected stationary points, so it can be concluded that the computed results and computational level L1 are reliable.

Table S1. Comparisons of relative Gibbs free energies for selected stationary points at the different levels L1~L4 (unit: kcal/mol).

	L1	L2	L3	L4
M3	0.0	0.0	0.0	0.0
^{os}TS3	4.2	4.3	5.9	4.2

2. Gibbs Free Energy Changes of the Stepwise PT-SET and SET-PT Pathways in Case Study 1

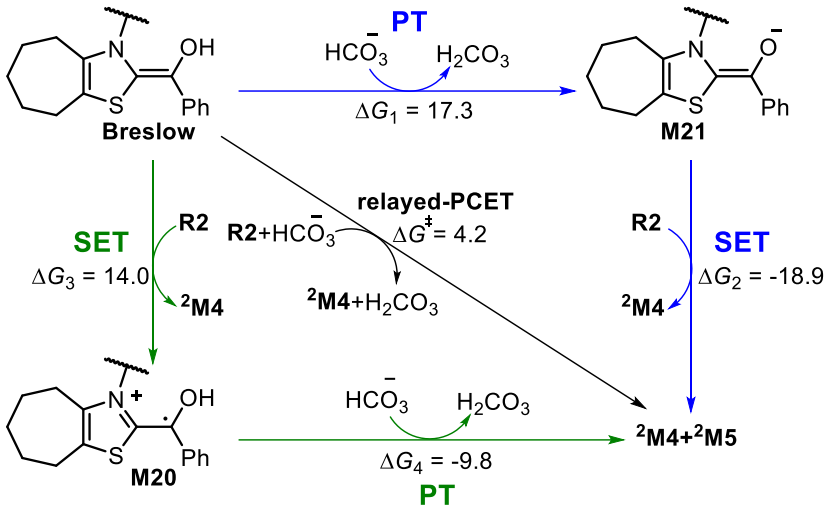


Fig. S1. The energy barrier and Gibbs energy changes of the possible pathways (unit: kcal/mol).

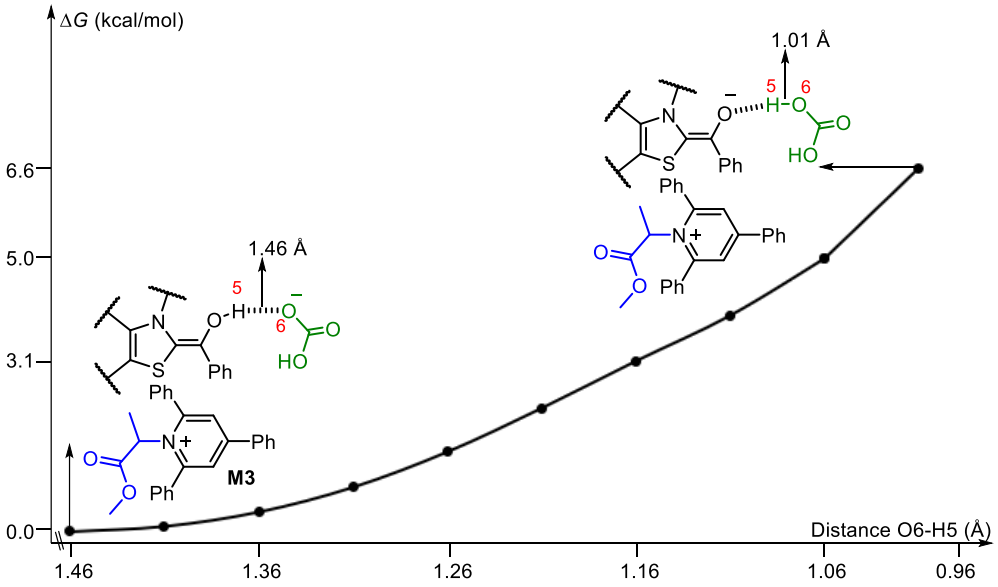


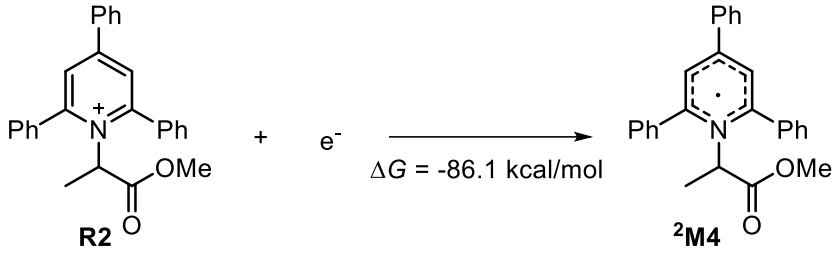
Fig. S2. The Gibbs free energy changes by reducing the O6–H5 distance in the first proton transfer process of the stepwise PT-SET pathway.

3. The Oxidation Potential

The oxidation potentials of intermediates Breslow, **^{2}M5**, and **R2** substrates (Sub) were calculated the reaction Gibbs free energies of the following reduction half-reaction:

$$Sub^{\bullet+} + e^- \longrightarrow Sub$$

For example, to calculate the oxidation potential of **R2**, the reaction Gibbs free energy of the following reduction half-reactions was calculated using the DFT-computed Gibbs free energies in DMSO solution and the Gibbs free energy of electron (−0.867 kcal/mol).[7]



Since $\Delta G = -nFE$, where n is the number of electron transferred (one), F is the Faraday constant (F = 96.485 kJ mol^{-1} V^{-1} = 23.083 kcal mol^{-1} V^{-1}), the absolute standard reduction potential can be calculated as: E = 4.76 V Then, the standard potential referenced to the SCE can be calculated from[8]

$$E^{\Theta,SCE}_{solvent} = E^{\Theta,abs}_{solvent} - E^{abs}_{SCE,aq} + E_L$$

where $E^{\Theta,abs}_{SCE,aq}$ is the absolute standard potential for the aqueous saturated calomel electrode (4.522 V) and E_L is the interliquid (intersolvent) potential. Because the experimental value of interliquid potential of toluene is not available, we used the EL value of ethanol (0.030 V).[9] Thus, the oxidation potential of **R2** can be calculated as follows:

$$E^{\Theta,abs}_{SCE,aq} = 3.728 \text{ eV} - 4.522\text{V} + 0.030\text{V} = -0.76 \text{ V}$$

The oxidation potentials of other substrates were also calculated using this approach. The reaction Gibbs free energies of the following substrate reduction half reactions were calculated using the above method and presented as follows:

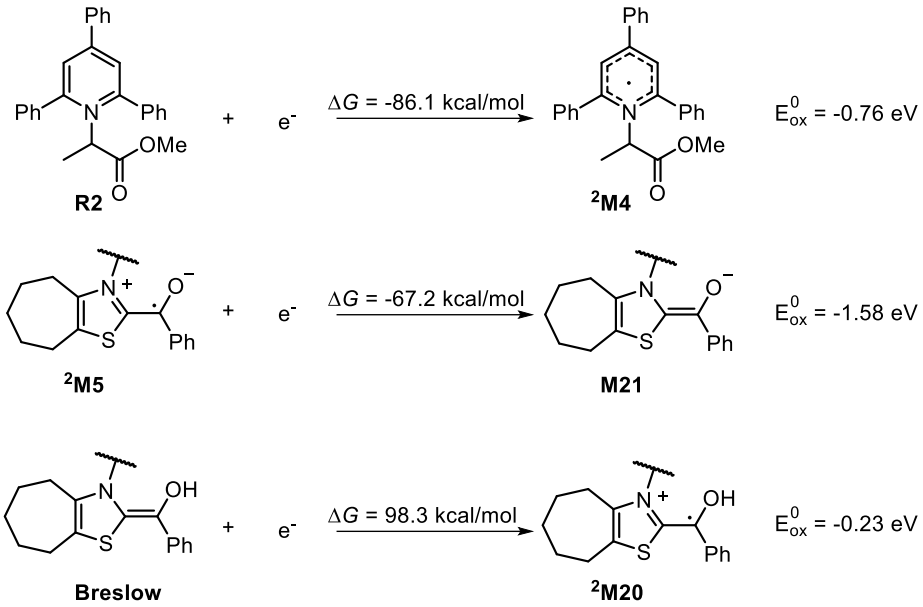


Fig. S3. Calculation results of oxidation potentials of the substrates.

4. The Possible Self-Coupling Pathway between Two ^{2}M5 Intermediates

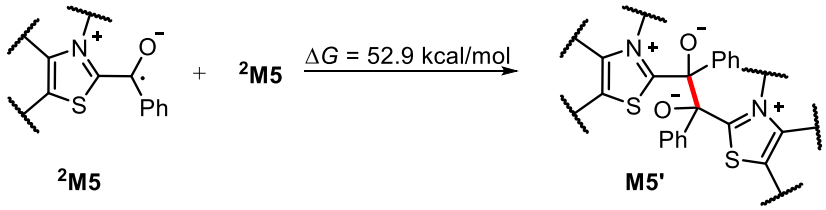
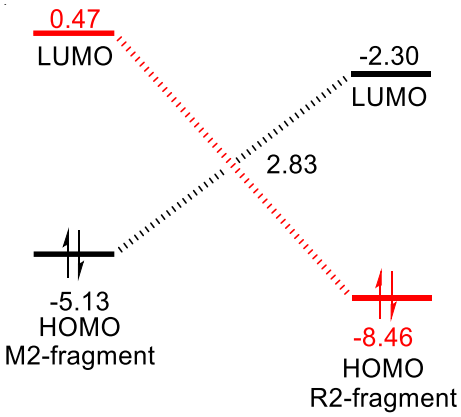


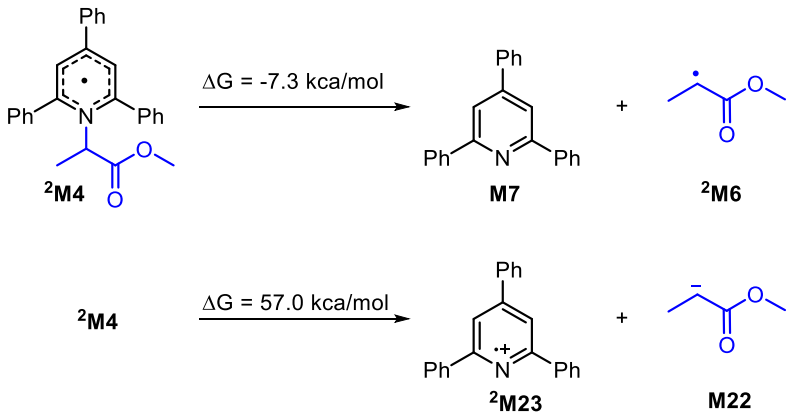
Fig. S4. The possible self-coupling pathway between two **^{2}M5** intermediates.

5. Energy Gap involved in Relayed-PCET Process of Case Study 1



Scheme S1. The energy gap between LUMO (R2-fragment) and HOMO (M2-fragment) involved in the relayed-PCET of case study 1. (Unit: eV)

6. Possible Pathways of N-C Bond Cleavage in Case Study 1



Scheme S2. The Gibbs free energy changes of possible pathways of N-C bond cleavage in case study 1.

7. Open-Shell Singlet and Triplet Diradical Intermediates ^{os}M9-F and ^{t}M9-F

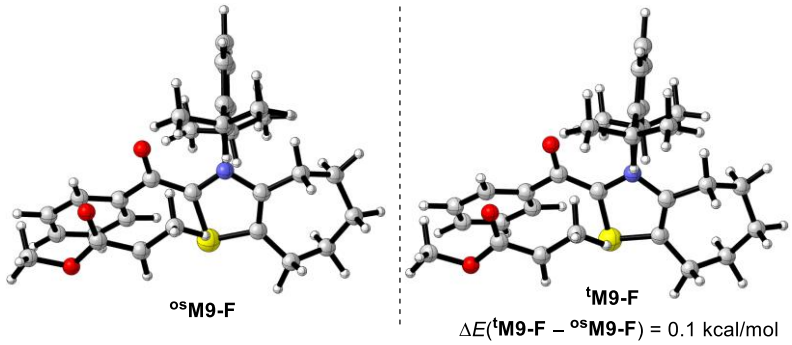


Fig. S5. Open-shell singlet and triplet diradical intermediates **^{os}M9-F** and **^{t}M9-F**.

8. Three Dimensional Structures of the Transition States involved in Case Study 1

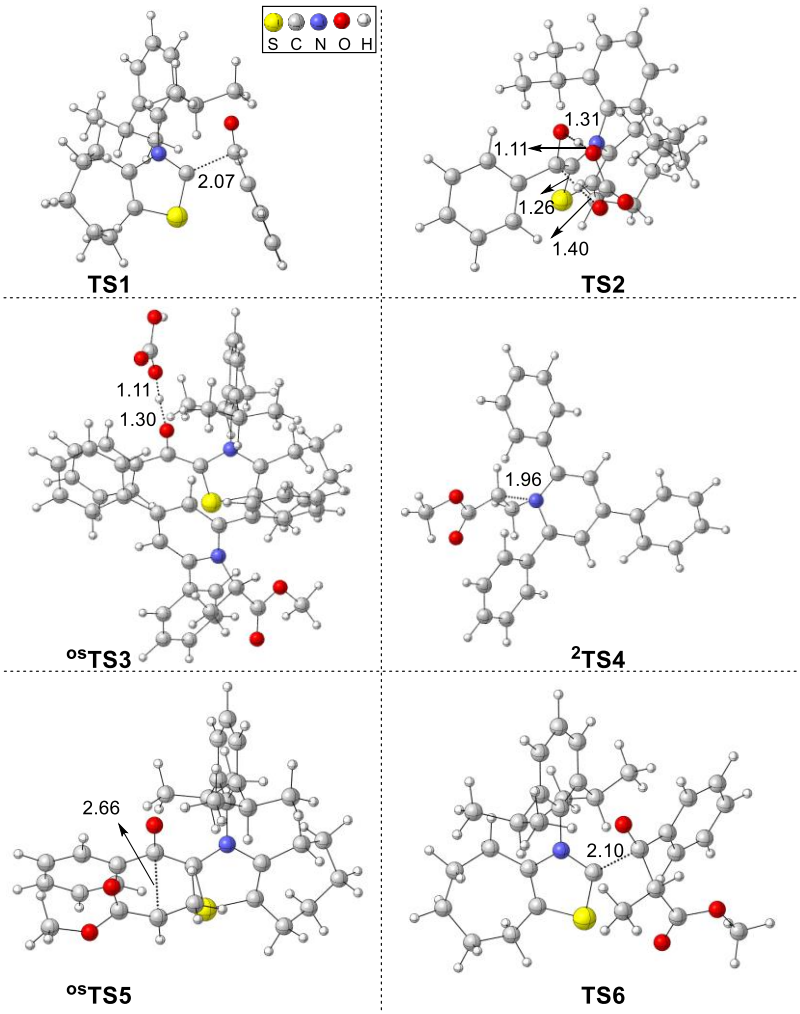


Fig. S6. Three dimensional structures of the transition states involved in case study 1. (unit: Å)

9. Evolution of Spin Population Value during Radical-Radical Cross-Coupling Process in Case Study 1

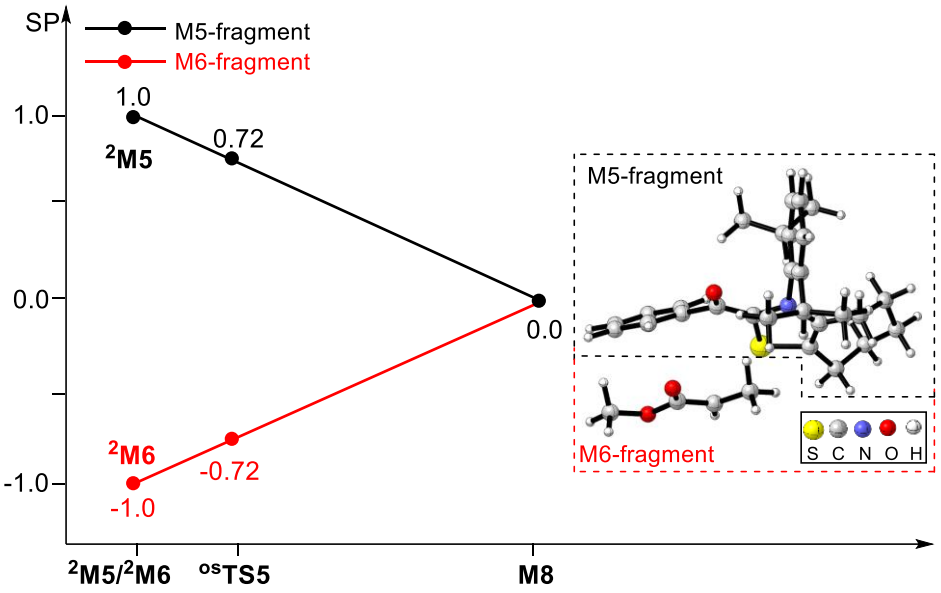


Fig. S7. Evolution of spin population (SP) values during radical-radical cross-coupling process. The SP(M5) represents the sum of SP values of the atoms in M5-fragment, and the SP(M6) represents the sum of SP values of atoms in M6-fragment.

10. FMO Diagram of Key Structures of Radical-Radical Cross-Coupling Process in Case Study 1

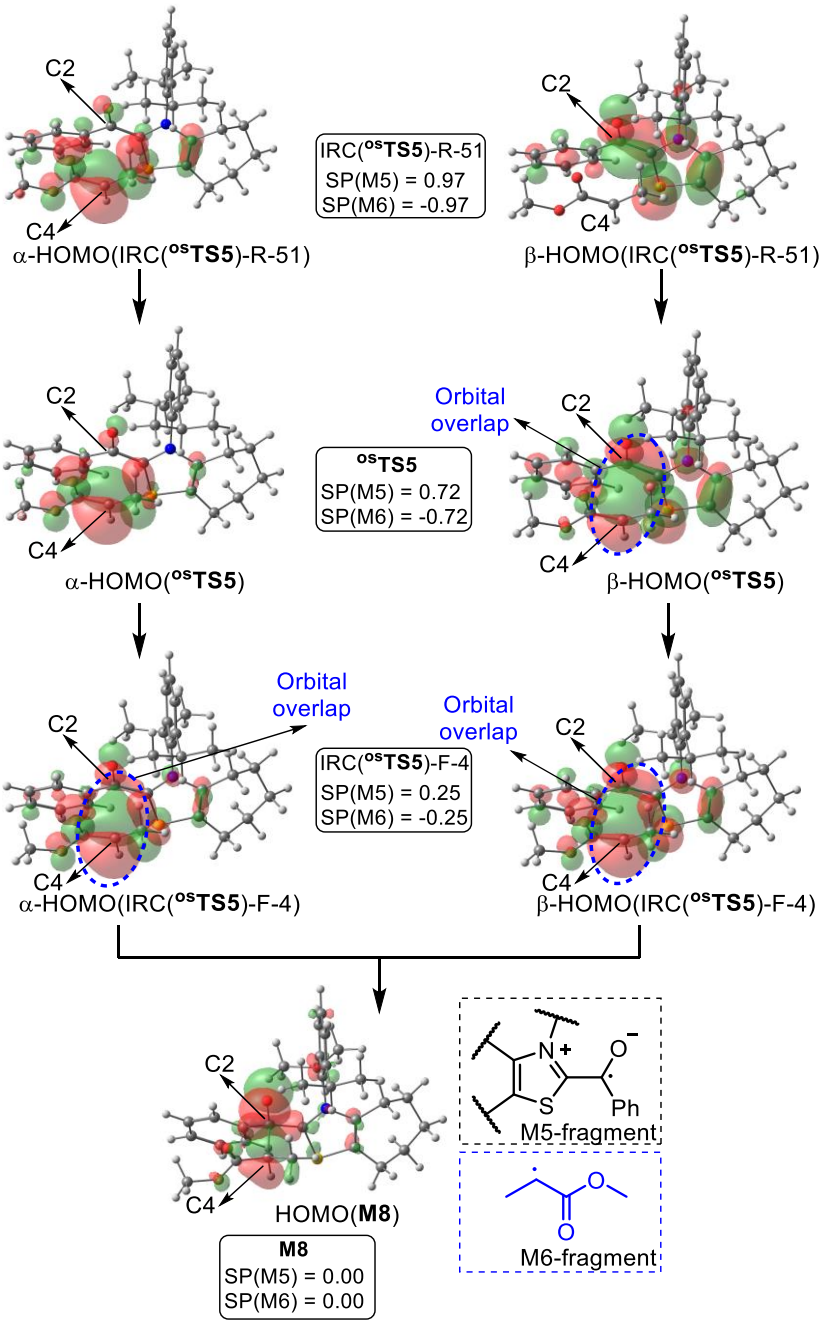
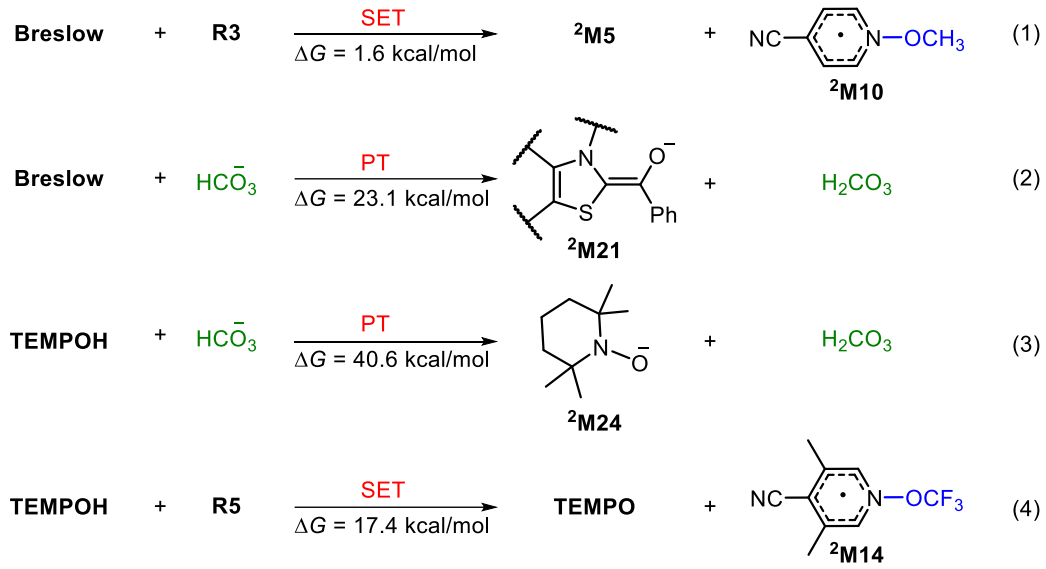


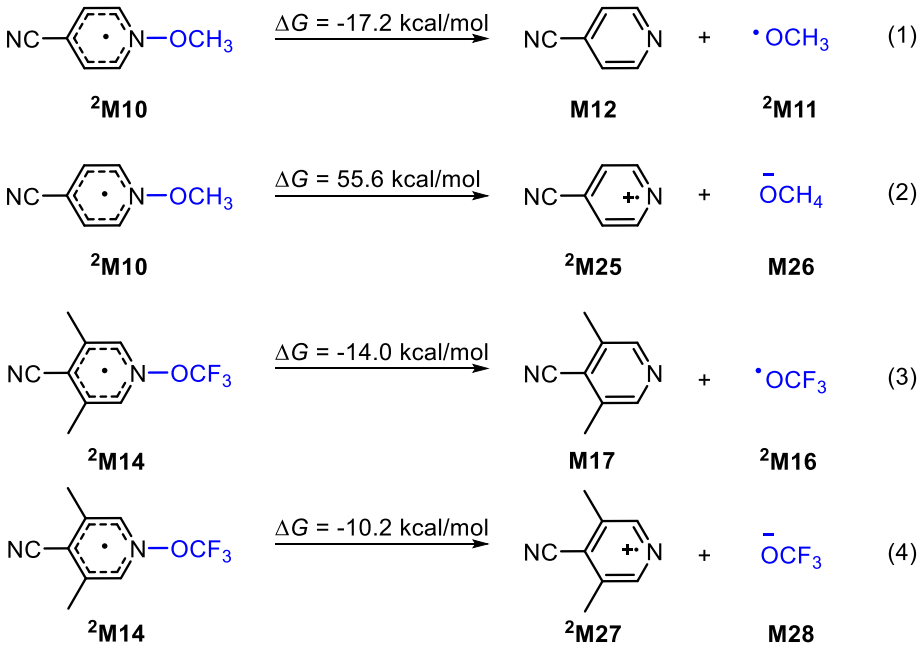
Fig. S8. FMO diagram of key structures of radical-radical cross-coupling process (the SP(M5) represents the sum of SP values of the atoms in M5-fragment, and the SP(M6) represents the sum of SP values of atoms in M6-fragment).

11. The Gibbs Free Energy Changes of the First SET and PT Processes in the SET-PT and PT-SET Pathways



Scheme S3. The Gibbs free energy changes of the first SET and PT processes in the stepwise SET-PT and PT-SET pathways in case studies 2-3.

12. Possible N-O Bond Cleavage Pathways in Case Studies 2 and 3



Scheme S4. The Gibbs free energy changes of possible N-O bond cleavage pathway in case studies 2 and 3.

13. Three Dimensional Structures of the Transition States involved in Other Case Studies

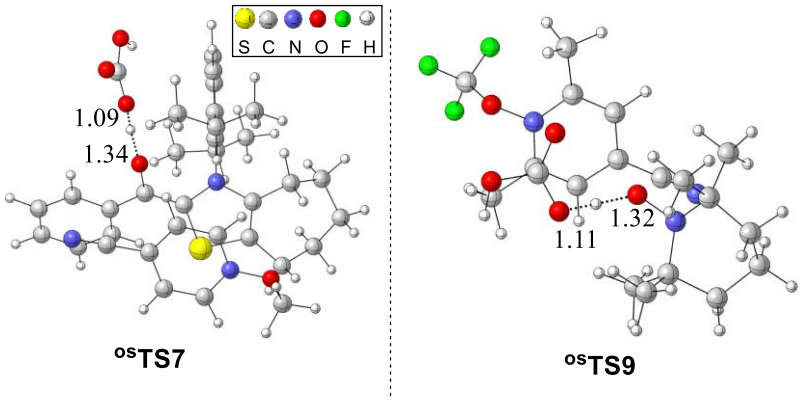


Fig. S9. Three dimensional structures of the transition states involved in other case studies (unit: Å).

14. ELF Analysis Graphs in a Selected Plane of ^{2}TS10 along the IRC Results

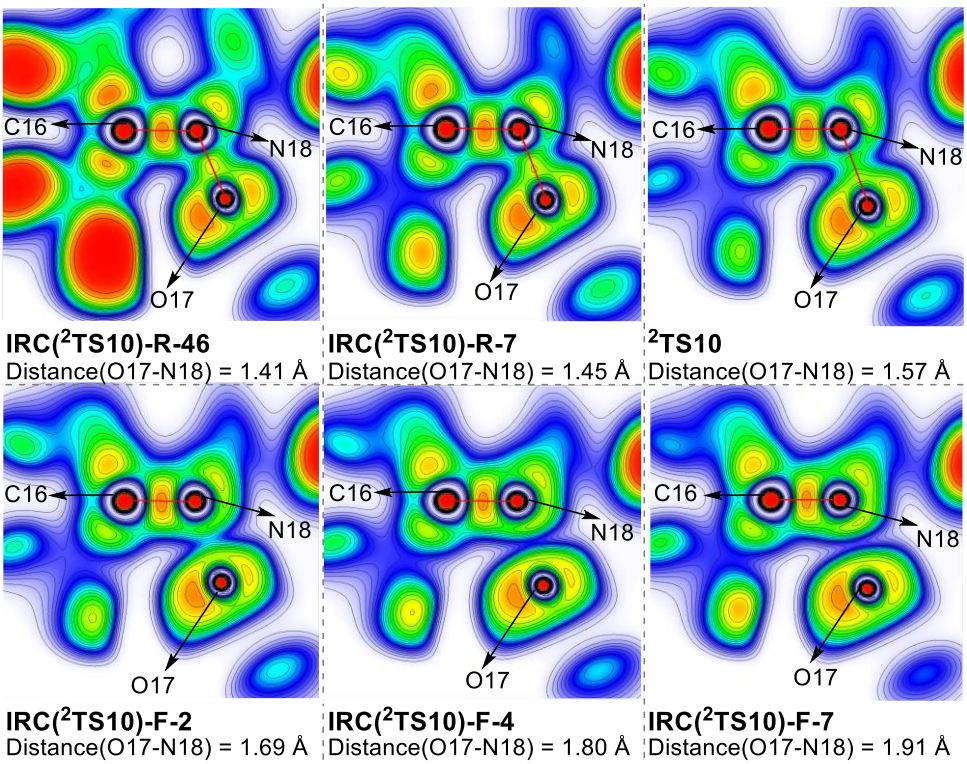


Fig. S10. ELF analysis graphs in a selected plane of **^{2}TS10** along the IRC results (F represents the forward direction, and R represents the reverse direction).

15. FMO Diagram of Key Structures of Relayed-PCET Process in Other Case Studies

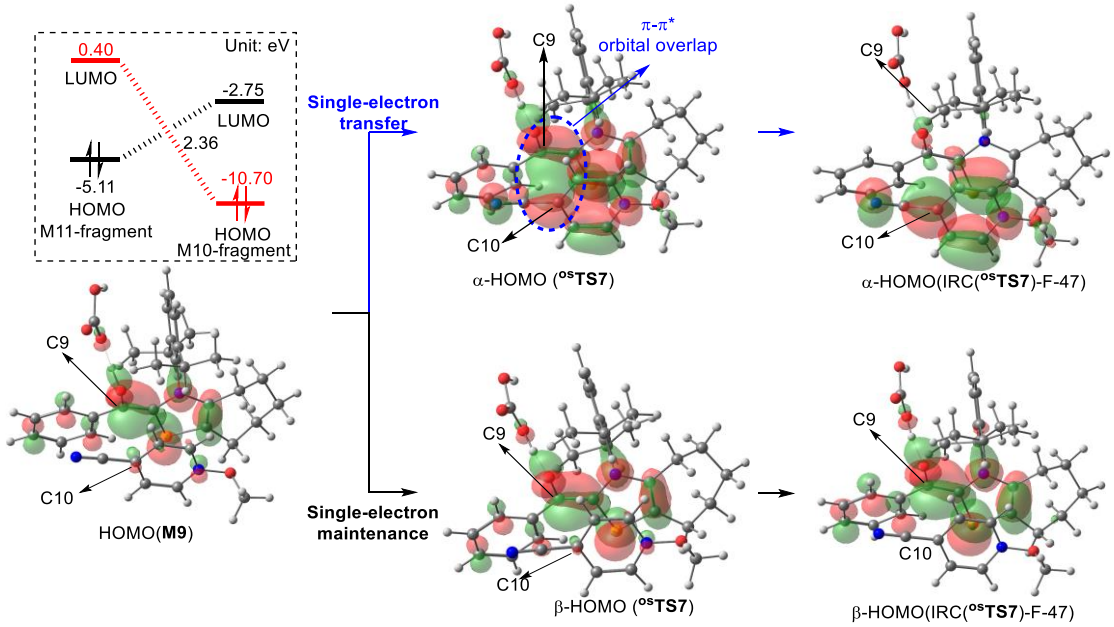


Fig. S11. FMO diagram of key structures of relayed-PCET process and energy gap between FMOs involved in transition state **^{os}TS7** in case study 2.

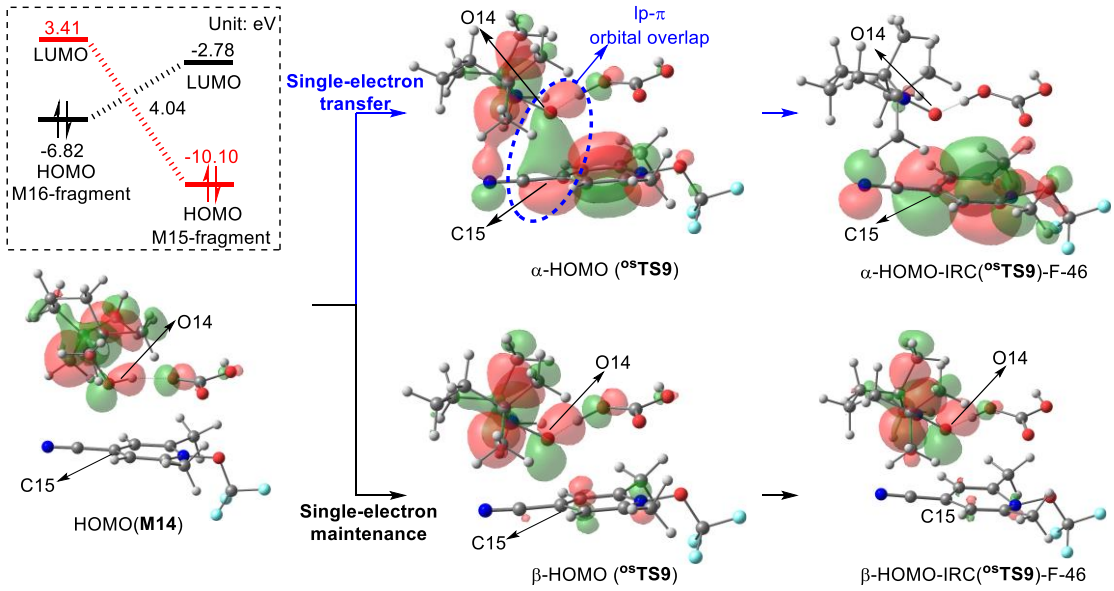


Fig. S12. FMO diagram of key structures of relayed-PCET process and energy gap between FMOs involved in transition state **^{os}TS9** in case study 3.

16. N-N Bond Cleavage Model

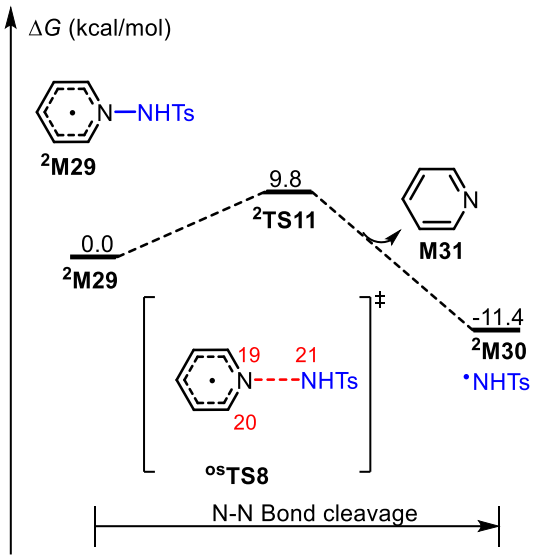


Fig. S13. Gibbs free energy profile of the N-N bond cleavage model.

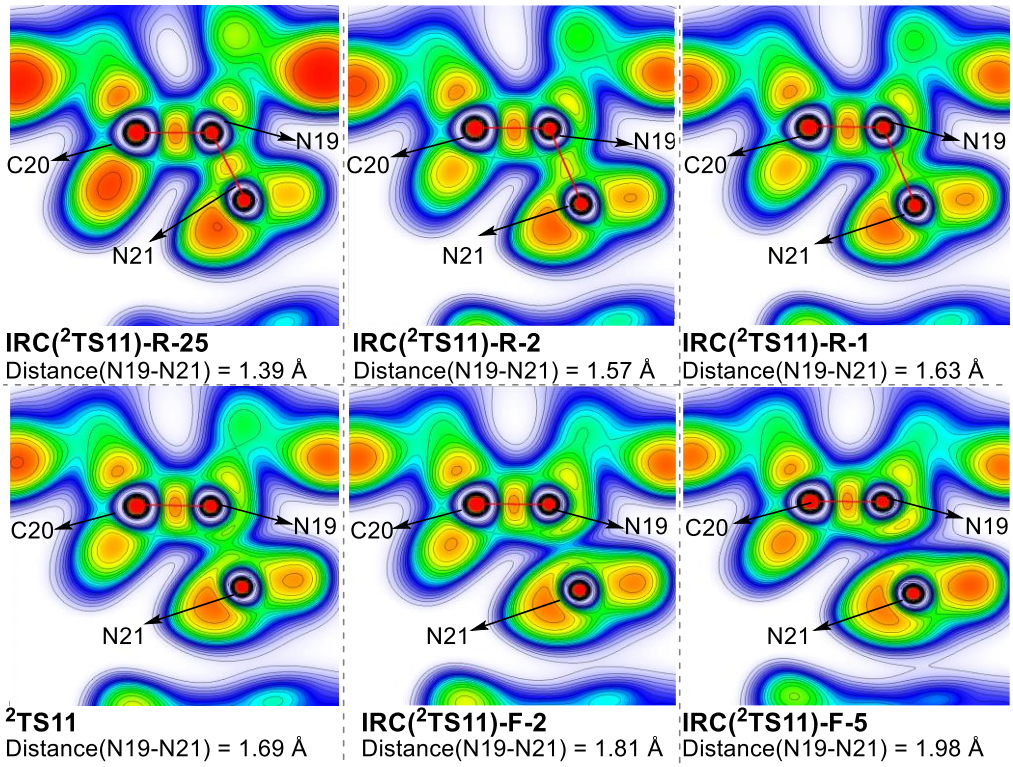


Fig. S14. ELF analysis graphs in a selected plane along the IRC results of transition state **^{2}TS11** (F represents the forward direction, and R represents the reverse direction).

17. Absolute SPE, GFEC, and GFE of the Optimized Structures

Table S2. The single-point energies (SPE) at M06-2X/6-311++G(d,p)/IEF-PCM$_{DMSO}$ level, Gibbs free energy corrections (GFEC) at M06-2X/6-31G(d,p)/IEF-PCM$_{DMSO}$ level, and Gibbs free energies (GFE = SPE + GFEC) of the stationary points involved in case study 1 (unit: a.u.).

	SPE (a.u.)	GFEC (a.u.)	GFE (a.u.)
pre-NHC	-1231.628697	0.392991	-1231.235706
CO_3^{2-}	-264.046117	-0.01094	-264.057057
NHC	-1231.150299	0.379690	-1230.770609
R1	-345.523172	0.080499	-345.442673
R2	-1248.193935	0.391717	-1247.802218
HCO_3^-	-264.552811	0.001269	-264.5515420
H_2CO_3	-265.007231	0.014281	-264.99295
TS1	-1576.672305	0.483485	-1576.188820
M1	-1576.682767	0.486590	-1576.196177
TS2	-1841.237011	0.502479	-1840.734532
M2	-1841.274106	0.509539	-1840.764567
M3	-3089.492459	0.928533	-3088.563926
^{os}TS3	-3089.481146	0.923977	-3088.557169
^{2}M4	-1248.326764	0.388789	-1247.937975
^{2}M5	-1576.10735	0.471694	-1575.635656
^{2}TS4	-1248.300549	0.385790	-1247.914759
^{2}M6	-307.008051	0.074222	-306.933829
M7	-941.30564	0.286825	-941.018815
^{os}TS8-F	-1883.127647	0.571878	-1882.555769
^{t}TS8-F	-1883.127436	0.570391	-1882.557045
^{os}TS5	-1883.123939	0.573394	-1882.550545
M8	-1883.163045	0.580995	-1882.58205
TS6	-1883.148253	0.580339	-1882.567914
P	-652.000444	0.171494	-651.82895
M19	-1576.705440	0.485962	-1576.219478
^{2}M20	-1576.545884	0.484429	-1576.061455

^{2}M21	-1576.213679	0.472393	-1575.741286
M22	-307.145411	0.072928	-307.072483
M23	-941.061015	0.283380	-940.777635
M5′	-3152.172265	0.988252	-3151.184013
M3(L2)	-3089.513453	0.928533	-3088.584892
^{os}TS3(L2)	-3089.502055	0.923977	-3088.578078
M3(L3)	-3089.748762	0.928533	-3088.820201
^{os}TS3(L3)	-3089.734796	0.923977	-3088.810819
M3(L4)	-3089.491501	0.928533	-3088.56294
^{os}TS3(L4)	-3089.480211	0.923977	-3088.556234

Table S3. The single-point energies (SPE) at M06-2X/6-311++G(d,p)/IEF-PCM$_{DMSO}$ level, Gibbs free energy corrections (GFEC) at M06-2X/6-31G(d,p)/IEF-PCM$_{DMSO}$ level, and Gibbs free energies (GFE = SPE + GFEC) of the stationary points involved in other case studies (unit: a.u.).

	SPE (a.u.)	GFEC (a.u.)	GFE (a.u.)
R3	-455.357978	0.099821	-455.258157
M9	-2296.655317	0.632925	-2296.022392
^{os}TS7	-2296.649054	0.628248	-2296.020806
^{2}M10	-455.508796	0.095188	-455.413608
^{2}M11	-1576.10735	0.471694	-1575.63566
^{2}TS8	-455.489038	0.093189	-455.395849
^{2}M12	-340.482216	0.014762	-340.423969
M13	-115.034831	0.058247	-115.020069
TEMPOH(R4)	-484.243093	0.240265	-484.002828
R5	-753.094726	0.073157	-753.021569
M14	-1580.552346	0.410003	-1580.142343
^{os}TS9	-1580.528676	0.406399	-1580.122277
^{2}M15	-831.879821	0.121982	-831.757839
^{2}M16	-483.631594	0.226748	-483.404846
^{2}TS10	-831.877933	0.121822	-831.756111
^{2}M17	-412.776775	-0.01174	-412.788514
M18	-419.103419	0.108726	-418.994693

^{2}M24	-483.723382	0.226687	-483.496695
^{2}M25	-340.20353	0.055983	-340.147547
^{2}M26	-115.194901	0.014416	-115.180485
^{2}M27	-418.833707	0.106480	-418.727227
^{2}M28	-413.039208	-0.010650	-413.04986
^{2}M29	-1122.996281	0.189516	-1122.80677
^{2}TS11	-1122.980146	0.188959	-1122.79119
^{2}M30	-874.751366	0.104721	-874.646645
^{2}M31	-248.243764	0.06238	-248.181384

18. The Energies, Cartesian Coordinates, and Frequencies of the Stationary Points

pre-NHC
Zero-point correction= 0.444143
Thermal correction to Energy= 0.466116
Thermal correction to Enthalpy= 0.467060
Thermal correction to Gibbs Free Energy= 0.392991
Sum of electronic and zero-point Energies= -1230.973736
Sum of electronic and thermal Energies= -1230.951764
Sum of electronic and thermal Enthalpies= -1230.950819
Sum of electronic and thermal Free Energies= -1231.024888

Cartesian coordinates

C	-3.729114	0.412062	-1.847625
C	-4.265230	-0.073022	-0.498388
C	-3.561525	-1.315252	0.066917
C	-2.318583	1.006822	-1.834216
C	-2.170083	-1.035476	0.553604
C	-1.192554	-0.006498	-1.576389
C	-1.145840	-0.480226	-0.155403
H	-4.414475	1.176046	-2.228191
H	-5.323205	-0.325507	-0.617579
H	-3.507056	-2.093732	-0.704505
H	-2.260682	1.810236	-1.088688
H	-1.323510	-0.876632	-2.231727
C	-0.126999	-0.799889	1.865771
H	-3.761346	-0.417622	-2.566675
H	-4.212196	0.736721	0.238927

H	-4.149959	-1.729901	0.889115
H	-2.126140	1.465755	-2.808803
H	-0.225774	0.435617	-1.832134
N	0.003560	-0.363693	0.623039
C	1.264618	0.174252	0.141760
C	1.435994	1.563557	0.165562
C	2.226650	-0.728945	-0.325316
C	2.667677	2.051021	-0.274458
C	3.439338	-0.185327	-0.754854
C	3.659868	1.186545	-0.724114
H	2.850405	3.121072	-0.265278
H	4.217642	-0.847607	-1.121330
H	4.610050	1.586705	-1.061932
C	0.357367	2.518869	0.645465
C	0.054961	3.588167	-0.410780
H	-0.798792	4.193725	-0.094441
H	0.907758	4.259386	-0.548934
H	-0.181329	3.137797	-1.379738
C	1.995787	-2.229185	-0.385499
S	-1.672258	-1.391530	2.168843
H	-0.566636	1.953886	0.815241
H	0.970497	-2.442230	-0.065067
C	0.761260	3.160224	1.978624
H	1.678686	3.745446	1.859337
H	-0.027684	3.830847	2.329677
H	0.938693	2.401864	2.746123
C	2.947060	-2.966767	0.564050
H	2.742645	-4.040518	0.541179
H	3.988820	-2.814129	0.264932
H	2.835291	-2.615434	1.593390
C	2.141243	-2.745948	-1.821913
H	1.916702	-3.815338	-1.857733
H	1.459119	-2.226380	-2.500562
H	3.162164	-2.604309	-2.189148
H	0.680142	-0.765329	2.584984

Vibrational frequencies

18.4913	33.9756	49.7700
64.7518	71.5870	81.6406
98.7502	113.5461	130.1967
149.3363	196.5353	218.9578
222.8461	233.0879	245.5795
250.4442	254.0616	267.1884
278.7900	297.7052	308.3173

322.9212	334.5551	358.7808
376.9377	400.9459	409.4944
447.6350	467.1427	496.1541
515.4408	529.7627	562.1224
580.4966	616.7825	621.3995
652.4319	659.7425	715.5085
732.2973	779.2200	789.0298
812.0291	820.6504	830.8887
838.1438	839.7226	896.5807
908.8410	915.7690	933.4374
937.6509	950.4610	956.5432
969.4299	973.3201	975.6093
978.2071	985.2651	1013.1534
1028.7453	1056.4737	1074.4545
1084.8184	1093.9608	1124.9263
1128.5851	1145.0749	1147.6588
1155.4129	1173.2918	1184.7909
1195.1634	1211.2078	1235.8303
1249.5772	1254.5409	1265.9391
1294.1659	1297.8122	1303.9671
1306.9423	1330.8290	1340.0251
1346.6234	1363.1670	1372.0586
1377.5871	1384.5132	1397.8292
1399.7825	1408.8639	1409.6443
1411.9297	1427.9302	1429.6713
1429.8901	1477.0495	1479.4758
1485.2878	1488.8252	1489.3531
1492.7648	1496.9170	1498.2562
1499.6760	1501.6842	1507.2189
1508.5344	1510.8894	1517.9303
1533.2737	1537.7277	1663.6011
1675.6284	1690.8139	3054.5095
3063.2502	3063.8489	3064.3894
3066.5266	3067.9694	3069.7498
3072.9271	3076.7221	3083.8400
3095.1700	3114.7567	3123.6925
3126.1999	3134.9664	3137.0570
3143.2051	3144.8755	3145.1515
3148.8274	3151.9358	3154.1133
3154.4049	3155.9030	3211.6541
3215.3690	3238.4730	3288.2666

CO_3^{2-}

Zero-point correction= 0.014588

Thermal correction to Energy= 0.017736
Thermal correction to Enthalpy= 0.018680
Thermal correction to Gibbs Free Energy= -0.010940
Sum of electronic and zero-point Energies= -263.876007
Sum of electronic and thermal Energies= -263.872859
Sum of electronic and thermal Enthalpies= -263.871914
Sum of electronic and thermal Free Energies= -263.901535

Cartesian coordinates

C	-0.000072	-0.000015	-0.000222
O	-0.384655	1.237683	0.000072
O	1.264661	-0.285837	0.000087
O	-0.879952	-0.951834	0.000008

Vibrational frequencies

697.5604	702.9251	896.7684
1086.2501	1509.3326	1510.6341

NHC

Zero-point correction= 0.430615 (Hartree/Particle)
Thermal correction to Energy= 0.452501
Thermal correction to Enthalpy= 0.453446
Thermal correction to Gibbs Free Energy= 0.379690
Sum of electronic and zero-point Energies= -1230.501500
Sum of electronic and thermal Energies= -1230.479614
Sum of electronic and thermal Enthalpies= -1230.478670
Sum of electronic and thermal Free Energies= -1230.552426

Cartesian coordinates

C	-3.66272200	0.32587500	-1.98169700
C	-4.23460900	-0.03598400	-0.60760400
C	-3.57465300	-1.24651200	0.06637100
C	-2.23106000	0.86986300	-1.99860900
C	-2.18492400	-0.96958500	0.56086300
C	-1.14669200	-0.14877300	-1.61837900
C	-1.14097500	-0.49638600	-0.15712500
H	-4.31769600	1.07732000	-2.43592300
H	-5.30021100	-0.25815500	-0.72867700
H	-3.54533500	-2.08429400	-0.64342500
H	-2.15706500	1.74087900	-1.33408700
H	-1.29428000	-1.06745100	-2.20250100
C	-0.04994200	-0.65844500	1.95974100
H	-3.71224100	-0.55902100	-2.63154300
H	-4.16463500	0.82884300	0.06367100

H	-4.19177500	-1.57489000	0.90758200
H	-2.01269500	1.22704500	-3.01057700
H	-0.16544700	0.24235800	-1.89865000
N	0.00672900	-0.34355400	0.65180300
C	1.24228800	0.16942800	0.10460300
C	1.43104900	1.55730600	0.07900100
C	2.18560700	-0.73997200	-0.39040700
C	2.64146200	2.03336400	-0.42957000
C	3.38196800	-0.21777100	-0.88825800
C	3.60985200	1.15409300	-0.90315000
H	2.82955600	3.10192500	-0.45705900
H	4.14260000	-0.89055100	-1.27124600
H	4.54558900	1.54138900	-1.29361800
C	0.37707100	2.50156900	0.63117500
C	0.24657700	3.79105000	-0.18175500
H	-0.60602700	4.37184700	0.18120500
H	1.13565200	4.42184500	-0.08603700
H	0.09073800	3.57841700	-1.24373300
C	1.93470000	-2.23734600	-0.34263700
S	-1.66896500	-1.19470500	2.21078500
H	-0.59059700	1.98767800	0.58805600
H	0.85012400	-2.39435900	-0.31477700
C	0.67640500	2.80400800	2.10563500
H	1.64430800	3.30857300	2.19752900
H	-0.09277800	3.45776900	2.52782100
H	0.71080600	1.87809400	2.68664400
C	2.52428900	-2.82115300	0.94853800
H	2.32326400	-3.89496500	1.01088100
H	3.60952200	-2.67348300	0.96754300
H	2.09073300	-2.32929800	1.82366500
C	2.47467600	-2.97061700	-1.57226400
H	2.15946300	-4.01734900	-1.54513600
H	2.10409200	-2.52325700	-2.49898900
H	3.56848600	-2.96083000	-1.60063400

Vibrational frequencies

30.6652	36.3525	44.7363
51.5413	61.5298	79.2986
92.0407	117.8646	135.7067
148.4748	198.8582	219.5350
224.2794	241.4155	243.9346
257.8909	272.8022	280.1228
291.4385	301.2863	304.3275
326.6450	335.6607	361.9138

376.6960	396.1840	409.7612
440.5363	470.8475	495.1424
516.2215	529.7680	566.0188
570.8222	612.5212	621.9385
652.7658	653.8466	708.1731
723.6484	774.5234	786.4683
808.9275	819.2492	829.9985
833.6334	837.1077	901.1252
914.4995	922.9782	930.3512
933.1414	940.2055	966.3958
969.0953	977.8054	979.5297
981.4751	1007.0160	1017.0537
1060.7083	1074.9593	1084.7572
1095.9962	1122.5673	1126.5669
1146.9404	1152.8398	1158.6946
1171.8629	1181.1645	1193.9552
1213.1049	1237.2670	1246.1235
1250.8083	1285.5271	1295.5326
1298.3771	1304.3867	1324.6077
1329.2803	1338.2137	1344.1279
1367.4427	1375.4948	1382.2325
1390.0150	1397.6810	1398.9350
1400.7957	1402.9711	1409.7124
1413.8149	1420.4858	1424.2852
1477.0639	1481.7042	1484.4789
1488.4841	1490.8366	1491.9122
1493.8788	1495.6190	1499.8589
1506.4263	1510.6395	1513.3643
1515.8803	1528.7524	1533.8350
1678.0809	1688.2002	1697.9190
3051.1107	3052.2919	3053.1161
3053.4607	3054.8009	3059.6570
3061.3001	3062.2917	3065.9122
3077.4787	3081.2242	3104.2037
3110.0690	3112.7366	3123.2924
3132.4111	3134.8918	3136.5305
3140.6919	3143.9348	3145.5796
3151.2875	3151.5722	3152.1310
3212.6255	3221.3965	3239.2039

R1

Zero-point correction= 0.111049 (Hartree/Particle)
Thermal correction to Energy= 0.117334
Thermal correction to Enthalpy= 0.118278

Thermal correction to Gibbs Free Energy= 0.080499
Sum of electronic and zero-point Energies= -345.322585
Sum of electronic and thermal Energies= -345.316300
Sum of electronic and thermal Enthalpies= -345.315356
Sum of electronic and thermal Free Energies= -345.353135

Cartesian coordinates

C	1.98641200	0.47192700	-0.00009000
O	2.83174700	-0.39831900	0.00013500
H	2.27413700	1.54194400	-0.00032600
C	0.52973900	0.21403900	-0.00004400
C	-0.35772300	1.29151200	0.00000900
C	0.04826800	-1.09902200	-0.00005600
C	-1.72997300	1.05869300	0.00004100
H	0.02939000	2.30737100	0.00002300
C	-1.32086200	-1.32965700	-0.00002000
H	0.76005600	-1.91869300	-0.00009800
C	-2.20805500	-0.25049100	0.00002700
H	-2.42400100	1.89228300	0.00008200
H	-1.70244400	-2.34525400	-0.00002000
H	-3.27795200	-0.43311100	0.00005600

Vibrational frequencies

116.5577	221.0833	244.9528
417.6797	445.8006	463.4758
623.9146	658.2830	707.3335
769.5227	847.1859	879.1974
959.0281	1011.0752	1018.9834
1037.2456	1054.9485	1059.6937
1113.1739	1180.4337	1189.1914
1249.2144	1339.1209	1367.7703
1436.6740	1507.4746	1546.9024
1678.2032	1695.1844	1833.2983
2998.5849	3197.5311	3207.5875
3215.1394	3223.3536	3229.9012

R2

Zero-point correction= 0.448577
Thermal correction to Energy= 0.473995
Thermal correction to Enthalpy= 0.474939
Thermal correction to Gibbs Free Energy= 0.391717
Sum of electronic and zero-point Energies= -1247.455532
Sum of electronic and thermal Energies= -1247.430115
Sum of electronic and thermal Enthalpies= -1247.429170

Sum of electronic and thermal Free Energies= -1247.512393

Cartesian coordinates

N	0.525343	0.297061	0.338597
C	0.172644	-1.022023	0.234657
C	-1.152437	-1.372976	0.073736
H	-1.381712	-2.426805	-0.030400
C	-2.160555	-0.404224	0.002389
C	-1.753322	0.929534	0.047770
H	-2.472043	1.736356	-0.031126
C	-0.421251	1.274618	0.202009
C	-3.579137	-0.775668	-0.149601
C	-4.064764	-1.954337	0.431169
H	-3.402394	-2.585965	1.014991
C	-5.404409	-2.298987	0.296564
H	-5.775525	-3.206649	0.759986
C	-6.267524	-1.478904	-0.428106
H	-7.311980	-1.751905	-0.536097
C	-5.789004	-0.309182	-1.015539
H	-6.455215	0.325532	-1.589629
C	-4.453032	0.045769	-0.873503
H	-4.082958	0.946325	-1.353484
C	1.206243	-2.097540	0.216312
C	1.796207	-2.435638	-1.005925
H	1.528624	-1.884967	-1.902415
C	2.722904	-3.471602	-1.063397
H	3.184009	-3.727672	-2.011639
C	3.046860	-4.182829	0.090098
H	3.773002	-4.987482	0.043672
C	2.422737	-3.877834	1.297354
H	2.653919	-4.447811	2.190489
C	1.491720	-2.845216	1.361312
H	0.987178	-2.620224	2.296039
C	-0.050084	2.712558	0.194568
C	0.790027	3.219253	-0.804966
H	1.220404	2.545083	-1.540651
C	1.064553	4.581161	-0.846479
H	1.712621	4.974652	-1.621886
C	0.505734	5.436865	0.102393
H	0.724759	6.498760	0.068026
C	-0.333894	4.932541	1.092143
H	-0.767831	5.597862	1.830467
C	-0.620085	3.570992	1.137395
H	-1.274516	3.170732	1.905596

C	1.898682	0.678136	0.791326
H	1.944944	1.761988	0.691757
C	2.140350	0.334520	2.252972
H	2.252911	-0.735976	2.412640
H	1.318569	0.717020	2.861401
C	2.992548	0.170954	-0.140052
O	4.041406	-0.275832	0.247032
O	2.677684	0.397011	-1.415180
C	3.689822	0.035794	-2.368866
H	3.254352	0.225244	-3.346744
H	4.579592	0.647286	-2.213133
H	3.946364	-1.019230	-2.254199
H	3.063606	0.824571	2.564961

Vibrational frequencies

17.7218	37.8229	41.0889
48.4306	54.1346	54.6661
64.7461	86.1950	101.7549
105.8849	121.0093	124.7039
156.2979	159.4577	173.0448
214.3189	226.8632	234.8340
236.3252	244.4039	269.0167
273.2308	284.9886	297.8209
342.8781	360.2395	408.6301
414.8495	415.8671	419.1734

HCO_3^-

Zero-point correction= 0.027008
Thermal correction to Energy= 0.030497
Thermal correction to Enthalpy= 0.031441
Thermal correction to Gibbs Free Energy= 0.001269
Sum of electronic and zero-point Energies= -264.412028
Sum of electronic and thermal Energies= -264.408538
Sum of electronic and thermal Enthalpies= -264.407594
Sum of electronic and thermal Free Energies= -264.437767

Cartesian coordinates

C	-0.13741900	0.06246000	0.00005300
O	0.09021200	1.29047100	0.00000200
O	1.00492300	-0.75708100	0.00001600
H	1.74622700	-0.13923200	0.00004000
O	-1.21034900	-0.56283000	-0.00006300

Vibrational frequencies

505.6855 572.4718 671.5362
829.0561 970.5900 1212.2796
1393.5246 1825.3832 3874.4270

H_2CO_3
Zero-point correction= 0.040178
Thermal correction to Energy= 0.043908
Thermal correction to Enthalpy= 0.044852
Thermal correction to Gibbs Free Energy= 0.014281
Sum of electronic and zero-point Energies= -264.874761
Sum of electronic and thermal Energies= -264.871031
Sum of electronic and thermal Enthalpies= -264.870087
Sum of electronic and thermal Free Energies= -264.900657

Cartesian coordinates

C	-0.000020	0.097899	0.000021
O	0.000262	1.305138	-0.000025
O	-1.082419	-0.677035	-0.000029
H	-1.857193	-0.096315	-0.000084
O	1.082180	-0.677378	0.000043
H	1.857135	-0.096880	0.000047

Vibrational frequencies
484.3474 561.8535 568.9412
608.0518 803.9819 1032.5632
1173.0469 1294.4879 1510.0888
1878.5695 3858.2215 3861.8533

TS1
Zero-point correction= 0.543678
Thermal correction to Energy= 0.572385
Thermal correction to Enthalpy= 0.573329
Thermal correction to Gibbs Free Energy= 0.483485
Sum of electronic and zero-point Energies= -1575.822426
Sum of electronic and thermal Energies= -1575.793719
Sum of electronic and thermal Enthalpies= -1575.792775
Sum of electronic and thermal Free Energies= -1575.882619

Cartesian coordinates

C	-3.85968200	3.30898300	0.16113600
C	-2.59782700	4.10134700	-0.18792400
C	-1.36371600	3.73763900	0.64602700
C	-3.83771100	1.82591500	-0.21651700
C	-0.79732100	2.37985400	0.34316900

C	-2.89753700	0.94581900	0.61918500
C	-1.44099100	1.18702800	0.34622700
H	-4.70814300	3.77668900	-0.34958200
H	-2.80173800	5.16542300	-0.02990200
H	-1.62303300	3.78137400	1.71226400
H	-3.57704900	1.72237500	-1.27745500
H	-3.09496000	1.11218400	1.68721500
C	0.72267000	0.43563500	-0.18467900
H	-4.05736000	3.40318400	1.23789300
H	-2.36389700	3.97640100	-1.25212100
H	-0.58431300	4.48810200	0.48673500
H	-4.84925700	1.42413600	-0.09911900
H	-3.12342600	-0.10550700	0.42283700
N	-0.55130700	0.12833800	0.05933200
C	-0.99018600	-1.25386300	0.08932900
C	-1.33329300	-1.88641300	-1.10640200
C	-1.07756200	-1.87745300	1.34277800
C	-1.81256500	-3.19754900	-1.02269000
C	-1.55518000	-3.18714400	1.37530900
C	-1.92751900	-3.83951600	0.20253400
H	-2.09482300	-3.71946100	-1.93268700
H	-1.63799700	-3.70592600	2.32439700
H	-2.30356200	-4.85664900	0.24746900
C	-1.18304900	-1.21986300	-2.46041100
C	-2.54801200	-0.99745000	-3.12118500
H	-2.42802300	-0.49274200	-4.08427200
H	-3.05244300	-1.95255800	-3.30096100
H	-3.19901900	-0.38539700	-2.48943800
C	-0.58363600	-1.17626100	2.59642700
S	0.88308500	2.12915800	-0.04005700
H	-0.71797500	-0.23973800	-2.31336000
H	-0.75085300	-0.09957700	2.47489400
C	-0.25687500	-2.04854700	-3.36078600
H	-0.74510700	-2.97874300	-3.67014100
H	-0.00524400	-1.48822000	-4.26604600
H	0.66280600	-2.30741300	-2.82802000
C	0.92989300	-1.40138600	2.73294200
H	1.32666400	-0.83674300	3.58217300
H	1.13207700	-2.46503300	2.90111600
H	1.45718200	-1.10240100	1.82154700
C	-1.31815000	-1.60985300	3.86520200
H	-1.00520700	-0.98326100	4.70460100
H	-2.40228800	-1.51752900	3.75170200
H	-1.08731000	-2.64644800	4.12925800

C	2.10687500	-0.89157700	-0.97045000
O	1.90552200	-2.05130900	-0.57129000
H	1.75500900	-0.57980100	-1.97887200
C	3.33817800	-0.12073000	-0.55138600
C	3.72614400	1.01575100	-1.26206400
C	4.11505400	-0.56292600	0.51857900
C	4.86673700	1.72366800	-0.89190100
H	3.13003000	1.34206500	-2.11254500
C	5.25656600	0.14306400	0.89117100
H	3.81227900	-1.46708300	1.03890700
C	5.63174600	1.28919800	0.18971300
H	5.16282300	2.60698500	-1.44903100
H	5.85900000	-0.20066700	1.72656700
H	6.52249100	1.83732600	0.47990200

Vibrational frequencies

-140.8025	18.8189	29.6112
37.9049	40.6064	45.1343
56.8633	66.0009	73.7143
82.9269	85.4257	88.4107
113.5616	120.0583	141.1356
153.9354	202.7354	216.3982
219.1715	225.9574	238.1202
246.8102	259.6185	262.3463
272.7154	288.3537	298.7973
307.3938	317.7457	328.6381
334.9106	355.4167	366.2059
385.3512	407.1054	419.0011
420.6561	446.3588	468.9936
477.5996	493.7406	509.7470
531.0288	553.4794	568.1661
576.1289	613.6219	621.0036
626.4572	654.3860	657.6069
667.8814	713.5913	721.8466
730.3073	778.2049	782.8019
789.9572	816.4287	831.1306
832.0620	836.0807	852.3069
868.7910	886.7694	905.4062
915.8664	932.1413	933.7832
937.9920	942.2857	957.7665
967.3101	974.0112	979.2787
981.5857	984.1692	1009.9591
1011.1316	1013.4095	1017.7860
1028.9132	1061.9468	1065.3600

1076.9267	1086.0081	1099.4191
1105.6412	1117.0074	1121.6567
1125.3399	1145.0067	1146.5538
1158.5861	1169.9395	1175.2075
1182.6996	1187.2510	1191.6308
1213.2397	1228.0826	1239.3124
1250.9881	1253.4166	1284.6376
1294.3724	1299.8031	1304.0891
1323.5190	1331.5457	1332.3106
1338.7955	1349.4771	1358.8665
1374.8352	1378.6810	1383.6958
1392.2655	1400.5930	1404.1848
1404.6663	1406.2486	1414.3531
1415.4588	1425.4687	1426.0106
1448.0424	1478.7063	1484.5170
1485.1584	1486.2173	1490.4838
1495.3334	1497.7333	1499.3922
1500.2417	1501.2541	1503.7797
1506.9733	1518.0636	1519.9197
1527.8542	1534.6253	1547.3609
1646.9675	1679.6054	1689.3538
1691.2011	1693.8084	1693.9350
2923.0689	3050.0907	3052.8007
3055.0320	3060.5888	3061.9637
3062.6487	3063.5130	3067.3604
3069.8973	3081.8159	3107.3134
3108.3930	3115.7131	3117.5058
3127.5855	3134.5887	3138.7250
3138.8888	3144.1775	3149.5638
3150.0419	3150.3429	3153.1947
3156.5017	3190.2860	3201.2388
3205.4115	3214.7078	3217.4916
3222.2738	3227.7035	3234.1834

M1

Zero-point correction= 0.545233
Thermal correction to Energy= 0.573694
Thermal correction to Enthalpy= 0.574639
Thermal correction to Gibbs Free Energy= 0.486590
Sum of electronic and zero-point Energies= -1575.830611
Sum of electronic and thermal Energies= -1575.802149
Sum of electronic and thermal Enthalpies= -1575.801205
Sum of electronic and thermal Free Energies= -1575.889253

Cartesian coordinates

C	3.49593400	3.56586100	-0.11819100
C	2.16484800	4.24595900	0.20823600
C	0.98356800	3.77833600	-0.65173100
C	3.58918400	2.07856900	0.23045900
C	0.52117800	2.38646200	-0.33062600
C	2.72392900	1.14424800	-0.62893800
C	1.25481700	1.24745900	-0.33136800
H	4.28990100	4.09166000	0.42239500
H	2.27927700	5.32365500	0.05443800
H	1.26550200	3.81852500	-1.71184700
H	3.33645400	1.92872200	1.28737600
H	2.88667600	1.36710100	-1.69227000
C	-0.80559000	0.37111600	0.25884600
H	3.71173500	3.69670300	-1.18743500
H	1.91962100	4.09901700	1.26683800
H	0.14470600	4.46822900	-0.52614500
H	4.62925900	1.76116300	0.10612000
H	3.04859500	0.11410000	-0.47222400
N	0.47188900	0.11898500	-0.01400600
C	1.07641600	-1.20649400	-0.04116300
C	1.49794400	-1.78135700	1.15700800
C	1.31628100	-1.77277400	-1.30085500
C	2.18586600	-2.99533600	1.07324400
C	2.00434500	-2.98521100	-1.33092000
C	2.43947800	-3.59102600	-0.15522700
H	2.52156000	-3.47916300	1.98606100
H	2.20430900	-3.46296300	-2.28426800
H	2.97808600	-4.53216000	-0.20022200
C	1.18438200	-1.17883200	2.51277400
C	2.45497700	-0.93499700	3.33246400
H	2.20403800	-0.46437300	4.28738400
H	2.96935200	-1.87629900	3.54968700
H	3.15312100	-0.28325300	2.79879300
C	0.77123000	-1.13784000	-2.56899000
S	-1.12637700	2.03684600	0.08143300
H	0.69944200	-0.20856100	2.35994600
H	0.70663700	-0.05485200	-2.41230800
C	0.19671300	-2.08716600	3.25861000
H	0.68623800	-3.02577200	3.54180500
H	-0.15319600	-1.60206600	4.17501900
H	-0.65323800	-2.31976600	2.60964800
C	-0.65513000	-1.65597700	-2.80783800
H	-1.13849400	-1.10116300	-3.61781400

H	-0.61861800	-2.71414000	-3.09212000
H	-1.24528200	-1.57896200	-1.88852500
C	1.65941000	-1.36267100	-3.79277100
H	1.27388400	-0.78549600	-4.63768300
H	2.69090100	-1.05027800	-3.60386200
H	1.66894300	-2.41431500	-4.09517800
C	-1.82170600	-0.69384200	0.80318900
O	-1.53891800	-1.92028000	0.42009400
H	-1.70939200	-0.48916600	1.91006500
C	-3.23966600	-0.18812200	0.45424500
C	-3.86916400	0.83513100	1.16685400
C	-3.92311000	-0.80430000	-0.59295700
C	-5.14878900	1.26216200	0.81264600
H	-3.36263700	1.29282700	2.01530200
C	-5.20132700	-0.38283100	-0.94918200
H	-3.43345600	-1.63194000	-1.09652200
C	-5.81530300	0.65690200	-0.25112100
H	-5.62965600	2.05758900	1.37389600
H	-5.72496100	-0.86920800	-1.76696500
H	-6.81343900	0.98384000	-0.52520700

Vibrational frequencies

22.4532	34.5255	41.6960
45.7416	54.3134	59.0850
74.5123	84.9104	89.8048
100.1741	115.5089	127.8115
131.6134	151.0281	172.4285
200.2148	214.0747	224.1640
238.0098	245.1587	247.7578
256.7972	266.8479	281.1756
290.0297	299.3309	312.2424
323.8496	332.1922	339.5367
352.3777	358.6558	377.8372
408.2607	414.9847	423.5976
442.2846	447.8565	473.5490
491.2897	516.5385	530.2404
538.5653	567.2838	572.9937
605.8014	618.3527	628.4028
630.9725	654.6545	671.5698
714.5981	727.1696	729.3450
747.7093	779.7950	789.7577
809.6548	827.2392	831.1365
835.7256	839.3911	876.7906
890.5026	897.4978	913.6221

918.3469	938.4362	940.5511
946.1104	951.5271	956.5823
965.3285	975.9985	976.0957
987.9407	1006.6547	1009.4196
1010.1640	1015.8642	1026.4731
1052.7791	1063.8980	1074.3724
1088.1971	1093.1829	1103.9214
1107.4464	1125.0542	1132.8130
1145.2153	1149.7901	1165.2266
1170.4147	1176.2709	1182.3545
1184.9059	1192.1137	1203.8061
1214.4706	1241.1550	1248.7931
1253.8513	1261.2737	1294.2923
1295.9403	1300.7017	1304.2463
1309.6159	1324.5177	1329.4256
1334.7499	1342.4851	1348.8350
1355.8872	1375.0594	1377.1722
1384.2690	1384.7118	1397.6720
1400.3043	1400.6096	1408.3088
1408.8342	1420.9894	1422.6334
1427.2549	1481.3985	1484.6443
1485.7385	1488.6214	1490.1896
1493.1451	1495.6679	1497.4899
1499.8970	1500.4544	1502.0357
1508.1533	1510.9678	1519.6202
1524.1370	1528.9902	1537.3492
1541.2552	1675.6994	1677.6032
1685.2045	1692.5319	1693.2594
2703.6002	3046.3367	3051.4629
3052.3934	3057.6980	3058.8198
3063.8384	3064.5275	3067.1254
3071.2769	3082.9310	3097.4861
3113.6805	3114.5818	3122.0097
3125.0538	3129.1099	3131.6183
3141.3101	3143.2111	3145.1498
3146.1551	3148.3822	3150.2621
3155.1594	3178.7279	3201.7654
3204.5135	3215.5076	3219.2052
3226.4483	3229.5548	3238.2595

TS2

Zero-point correction= 0.566851
Thermal correction to Energy= 0.599365
Thermal correction to Enthalpy= 0.600310

Thermal correction to Gibbs Free Energy= 0.502479
Sum of electronic and zero-point Energies= -1840.260360
Sum of electronic and thermal Energies= -1840.227845
Sum of electronic and thermal Enthalpies= -1840.226901
Sum of electronic and thermal Free Energies= -1840.324732

Cartesian coordinates

C	4.646201	-2.044513	-1.747934
C	3.527581	-2.823917	-2.436230
C	2.377477	-3.229531	-1.512119
C	4.289580	-0.605805	-1.372338
C	1.542678	-2.093292	-0.992347
C	3.320174	-0.430033	-0.199631
C	1.917355	-0.926354	-0.428665
H	5.510290	-2.014928	-2.419660
H	3.945566	-3.743835	-2.859123
H	2.781506	-3.785734	-0.656310
H	3.887230	-0.091787	-2.253868
H	3.728761	-0.931238	0.689811
C	-0.399427	-0.732792	-0.169870
H	4.970402	-2.588248	-0.850364
H	3.130810	-2.238628	-3.274537
H	1.720513	-3.924054	-2.046392
H	5.209172	-0.079689	-1.099022
H	3.276049	0.633504	0.046392
N	0.808419	-0.171657	0.040385
C	1.057685	1.014041	0.845743
C	1.021514	2.275175	0.238451
C	1.448404	0.811978	2.174557
C	1.414383	3.365639	1.013727
C	1.826965	1.935978	2.913177
C	1.818892	3.199480	2.335523
H	1.395446	4.361398	0.583853
H	2.132292	1.821071	3.947809
H	2.123540	4.062692	2.919692
C	0.557271	2.437936	-1.197107
C	1.664079	2.059434	-2.191789
H	1.326083	2.243434	-3.216139
H	2.563264	2.659842	-2.015798
H	1.937361	1.003660	-2.118075
C	1.375526	-0.566136	2.813233
S	-0.196214	-2.263760	-0.952704
H	-0.285761	1.755135	-1.343567
H	1.558478	-1.316578	2.036865

C	0.040734	3.845590	-1.501824
H	0.856288	4.575474	-1.551375
H	-0.467837	3.838583	-2.470803
H	-0.689392	4.162936	-0.754473
C	-0.046603	-0.790754	3.348644
H	-0.168232	-1.816834	3.709654
H	-0.238680	-0.107173	4.183688
H	-0.790903	-0.580544	2.573699
C	2.417407	-0.784939	3.911036
H	2.393099	-1.828728	4.237630
H	3.427090	-0.557360	3.558089
H	2.212973	-0.164357	4.789635
C	-1.692994	-0.110341	0.070524
O	-1.688453	0.951909	0.926186
H	-1.941883	0.374640	-1.070924
C	-2.826547	-1.099713	0.274299
C	-3.310371	-1.901635	-0.766748
C	-3.464443	-1.157380	1.516479
C	-4.366781	-2.784978	-0.553354
H	-2.877747	-1.809610	-1.760721
C	-4.521611	-2.038491	1.731259
H	-3.123133	-0.484506	2.295296
C	-4.970842	-2.863149	0.700388
H	-4.728384	-3.399292	-1.372162
H	-5.001753	-2.079452	2.704469
H	-5.796080	-3.547609	0.866568
C	-2.833051	2.333241	-1.749611
O	-2.404660	1.164559	-2.133487
O	-2.740503	2.644239	-0.458471
H	-2.248035	1.877932	0.189905
O	-3.320797	3.160945	-2.539732

Vibrational frequencies

-1081.8670	17.2341	31.3394
38.0645	41.7905	44.7797
48.6675	54.6800	65.8531
76.2570	80.3542	90.8592
99.4181	112.9496	120.0832
131.1830	137.9149	147.5984
154.7782	183.9519	192.8334
213.2534	222.1709	228.4864
232.8099	249.0350	257.1655
263.7874	271.1006	283.7029
304.8183	309.1080	320.1781

331.1162	334.0478	342.0975
354.0003	360.6581	386.6652
407.1982	413.1238	422.1399
442.5975	447.6859	465.7322
484.9905	495.6873	532.9678
544.2879	554.9625	564.2577
578.9482	596.3152	601.4601
627.1075	631.7149	636.6794
648.6744	664.5242	709.5233
719.7710	723.5609	725.5069
760.0735	780.4548	793.5693
818.6410	823.0057	825.4566
831.2976	836.8940	854.8463
879.1121	893.6128	911.2240
916.7817	927.4196	934.6010
939.1241	943.5514	945.7828
963.0990	966.6072	978.8808
979.8452	982.8943	1001.3783
1006.6861	1011.5138	1015.1731
1017.3149	1030.2758	1060.8778
1075.6490	1077.2825	1085.8198
1088.8596	1099.9323	1104.4444
1121.0961	1130.2635	1148.1189
1150.0538	1161.8157	1168.5626
1173.8829	1175.9341	1179.7455
1182.9068	1190.0101	1200.3331
1213.7694	1231.2024	1246.7012
1254.3696	1277.6608	1289.0244
1291.7404	1303.1986	1306.2915
1317.2041	1322.5149	1326.6188
1338.2380	1341.3003	1349.8094
1359.5862	1371.8556	1384.5708
1387.2687	1390.5488	1395.0922
1401.9987	1405.6200	1406.8575
1410.2605	1419.4667	1421.5837
1425.6073	1461.0676	1471.6603
1481.3770	1481.8267	1484.1614
1488.7930	1490.6309	1492.4661
1494.7387	1497.1735	1498.0588
1503.0362	1509.5547	1513.1405
1518.1699	1520.3150	1526.6842
1533.5474	1538.4669	1631.3269
1668.4437	1674.9756	1688.8325
1689.4152	1716.1674	1720.6390

1793.9764	3043.7876	3050.0561
3055.3816	3056.2774	3058.7775
3060.3578	3063.6595	3063.7592
3066.8959	3097.8363	3108.0019
3110.9568	3115.8175	3117.8531
3124.3474	3129.5521	3133.3834
3138.7204	3142.3994	3144.2498
3149.5219	3154.4011	3161.9604
3165.5234	3192.9574	3197.8106
3208.1731	3209.5800	3216.5807
3221.0348	3230.6200	3231.0004

M2

Zero-point correction= 0.573678
Thermal correction to Energy= 0.606927
Thermal correction to Enthalpy= 0.607872
Thermal correction to Gibbs Free Energy= 0.509539
Sum of electronic and zero-point Energies= -1840.295825
Sum of electronic and thermal Energies= -1840.262575
Sum of electronic and thermal Enthalpies= -1840.261631
Sum of electronic and thermal Free Energies= -1840.359964

Cartesian coordinates

C	5.352143	0.811284	-0.096452
C	4.727530	2.165390	0.246298
C	3.669210	2.649457	-0.753073
C	4.422570	-0.400352	0.005706
C	2.380593	1.880916	-0.684148
C	3.291880	-0.450219	-1.029032
C	2.199183	0.556389	-0.794768
H	6.204119	0.645058	0.572219
H	5.527710	2.913043	0.286775
H	4.081836	2.596947	-1.770303
H	3.983110	-0.445067	1.010346
H	3.711763	-0.297764	-2.033199
C	-0.051503	1.195544	-0.534615
H	5.763727	0.858183	-1.114676
H	4.278032	2.123422	1.247093
H	3.459215	3.707558	-0.566989
H	5.027080	-1.306146	-0.114457
H	2.852164	-1.449990	-1.021180
N	0.859343	0.126281	-0.678376
C	0.588393	-1.136630	-0.026869
C	0.725094	-1.231499	1.370122

C	0.234781	-2.248615	-0.809086
C	0.520301	-2.476890	1.970072
C	0.054895	-3.475535	-0.167144
C	0.195997	-3.593498	1.209974
H	0.621781	-2.574597	3.047501
H	-0.209762	-4.349580	-0.755979
H	0.044698	-4.554774	1.691763
C	1.033866	-0.022324	2.239039
C	2.045930	-0.325345	3.349635
H	2.341732	0.604285	3.845146
H	1.619553	-0.980336	4.115987
H	2.946922	-0.807368	2.959377
C	0.039635	-2.155310	-2.311645
S	0.856466	2.723939	-0.352338
H	1.472570	0.753948	1.604374
H	0.021738	-1.093485	-2.565480
C	-0.259530	0.537515	2.848935
H	-0.700450	-0.197237	3.532084
H	-0.047475	1.449197	3.417834
H	-0.996791	0.761065	2.074242
C	-1.300834	-2.769721	-2.731527
H	-1.517398	-2.515953	-3.774483
H	-1.269509	-3.863349	-2.663620
H	-2.113070	-2.413095	-2.094895
C	1.186392	-2.830139	-3.075516
H	0.997731	-2.791192	-4.153315
H	2.148725	-2.347623	-2.885148
H	1.272646	-3.884178	-2.788449
C	-1.397556	1.058631	-0.646756
O	-1.903810	-0.131922	-1.082109
H	-2.208462	-0.682048	-0.262096
C	-2.370647	2.136860	-0.404688
C	-2.133999	3.223506	0.453210
C	-3.620114	2.065736	-1.046201
C	-3.090163	4.222024	0.623873
H	-1.215753	3.270577	1.030434
C	-4.571673	3.062727	-0.873808
H	-3.822558	1.211476	-1.682650
C	-4.310332	4.153695	-0.043308
H	-2.883898	5.048580	1.297268
H	-5.525184	2.989267	-1.388563
H	-5.054812	4.931525	0.092142
C	-3.026967	-2.536566	0.815793
O	-2.859161	-3.413735	1.872056

O	-2.503472	-1.396260	0.996069
O	-3.671330	-2.959157	-0.147782
H	-2.238873	-2.970926	2.466936

Vibrational frequencies

27.8398	32.4459	40.7321
43.9493	48.3363	57.8559
65.7227	74.7546	81.8836
93.4888	97.0719	98.3246
102.9486	111.2100	122.6137
134.2604	137.1614	147.9674
154.2251	172.7328	193.1666
203.4070	218.8711	222.7995
242.2681	247.6433	256.7274
267.2811	271.3343	278.9531
293.8664	308.2233	318.6575
323.0632	327.0443	344.0385
358.0549	372.5401	389.0175
405.5391	415.2288	422.9489
452.5666	459.5545	463.8633
491.5730	506.0680	517.3630
535.8987	538.3859	559.3768
570.0627	595.1493	610.4848
615.5798	630.0937	637.9876
648.2484	656.1047	662.3472
687.4282	706.4534	720.2058
721.4626	770.7781	787.4532
793.3960	813.6708	825.9849
829.2058	830.6893	833.3433
873.3638	885.3098	894.5520
914.1253	925.9900	930.2705
932.4859	938.2999	940.4157
948.6442	964.6247	965.4045
975.7382	981.5683	982.9804
993.6594	999.5959	1000.7151
1012.4368	1019.8257	1020.6979
1067.5645	1072.1180	1077.3664
1087.0756	1094.6588	1105.8734
1120.6342	1121.5817	1140.4970
1141.4589	1146.5058	1162.5577
1174.4868	1178.7458	1182.4089
1190.2105	1207.6204	1208.9057
1217.8271	1234.6278	1248.7772
1263.1064	1274.8414	1290.3009

1292.1100	1299.9680	1308.8320
1310.2116	1331.3072	1333.8935
1338.8100	1342.0351	1361.0160
1365.7383	1372.6422	1379.9849
1382.8064	1392.5380	1397.3775
1400.5996	1403.9456	1405.4954
1406.7603	1415.5458	1420.6762
1425.2858	1478.3479	1480.6111
1482.3240	1483.2826	1486.6415
1491.8749	1493.9767	1495.7067
1496.8178	1501.4904	1502.2065
1506.8740	1512.8057	1513.8853
1519.2816	1531.3210	1541.8341
1555.2724	1655.4713	1672.8563
1676.7957	1680.6454	1702.4243
1750.9971	1791.6512	2577.6480
3043.3706	3046.5754	3051.9472
3053.9472	3054.2359	3056.6311
3058.3288	3058.7162	3060.1941
3098.1828	3103.1612	3107.6281
3110.4423	3111.7064	3120.8497
3125.8224	3131.8121	3138.2738
3139.4126	3142.4893	3145.8476
3153.9616	3164.6421	3174.5030
3198.6853	3202.7072	3202.9607
3214.0982	3217.3147	3228.2727
3230.8840	3235.8667	3853.8099

M3

Zero-point correction= 1.023554
Thermal correction to Energy= 1.083458
Thermal correction to Enthalpy= 1.084403
Thermal correction to Gibbs Free Energy= 0.928533
Sum of electronic and zero-point Energies= -3087.774884
Sum of electronic and thermal Energies= -3087.714979
Sum of electronic and thermal Enthalpies= -3087.714035
Sum of electronic and thermal Free Energies= -3087.869905

Cartesian coordinates

C	-0.645417	-5.185280	-1.810778
C	-1.352169	-4.097396	-2.622497
C	-1.840155	-2.908245	-1.785711
C	0.706413	-4.800341	-1.203581
C	-0.734487	-2.018073	-1.299750

C	0.648299	-3.745616	-0.090889
C	0.351897	-2.356807	-0.586664
H	-0.492619	-6.054454	-2.460027
H	-2.221448	-4.545545	-3.117192
H	-2.422609	-3.291281	-0.934742
H	1.377740	-4.445324	-1.994394
H	-0.121868	-4.030424	0.638957
C	0.835049	-0.068088	-0.892592
H	-1.315761	-5.517253	-1.004645
H	-0.686364	-3.728497	-3.413178
H	-2.536779	-2.309588	-2.383779
H	1.161554	-5.704096	-0.784424
H	1.599459	-3.735484	0.445771
N	1.251796	-1.301826	-0.349390
C	2.661498	-1.621659	-0.245344
C	3.370036	-1.993633	-1.399437
C	3.263313	-1.599296	1.022008
C	4.704172	-2.387365	-1.247309
C	4.592322	-2.007331	1.126878
C	5.308524	-2.404515	0.001968
H	5.276080	-2.684970	-2.121261
H	5.076715	-2.007065	2.099322
H	6.343328	-2.719071	0.100871
C	2.757663	-1.924502	-2.790317
C	3.202168	-3.076539	-3.700085
H	2.587544	-3.092256	-4.604887
H	4.242593	-2.953161	-4.017066
H	3.116125	-4.049254	-3.208097
C	2.504041	-1.126761	2.247942
S	-0.697823	-0.310314	-1.746936
H	1.667020	-1.982416	-2.690636
H	1.628468	-0.587239	1.877550
C	3.106823	-0.585896	-3.458039
H	4.191347	-0.507060	-3.587886
H	2.636650	-0.521326	-4.444944
H	2.780374	0.260934	-2.850739
C	3.339031	-0.144886	3.075848
H	2.713173	0.315616	3.849556
H	4.162400	-0.652354	3.590619
H	3.758662	0.636919	2.434888
C	2.023269	-2.301964	3.106311
H	1.559624	-1.935037	4.027422
H	1.277718	-2.908736	2.580366
H	2.862733	-2.949757	3.383165

C	1.506995	1.104521	-0.701234
O	2.522816	1.080496	0.203874
H	3.450460	1.051110	-0.255733
C	1.270774	2.392003	-1.378395
C	0.183179	2.700213	-2.218020
C	2.214367	3.413870	-1.146173
C	0.041948	3.970411	-2.774803
H	-0.582157	1.969114	-2.447467
C	2.071926	4.673591	-1.709616
H	3.058518	3.196005	-0.502459
C	0.980329	4.967276	-2.526906
H	-0.814355	4.175157	-3.410889
H	2.816901	5.436719	-1.502573
H	0.864210	5.954128	-2.963342
C	5.633558	1.112856	0.064196
O	6.823964	0.442751	-0.136260
O	4.776680	0.947444	-0.857757
O	5.552287	1.791431	1.091588
H	6.671266	-0.109887	-0.914672
N	-2.944133	0.362071	1.110110
C	-2.914471	1.454895	0.283578
C	-1.869454	2.353168	0.352049
H	-1.887760	3.190630	-0.334570
C	-0.817425	2.185599	1.267299
C	-0.793798	0.964099	1.953737
H	0.033465	0.705068	2.603265
C	-1.835955	0.063211	1.871201
C	0.182055	3.237538	1.509258
C	-0.099300	4.569260	1.169543
H	-1.056917	4.833841	0.732907
C	0.828510	5.570785	1.422072
H	0.595222	6.597753	1.161266
C	2.053651	5.257079	2.009209
H	2.780571	6.040105	2.200209
C	2.344951	3.936766	2.344140
H	3.305151	3.680865	2.780483
C	1.415535	2.933009	2.101172
H	1.683682	1.905533	2.314874
C	-4.002526	1.669964	-0.706417
C	-4.141805	0.781167	-1.777875
H	-3.489732	-0.083215	-1.842945
C	-5.111773	1.008131	-2.748328
H	-5.209994	0.319039	-3.580776
C	-5.944135	2.121355	-2.655569

H	-6.704433	2.293413	-3.409928
C	-5.791307	3.021328	-1.603016
H	-6.429349	3.895776	-1.536767
C	-4.813212	2.806543	-0.636088
H	-4.683143	3.512255	0.179387
C	-1.764234	-1.209550	2.624840
C	-2.053336	-2.422370	1.986522
H	-2.372082	-2.414438	0.948659
C	-1.931932	-3.619419	2.683655
H	-2.156150	-4.556231	2.183198
C	-1.523362	-3.614412	4.017033
H	-1.431794	-4.549904	4.558700
C	-1.239275	-2.408953	4.654531
H	-0.928966	-2.401149	5.693906
C	-1.354146	-1.207573	3.961699
H	-1.146376	-0.266682	4.462334
C	-4.265397	-0.193067	1.547359
H	-4.026401	-1.023501	2.211698
C	-5.036386	0.858365	2.333865
H	-5.399316	1.656563	1.685618
H	-4.393788	1.277475	3.110833
C	-5.119388	-0.816576	0.447499
O	-6.285069	-0.554375	0.294155
O	-4.463392	-1.762950	-0.227269
C	-5.262718	-2.461429	-1.197137
H	-4.615650	-3.220264	-1.629707
H	-6.122481	-2.919599	-0.707226
H	-5.608198	-1.762607	-1.962088
H	-5.897412	0.383250	2.805455

Vibrational frequencies

16.2558	26.5002	27.5415
31.5443	34.0167	37.7419
40.1038	44.9065	48.6848
49.3504	52.2975	55.6209
59.4462	63.3236	66.0054
71.1187	75.4282	79.9723
82.7692	87.7969	91.9262
94.1577	96.6446	97.5127
104.0324	107.4668	110.1095
111.9812	113.5620	122.1842
124.3376	130.8785	133.7438
144.8977	145.7053	156.9819
158.0390	170.5773	180.8624

186.8100	189.1431	195.9627
211.2241	227.3307	234.0512
236.5121	238.1875	239.7750
243.2925	247.7059	257.5412
262.3080	265.5753	270.2731
272.9991	278.2224	280.2379
288.8307	297.3250	302.6338
305.9362	316.4048	320.2407
328.6131	331.8163	348.4802
363.3293	367.2478	376.8840
387.2960	393.0063	410.8616
413.2417	413.9409	416.6191
418.1939	420.3245	423.2598
426.5434	449.9497	452.9466
457.6078	473.0480	480.4037
502.8963	514.0065	516.4156
523.2395	530.2817	533.5398
561.8547	568.1729	576.6739
592.8535	599.6972	607.0530
612.1960	612.5634	622.6672
625.7303	627.3180	629.2092
634.2334	635.7109	640.6544
645.4280	649.4697	654.6865
663.7638	667.1087	682.5614
684.0588	702.5189	703.9350
704.5809	712.0236	720.4226
725.9219	752.7185	773.5354
776.6218	777.9762	783.2510
791.5371	791.7413	794.7600
811.4097	816.1742	825.9798
829.5250	831.0406	832.6739
847.6780	853.2886	860.5614
865.5287	871.3105	884.4105
887.6314	895.2762	903.8297
909.1734	914.4789	917.3577
925.7785	929.6997	932.0981
935.4343	935.8179	952.0405
955.8312	965.9858	967.3961
973.7354	974.4617	979.4144
982.6489	983.8170	991.7893
993.9354	999.0057	1003.2471
1005.6527	1006.0535	1009.2737
1013.1329	1014.9298	1015.7990
1017.6928	1018.7785	1024.8929

1027.5516	1033.7564	1038.2919
1048.1010	1054.4000	1068.5624
1068.8716	1071.0776	1075.7586
1078.7074	1083.3010	1086.2582
1092.8151	1094.4021	1111.5706
1115.6349	1119.7705	1122.6217
1123.9590	1132.3630	1135.2050
1138.2755	1147.5988	1149.3982
1154.4465	1165.6862	1176.3836
1180.3576	1180.7403	1182.2328
1182.2748	1187.4565	1187.9611
1188.5878	1192.0859	1194.5497
1208.9716	1210.2270	1211.6554
1218.5765	1220.7816	1226.3446
1227.1466	1231.2367	1253.7449
1264.8929	1279.6569	1280.3554
1280.9527	1288.4211	1292.1541
1292.9315	1299.9181	1308.9192
1310.6987	1315.1706	1327.6708
1332.8694	1335.7814	1337.4377
1338.9043	1342.6684	1348.6330
1360.2643	1363.0423	1365.6585
1370.3212	1372.1612	1373.4274
1376.3710	1380.5003	1383.1257
1393.9371	1397.9365	1400.9797
1401.7758	1402.9973	1404.1914
1406.0890	1414.7491	1421.4314
1423.0263	1424.7310	1425.5979
1467.8739	1471.4020	1472.6019
1478.0362	1481.6156	1484.1567
1487.5724	1488.1029	1488.5027
1489.1737	1490.8221	1491.9932
1496.3944	1496.8508	1498.5137
1499.3356	1500.5434	1500.6894
1504.0901	1504.4459	1507.8573
1513.6072	1514.5092	1520.9905
1521.7491	1528.7451	1531.5492
1549.4362	1551.7578	1554.7781
1561.3174	1619.2066	1636.0514
1663.2589	1666.4244	1670.6528
1672.3518	1674.7862	1678.9761
1685.9695	1691.3861	1692.4412
1693.4902	1699.9611	1741.5984
1780.5442	1875.4816	2515.7845

3038.8808	3040.9054	3047.1669
3050.5499	3053.7027	3059.6185
3062.9492	3064.8431	3069.0369
3094.5961	3098.4281	3098.7582
3099.2412	3101.5234	3105.4112
3113.2672	3117.8312	3124.6567
3134.0479	3135.3418	3139.1198
3139.7158	3140.8759	3152.7793
3154.6060	3162.1250	3171.0824
3184.1581	3187.3357	3188.6144
3196.4860	3199.8142	3203.8702
3204.2951	3207.1576	3209.1737
3209.8885	3213.4373	3213.5406
3214.5601	3223.8749	3224.7675
3225.0552	3228.0557	3230.8334
3231.2703	3234.8641	3239.9580
3241.3568	3241.6237	3243.4520
3243.9210	3246.3193	3247.0323
3248.2297	3268.3615	3858.8550

^{os}TS3

Zero-point correction= 1.018351
Thermal correction to Energy= 1.077970
Thermal correction to Enthalpy= 1.078914
Thermal correction to Gibbs Free Energy= 0.923977
Sum of electronic and zero-point Energies= -3087.772116
Sum of electronic and thermal Energies= -3087.712497
Sum of electronic and thermal Enthalpies= -3087.711553
Sum of electronic and thermal Free Energies= -3087.866490

Cartesian coordinates

C	-1.299391	-4.788498	-2.407198
C	-1.874371	-3.551505	-3.099826
C	-2.244895	-2.398018	-2.156516
C	0.076905	-4.612823	-1.762571
C	-1.054125	-1.683301	-1.585786
C	0.103589	-3.680268	-0.544638
C	-0.025502	-2.224643	-0.895745
H	-1.231524	-5.593952	-3.146483
H	-2.780087	-3.847769	-3.639934
H	-2.871505	-2.780487	-1.337691
H	0.791057	-4.244004	-2.508714
H	-0.710647	-3.951223	0.139880
C	0.722238	-0.007730	-0.984622

H	-2.009430	-5.131310	-1.641182
H	-1.162337	-3.180195	-3.847961
H	-2.863582	-1.681410	-2.706844
H	0.434673	-5.595660	-1.439033
H	1.035978	-3.829485	0.002604
N	0.977519	-1.312848	-0.560025
C	2.344039	-1.795452	-0.431850
C	3.095734	-1.985621	-1.603240
C	2.852155	-2.107695	0.837168
C	4.400756	-2.470177	-1.468695
C	4.159079	-2.589384	0.919690
C	4.934048	-2.764312	-0.221668
H	5.006395	-2.617346	-2.358359
H	4.575707	-2.828142	1.894634
H	5.949897	-3.138437	-0.137000
C	2.566625	-1.657693	-2.991573
C	2.873710	-2.762539	-4.010797
H	2.342188	-2.561723	-4.945473
H	3.941889	-2.803486	-4.245111
H	2.572773	-3.749081	-3.648433
C	2.033195	-1.941835	2.102491
S	-0.795878	0.028028	-1.852312
H	1.476473	-1.559722	-2.935383
H	1.050140	-1.556807	1.812934
C	3.147384	-0.325405	-3.486338
H	4.237140	-0.401171	-3.568695
H	2.746576	-0.079949	-4.475029
H	2.917156	0.495058	-2.802750
C	2.688158	-0.925361	3.044162
H	2.007772	-0.686271	3.871173
H	3.606208	-1.334289	3.481272
H	2.950015	-0.015547	2.499845
C	1.835113	-3.282636	2.820006
H	1.293518	-3.128964	3.756934
H	1.258489	-3.988958	2.214782
H	2.799518	-3.744017	3.057635
C	1.546591	1.059916	-0.607605
O	2.434007	0.818962	0.317558
H	3.679017	0.710277	-0.048646
C	1.581745	2.379968	-1.281997
C	0.637410	2.869201	-2.202628
C	2.665140	3.215209	-0.953897
C	0.775441	4.137596	-2.761338
H	-0.221652	2.281079	-2.502171

C	2.804041	4.474449	-1.521112
H	3.386694	2.859253	-0.228509
C	1.858891	4.947706	-2.429273
H	0.028522	4.490239	-3.466058
H	3.650517	5.094959	-1.242031
H	1.962121	5.934074	-2.870088
C	5.521909	0.478693	0.651065
O	6.713306	-0.095671	0.355246
O	4.721720	0.530988	-0.372901
O	5.317909	0.890824	1.778263
H	6.649521	-0.432473	-0.549666
N	-2.734530	0.441619	1.124460
C	-2.625405	1.564715	0.310442
C	-1.533475	2.389338	0.393052
H	-1.504461	3.234746	-0.285338
C	-0.453871	2.128846	1.268577
C	-0.500267	0.868885	1.922328
H	0.357261	0.505218	2.478357
C	-1.598460	0.056946	1.852027
C	0.564477	3.138998	1.561122
C	0.392479	4.472025	1.143398
H	-0.503046	4.764604	0.605883
C	1.345613	5.439529	1.425845
H	1.187144	6.459879	1.090911
C	2.499281	5.106049	2.135670
H	3.244584	5.863747	2.355957
C	2.683091	3.792875	2.560880
H	3.578034	3.516669	3.109877
C	1.729374	2.820405	2.281083
H	1.903198	1.804521	2.609474
C	-3.720125	1.882548	-0.639195
C	-4.145584	0.944832	-1.587036
H	-3.695150	-0.042206	-1.589853
C	-5.133589	1.274661	-2.508464
H	-5.448383	0.542711	-3.245879
C	-5.707491	2.544697	-2.493198
H	-6.481523	2.799628	-3.209529
C	-5.280771	3.487814	-1.560741
H	-5.721954	4.478840	-1.546151
C	-4.287916	3.161611	-0.642150
H	-3.955876	3.892833	0.089703
C	-1.629906	-1.247241	2.549499
C	-2.129965	-2.384175	1.901115
H	-2.506593	-2.289800	0.886645

C	-2.157123	-3.609853	2.558490
H	-2.543611	-4.485796	2.046346
C	-1.697120	-3.712105	3.870777
H	-1.728066	-4.666915	4.385307
C	-1.204616	-2.583090	4.522456
H	-0.853688	-2.655169	5.546884
C	-1.165892	-1.356572	3.866204
H	-0.805331	-0.471207	4.381892
C	-4.054803	0.164931	1.753673
H	-3.878046	-0.648461	2.460440
C	-4.569772	1.375406	2.522098
H	-4.864391	2.179873	1.845827
H	-3.787234	1.735064	3.194531
C	-5.113045	-0.391091	0.806530
O	-6.244312	0.023889	0.751077
O	-4.675826	-1.458898	0.130169
C	-5.649596	-2.068153	-0.728470
H	-5.167231	-2.944161	-1.156890
H	-6.530591	-2.354933	-0.153232
H	-5.941272	-1.366703	-1.514006
H	-5.441066	1.089305	3.112963

Vibrational frequencies

-1162.6049	11.2171	21.5395
28.6998	34.6314	35.9151
38.5076	41.0922	45.2736
52.6100	53.4470	56.0605
60.4807	63.4615	66.4184
68.6973	69.5162	74.6240
86.5485	89.1815	92.5826
95.2475	97.1096	98.0752
105.3164	107.6578	109.6610
113.2417	114.5989	117.9740
123.7963	129.3880	137.4403
139.5328	145.4511	151.5043
155.6882	164.0648	168.1227
175.4461	189.2583	190.4352
196.0549	209.9696	222.1850
230.0557	232.0604	234.3754
245.0518	248.4379	254.5780
255.2839	264.1202	266.2375
269.4612	273.7020	279.3699
280.7405	289.2886	294.8261
299.6463	306.3758	321.2432

325.4209	333.3843	337.3314
353.4550	357.6458	373.0583
384.6834	397.5433	406.6555
408.4236	412.8755	415.6974
419.1577	424.9373	425.6714
429.3539	442.4743	454.1573
465.1278	466.0858	473.1621
474.1423	502.7824	513.0001
514.9888	524.7497	525.2808
550.9611	563.0649	569.1103
570.9461	578.1762	596.7195
603.4026	607.1118	620.5316
621.9984	623.7636	625.6056
626.8100	630.8082	633.2346
643.2857	648.6495	653.5604
654.7189	660.8488	672.5711
680.0858	694.0473	700.9763
707.4232	718.8337	719.4661
724.9774	731.0927	751.4113
769.5988	776.0574	777.0385
783.7345	790.3907	791.8269
798.4530	810.9953	814.5902
818.6318	827.8308	830.9596
834.3500	840.2262	849.9532
853.4758	858.1975	873.7714
876.8824	880.0758	894.9396
898.3174	901.1861	916.3344
917.0461	922.3059	924.7086
930.3004	935.3637	936.5091
947.3207	957.2970	957.4758
966.9264	969.1990	971.5171
974.0419	980.3736	986.8225
993.8904	994.6519	1004.6088
1005.2267	1007.2448	1007.7130
1008.3914	1010.6461	1011.6851
1014.3343	1017.8463	1019.3435
1028.0542	1029.0938	1041.7580
1051.4936	1056.9348	1063.3105
1069.3158	1070.8849	1072.3906
1073.2477	1078.8083	1081.3080
1083.6975	1096.3602	1098.6125
1111.8566	1115.7280	1119.8469
1121.0254	1124.3816	1128.4238
1138.9834	1143.9734	1145.5962

1153.7605	1162.6978	1171.9735
1173.1510	1177.2961	1178.8162
1180.2704	1182.3096	1183.8052
1184.9364	1188.1407	1189.5260
1196.2651	1197.5063	1207.3409
1207.7205	1222.1132	1223.9366
1227.8122	1234.6935	1240.9655
1249.9688	1250.8657	1277.5773
1278.6128	1280.1762	1289.0583
1291.1935	1298.3172	1304.2205
1308.9875	1313.6252	1326.6102
1327.2207	1331.2548	1331.4124
1339.2187	1340.5494	1347.0911
1350.6773	1354.2564	1361.0837
1364.1421	1368.4927	1370.1718
1372.6426	1376.8153	1383.4340
1386.1135	1393.1783	1399.4748
1402.4939	1403.3029	1408.5129
1414.5870	1417.5070	1420.1013
1422.0289	1424.7794	1428.1553
1433.7842	1448.2835	1467.5642
1474.0632	1477.1701	1487.2886
1487.4976	1487.8366	1488.7319
1489.2372	1489.9978	1491.8691
1492.7416	1494.0365	1495.3183
1498.2887	1499.0709	1499.9907
1503.0672	1504.0290	1505.0034
1505.6344	1514.7957	1517.0071
1520.0172	1520.5464	1530.3655
1533.6624	1548.8725	1549.6568
1561.1401	1573.0157	1586.8100
1650.6350	1661.1835	1661.3002
1666.4998	1672.3852	1677.8507
1680.9174	1684.0098	1689.6534
1691.7814	1692.8021	1695.4679
1698.4763	1868.7893	1914.9011
3041.1053	3045.6704	3046.8911
3059.1827	3061.9311	3062.1033
3065.1691	3069.8067	3075.2221
3087.5314	3094.7423	3100.4186
3105.0535	3106.3551	3107.2743
3111.7493	3121.1255	3123.2111
3136.1125	3141.3163	3142.4430
3142.7265	3151.2309	3152.6257

3157.4538	3162.4206	3173.6972
3182.8675	3186.0435	3189.8740
3191.3042	3197.6545	3200.0024
3200.7128	3201.6113	3205.7344
3206.9825	3209.4149	3212.8348
3213.5290	3214.9671	3215.0973
3215.3973	3216.5083	3223.1945
3224.0073	3224.2193	3227.5692
3227.8184	3228.2914	3231.6982
3234.2522	3238.6346	3257.5998
3264.0586	3265.1287	3853.2995

^{2}M4

Zero-point correction= 0.445647
Thermal correction to Energy= 0.471134
Thermal correction to Enthalpy= 0.472078
Thermal correction to Gibbs Free Energy= 0.388789
Sum of electronic and zero-point Energies= -1247.582807
Sum of electronic and thermal Energies= -1247.557320
Sum of electronic and thermal Enthalpies= -1247.556376
Sum of electronic and thermal Free Energies= -1247.639664

Cartesian coordinates

N	0.546409	0.257335	0.101895
C	0.038979	-1.046765	-0.100103
C	-1.303668	-1.283491	-0.147216
H	-1.623059	-2.302011	-0.345787
C	-2.261839	-0.234386	-0.080117
C	-1.725135	1.075276	-0.083600
H	-2.381105	1.933577	-0.180131
C	-0.379406	1.322066	-0.008282
C	-3.700852	-0.501041	-0.111643
C	-4.211573	-1.737199	0.328365
H	-3.532932	-2.487105	0.722995
C	-5.575324	-2.002912	0.301716
H	-5.939594	-2.962866	0.654460
C	-6.473868	-1.041945	-0.159653
H	-7.538668	-1.248969	-0.178121
C	-5.986127	0.189605	-0.596267
H	-6.672333	0.944869	-0.966900
C	-4.622928	0.456765	-0.575224
H	-4.268972	1.411422	-0.950875
C	1.022055	-2.129624	-0.323448
C	2.024417	-1.983576	-1.292737

H	2.085796	-1.057506	-1.856588
C	2.926371	-3.015235	-1.531176
H	3.691060	-2.895537	-2.292632
C	2.842504	-4.203444	-0.805643
H	3.551886	-5.003824	-0.988497
C	1.841928	-4.360361	0.151039
H	1.771153	-5.282823	0.718228
C	0.935251	-3.331361	0.389192
H	0.161131	-3.446532	1.142954
C	0.163487	2.690654	-0.109682
C	1.372550	2.928969	-0.781778
H	1.920992	2.088705	-1.196008
C	1.860944	4.224069	-0.917003
H	2.794410	4.392168	-1.444906
C	1.157038	5.302482	-0.383550
H	1.541739	6.311563	-0.488633
C	-0.039250	5.074272	0.294893
H	-0.586539	5.905487	0.727987
C	-0.528975	3.780828	0.437442
H	-1.445461	3.608399	0.993675
C	1.532157	0.397025	1.208034
H	1.672694	1.473181	1.343264
C	1.019868	-0.211721	2.506462
H	0.974724	-1.300990	2.437631
H	0.019624	0.176573	2.714911
C	2.922291	-0.127054	0.859364
O	3.548267	-0.902460	1.541855
O	3.409458	0.452159	-0.241549
C	4.729667	0.042553	-0.614635
H	4.966796	0.594082	-1.521661
H	5.437632	0.283878	0.180054
H	4.745486	-1.033444	-0.801258
H	1.683484	0.052071	3.331639

Vibrational frequencies

21.6642	44.9263	48.3586
50.7827	54.8405	61.2821
74.7307	83.1200	95.4166
104.9710	121.3658	138.3361
149.3375	153.7057	181.2772
214.7651	226.4847	239.7005
246.8033	246.8572	258.8383
265.8353	295.8708	298.3678
347.9751	376.6800	403.8926

416.3770	418.4683	421.2867
424.6409	464.8483	484.2914
509.4351	515.8871	574.4194
590.5150	599.6276	617.0722
624.7027	627.5778	631.6288
638.7541	651.2396	677.7724
715.4237	719.3861	719.6048
723.7070	762.9364	783.4445
785.3980	790.3307	808.7021
846.6845	855.1931	874.0709
876.5755	882.8264	894.8337
902.3815	917.5658	942.2853
955.8501	956.5663	1001.3454
1004.1192	1005.6019	1008.8155
1009.4753	1011.6302	1015.2412
1024.7855	1026.9428	1027.0970
1038.0062	1054.9984	1058.2095
1071.2460	1072.9928	1080.7507
1088.7468	1119.4349	1120.8141
1124.3283	1137.3747	1173.2496
1175.1311	1177.7056	1180.0657
1182.8003	1185.2951	1207.0978
1207.9433	1219.1927	1225.6421
1267.5046	1273.7920	1278.2569
1314.4089	1324.9535	1328.7032
1337.4472	1354.6009	1361.9134
1363.5161	1373.9279	1388.5357
1393.8491	1409.1437	1439.8424
1444.0199	1485.2718	1488.0682
1491.3968	1492.6192	1497.3708
1501.3985	1501.4866	1501.9637
1534.1192	1547.7439	1556.1628
1559.1143	1654.6286	1656.0243
1665.6475	1672.5925	1689.2184
1693.9182	1694.7369	1860.4956
3079.9378	3089.4062	3137.2687
3168.2455	3174.4801	3175.1972
3201.1953	3206.3956	3207.6036
3207.7828	3210.6566	3213.4239
3213.9275	3215.4226	3217.4894
3219.4009	3221.0324	3224.1015
3224.7128	3226.3545	3230.8988
3233.7547	3235.6157	3239.0627

^{2}M5

Zero-point correction= 0.533230
Thermal correction to Energy= 0.562185
Thermal correction to Enthalpy= 0.563129
Thermal correction to Gibbs Free Energy= 0.471694
Sum of electronic and zero-point Energies= -1575.271146
Sum of electronic and thermal Energies= -1575.242191
Sum of electronic and thermal Enthalpies= -1575.241247
Sum of electronic and thermal Free Energies= -1575.332682

Cartesian coordinates

C	3.842271	-3.244428	0.140241
C	2.559260	-4.057262	-0.049302
C	1.405635	-3.657635	0.880709
C	3.767051	-1.766991	-0.253253
C	0.784464	-2.335242	0.534413
C	2.870917	-0.900856	0.644964
C	1.402897	-1.137591	0.431250
H	4.636127	-3.714787	-0.449948
H	2.790259	-5.111366	0.137164
H	1.769170	-3.627358	1.916886
H	3.432000	-1.674381	-1.294752
H	3.112638	-1.100149	1.697385
C	-0.777725	-0.477927	-0.082535
H	4.156415	-3.314902	1.190919
H	2.221913	-3.983817	-1.090372
H	0.632376	-4.430777	0.848817
H	4.778774	-1.349172	-0.210582
H	3.092425	0.154654	0.471120
N	0.537567	-0.096163	0.086269
C	0.942400	1.285044	0.145074
C	1.643824	1.829525	-0.938888
C	0.651285	2.015019	1.304031
C	2.035062	3.165789	-0.851027
C	1.054741	3.352404	1.342763
C	1.737544	3.925003	0.276574
H	2.570760	3.621872	-1.678538
H	0.831080	3.949854	2.222155
H	2.043760	4.965201	0.324829
C	1.932091	1.019809	-2.189886
C	3.399736	1.115192	-2.616230
H	3.587600	0.450122	-3.464271
H	3.660080	2.131306	-2.928438
H	4.071778	0.828281	-1.800777

C	-0.095971	1.413008	2.481663
S	-0.930256	-2.194036	0.213231
H	1.717976	-0.031924	-1.971622
H	-0.212677	0.338676	2.305844
C	0.990345	1.456935	-3.318844
H	1.186349	2.499153	-3.594092
H	1.141240	0.836297	-4.207379
H	-0.050381	1.378157	-2.993273
C	-1.497670	2.026157	2.594288
H	-2.066713	1.536504	3.390265
H	-1.430455	3.093155	2.832788
H	-2.046379	1.923463	1.653848
C	0.686668	1.579452	3.788599
H	0.157919	1.085840	4.609013
H	1.684878	1.139635	3.707402
H	0.800602	2.635235	4.053535
C	-1.811310	0.372919	-0.573113
O	-1.578687	1.513371	-1.039437
C	-3.222070	-0.134429	-0.556028
C	-3.769624	-0.828104	0.528186
C	-4.040043	0.177422	-1.647893
C	-5.103750	-1.229800	0.505157
H	-3.161743	-1.030478	1.405650
C	-5.367787	-0.232204	-1.675228
H	-3.614348	0.743553	-2.470385
C	-5.902225	-0.940989	-0.598786
H	-5.521711	-1.758623	1.355803
H	-5.989006	0.003789	-2.533421
H	-6.940162	-1.257597	-0.617049

Vibrational frequencies

14.4779	20.3480	35.8536
43.5421	49.6825	53.3321
61.4821	66.8007	79.9592
89.3898	109.1258	113.5619
126.2481	136.4570	168.1669
200.3992	201.9261	212.9965
227.6467	233.5501	243.3942
256.4437	258.8526	264.6155
270.4654	287.0498	298.2258
316.1359	326.1687	330.4608
344.5002	357.3234	385.5897
401.8134	410.0229	419.3839
442.3402	447.0812	469.3136

481.0337	502.3052	525.1897
553.9918	561.8635	565.1162
598.7840	612.7928	626.4046
646.0188	653.3200	664.2995
686.2451	714.8512	722.0479
724.1853	776.1940	792.0300
795.9829	816.9300	828.4974
830.4505	834.5144	883.5942
893.3438	901.2691	915.2358
933.5872	935.0728	945.3345
949.6142	958.8927	967.2653
968.7902	975.0692	976.6050
987.8677	1005.1939	1009.3020
1010.7502	1018.2751	1029.4450
1063.1592	1070.7434	1074.5758
1084.0133	1098.8673	1113.4365
1121.0136	1122.5253	1144.7951
1149.1536	1164.1089	1170.5716
1173.1047	1177.8430	1184.7029
1192.1729	1195.8018	1211.0000
1238.2465	1247.2081	1252.4757
1284.7759	1291.9965	1293.7925
1303.4767	1318.5545	1324.7714
1335.5694	1346.6176	1354.9248
1355.7051	1356.8411	1374.7830
1383.5670	1390.3841	1395.7101
1398.2461	1401.7633	1405.2749
1406.2247	1414.9861	1420.7390
1424.9326	1467.3227	1478.2217
1481.7462	1483.1236	1488.3841
1490.1030	1491.5513	1492.7592
1494.0137	1497.0735	1497.4779
1505.1499	1506.6200	1509.6206
1511.9987	1526.6674	1532.2378
1544.2859	1624.1482	1672.0651
1677.0716	1684.4568	1688.6997
1692.8933	3050.1500	3051.8575
3054.4970	3056.3675	3058.6065
3060.0372	3064.7433	3065.5332
3069.9218	3099.6531	3100.3954
3105.6038	3110.3659	3117.3942
3119.2618	3136.9063	3138.2842
3138.7498	3144.2744	3145.3699
3145.7441	3153.2976	3153.8153

3154.6473	3202.2913	3207.3671
3212.8520	3214.9701	3216.1443
3224.5082	3228.6969	3236.1922

^{2}TS4

Zero-point correction= 0.442970
Thermal correction to Energy= 0.468470
Thermal correction to Enthalpy= 0.469414
Thermal correction to Gibbs Free Energy= 0.385790
Sum of electronic and zero-point Energies= -1247.558909
Sum of electronic and thermal Energies= -1247.533409
Sum of electronic and thermal Enthalpies= -1247.532465
Sum of electronic and thermal Free Energies= -1247.616089

Cartesian coordinates

N	0.511935	0.271050	-0.219094
C	0.007048	-0.996431	-0.328092
C	-1.350367	-1.260608	-0.261153
H	-1.696098	-2.281529	-0.388711
C	-2.274880	-0.211255	-0.145552
C	-1.754636	1.089154	-0.149990
H	-2.427814	1.939078	-0.142621
C	-0.385316	1.308328	-0.204675
C	-3.728931	-0.468318	-0.082530
C	-4.220827	-1.614992	0.556012
H	-3.526957	-2.304445	1.028028
C	-5.588311	-1.862936	0.617385
H	-5.950700	-2.752425	1.122773
C	-6.489494	-0.969651	0.041388
H	-7.556101	-1.162937	0.089482
C	-6.012109	0.173527	-0.597199
H	-6.706210	0.870584	-1.055663
C	-4.645406	0.422543	-0.659108
H	-4.284911	1.302756	-1.183033
C	0.998335	-2.072782	-0.548330
C	2.122488	-1.824798	-1.345162
H	2.257471	-0.835247	-1.771990
C	3.049698	-2.833740	-1.584277
H	3.909908	-2.636121	-2.216861
C	2.874199	-4.095997	-1.018933
H	3.602340	-4.879925	-1.200163
C	1.760776	-4.347746	-0.219277
H	1.623612	-5.325722	0.230638
C	0.825759	-3.343937	0.011697

H	-0.031634	-3.538829	0.650105
C	0.189365	2.672408	-0.263928
C	1.471400	2.862147	-0.800607
H	2.028064	1.996031	-1.144217
C	2.024372	4.136001	-0.876499
H	3.015497	4.266575	-1.299307
C	1.310673	5.240521	-0.415493
H	1.742605	6.234195	-0.475995
C	0.041497	5.060308	0.132277
H	-0.514875	5.912741	0.508573
C	-0.513233	3.787773	0.212274
H	-1.488902	3.662742	0.670935
C	1.571025	0.400516	1.423083
H	1.618207	1.484894	1.412253
C	0.709508	-0.236724	2.465760
H	0.660012	-1.318798	2.315897
H	-0.302078	0.179512	2.432972
C	2.873575	-0.233469	1.170443
O	3.265582	-1.265078	1.685949
O	3.615083	0.475489	0.294522
C	4.902207	-0.070400	0.010701
H	5.360923	0.603233	-0.710908
H	5.505550	-0.121954	0.919813
H	4.803916	-1.073767	-0.409835
H	1.118815	-0.057934	3.466445

Vibrational frequencies

-644.6122	23.0843	41.9888
43.4552	46.7353	55.2340
60.1356	66.4167	81.1841
90.5510	102.7175	120.8274
128.1567	157.7120	183.1938
196.1794	198.7549	222.9436
239.5948	241.3362	244.0297
245.7756	265.5459	284.6437
304.0732	330.8541	350.5164
404.7832	415.4421	418.0981
424.3464	424.8930	452.4007
475.5516	491.9537	513.9457
588.8906	615.7014	622.0517
626.1494	630.3592	633.4426
641.9175	656.8721	671.8102
682.1270	716.1383	718.2939
720.8277	747.7082	752.7718

784.7574	798.4904	802.7024
837.1485	853.7912	874.9522
881.6906	885.0769	886.2772
914.2291	921.9711	932.5475
954.5237	962.0876	963.8351
971.3070	1004.7949	1009.2103
1010.9314	1013.0712	1015.3999
1015.6614	1026.5559	1030.0983
1031.0277	1038.4447	1049.1654
1061.5379	1069.5227	1071.1743
1085.2442	1096.7891	1111.5773
1119.6328	1122.0002	1123.7292
1167.8778	1174.0466	1178.4384
1179.7580	1183.2886	1190.9103
1207.1024	1207.7256	1213.7385
1218.4830	1240.7769	1268.4635
1281.5535	1300.1575	1325.2792
1329.3938	1339.4885	1360.1750
1363.2099	1364.6513	1368.2440
1401.9386	1427.1405	1443.0686
1466.8849	1478.2353	1484.0379
1493.9318	1498.4520	1498.9570
1505.9056	1507.2017	1511.4100
1550.0357	1558.0039	1559.4342
1562.0801	1656.2873	1666.6659
1669.5326	1672.2884	1693.7589
1694.6376	1696.3218	1787.9208
3057.6592	3092.3865	3129.4730
3152.9790	3175.2815	3202.1034
3202.5165	3205.6546	3206.0717
3206.1365	3207.9029	3213.2861
3215.8390	3217.8126	3218.5465
3221.9258	3224.4804	3226.5369
3228.9411	3231.9484	3234.8414
3237.5487	3240.5860	3240.9806

^{2}M6

Zero-point correction= 0.106107
Thermal correction to Energy= 0.113404
Thermal correction to Enthalpy= 0.114349
Thermal correction to Gibbs Free Energy= 0.074222
Sum of electronic and zero-point Energies= -306.812541
Sum of electronic and thermal Energies= -306.805243
Sum of electronic and thermal Enthalpies= -306.804299

Sum of electronic and thermal Free Energies= -306.844425

Cartesian coordinates

C	1.210991	-0.670957	0.000146
H	1.147558	-1.752330	0.000348
C	2.522921	0.016030	-0.000293
H	2.388923	1.098272	-0.000307
H	3.112627	-0.270536	-0.878769
C	-0.026845	0.080951	0.000283
O	-0.109669	1.299675	0.000278
O	-1.109472	-0.724460	0.000358
C	-2.366429	-0.048521	-0.000442
H	-3.125668	-0.828203	-0.001603
H	-2.464765	0.577837	0.888879
H	-2.462986	0.578874	-0.889214
H	3.113611	-0.270646	0.877414

Vibrational frequencies

102.7370	115.0844	127.9173
197.3535	221.6562	346.9435
471.5868	596.1166	680.9716
725.6487	887.7418	993.4303
1036.3726	1090.5581	1175.5640
1179.9807	1216.5895	1253.1257
1404.6713	1441.7853	1478.3359
1480.3481	1486.3027	1501.0665
1522.3738	1767.7523	3060.5047
3088.5098	3116.9081	3171.8892
3178.7897	3205.5974	3251.2410

M7

Zero-point correction= 0.334829
Thermal correction to Energy= 0.352899
Thermal correction to Enthalpy= 0.353843
Thermal correction to Gibbs Free Energy= 0.286825
Sum of electronic and zero-point Energies= -940.759593
Sum of electronic and thermal Energies= -940.741523
Sum of electronic and thermal Enthalpies= -940.740579
Sum of electronic and thermal Free Energies= -940.807597

Cartesian coordinates

N	1.313527	0.022212	-0.067932
C	0.613835	1.162751	-0.034702
C	-0.783016	1.179856	0.002679

H	-1.317087	2.119547	0.089945
C	-1.483143	-0.027570	-0.000247
C	-0.741101	-1.209090	-0.042018
H	-1.245349	-2.168960	-0.037889
C	0.654137	-1.142609	-0.076124
C	-2.965557	-0.053010	0.064237
C	-3.721834	0.920835	-0.598181
H	-3.218751	1.686745	-1.181092
C	-5.111734	0.898165	-0.538458
H	-5.684648	1.654977	-1.064240
C	-5.764701	-0.095823	0.187670
H	-6.848590	-0.112636	0.235601
C	-5.020139	-1.068190	0.852259
H	-5.521882	-1.841149	1.425243
C	-3.630405	-1.048441	0.790034
H	-3.056101	-1.796460	1.328442
C	1.403085	2.424628	-0.010647
C	2.702567	2.417373	0.508410
H	3.110981	1.483687	0.880186
C	3.452549	3.587484	0.552912
H	4.456187	3.568760	0.965687
C	2.917306	4.781283	0.071203
H	3.503207	5.694151	0.103113
C	1.628696	4.795642	-0.457430
H	1.210068	5.718095	-0.846637
C	0.875634	3.625393	-0.498405
H	-0.118197	3.645804	-0.935283
C	1.487889	-2.375795	-0.109232
C	2.790931	-2.341463	0.400012
H	3.169293	-1.408705	0.804359
C	3.583845	-3.483813	0.392647
H	4.589650	-3.443645	0.798531
C	3.088785	-4.676826	-0.132050
H	3.707538	-5.568259	-0.139523
C	1.797128	-4.717487	-0.651600
H	1.408464	-5.638723	-1.073430
C	1.001078	-3.575236	-0.640624
H	0.005501	-3.617049	-1.071565

Vibrational frequencies

41.0900	44.7091	47.3177
49.1361	63.6525	67.5483
114.8245	121.9006	168.7025
239.1457	241.9694	251.7851

266.9168	290.4614	302.4587
400.2034	413.0379	416.8702
418.7377	422.1684	440.0020
495.7601	514.8892	589.1603
621.3029	625.2744	628.1557
633.2311	642.8038	653.3104
670.8885	683.5090	718.4793
719.6726	721.0340	765.4175
788.6839	805.8034	810.8749
843.8495	858.1541	878.3576
882.0892	883.0018	912.2878
929.4385	959.7759	964.8132
966.1310	1007.0192	1010.2290
1010.9643	1011.7854	1016.4436
1016.8439	1024.2681	1030.8677
1033.2314	1035.3620	1052.3682
1067.9335	1069.4554	1085.3198
1114.5263	1116.6494	1119.8298
1132.7182	1169.9404	1178.0071
1180.1129	1181.5862	1204.3640
1205.4670	1207.9888	1277.3189
1285.0558	1301.4619	1330.0549
1331.2260	1339.5333	1360.2777
1360.4414	1364.0888	1410.7095
1456.3225	1468.1304	1499.7729
1506.3003	1518.5215	1554.3350
1556.8638	1559.7159	1641.8954
1669.5830	1672.0897	1678.8518
1687.4402	1694.9079	1696.8932
1699.4940	3200.5310	3204.7213
3205.3606	3205.8649	3207.8258
3209.5996	3214.1532	3223.0190
3223.6712	3224.8089	3227.0039
3230.3006	3232.6061	3236.8245
3241.3054	3245.5854	3246.5526

^{os}TS8-F

Zero-point correction=	0.641197
Thermal correction to Energy=	0.678435
Thermal correction to Enthalpy=	0.679379
Thermal correction to Gibbs Free Energy=	0.571878
Sum of electronic and zero-point Energies=	-1882.094573
Sum of electronic and thermal Energies=	-1882.057335
Sum of electronic and thermal Enthalpies=	-1882.056391

Sum of electronic and thermal Free Energies= -1882.163892

Cartesian coordinates

C	4.52858800	-1.89323300	2.43489700
C	3.39191700	-2.91555600	2.51143800
C	2.02699700	-2.32549800	2.89157800
C	4.42831100	-0.86105400	1.30901900
C	1.40169800	-1.50628800	1.79983500
C	3.28423700	0.15230200	1.45331300
C	1.92980400	-0.43146000	1.17213100
H	5.47177900	-2.43705900	2.31550800
H	3.65415500	-3.66757600	3.26315500
H	2.13619200	-1.70331800	3.79008700
H	4.32961200	-1.37361200	0.34382900
H	3.28600300	0.56580100	2.47085000
C	-0.11115700	-0.55495400	0.05269700
H	4.59696900	-1.36431100	3.39572000
H	3.29872000	-3.44108700	1.55283400
H	1.34350700	-3.13585800	3.16146200
H	5.36715900	-0.29908400	1.27428500
H	3.45880700	0.98838800	0.77307200
N	1.09602000	0.10549100	0.18446100
C	1.63669900	0.90020500	-0.89916200
C	2.06911200	0.22653000	-2.05301400
C	1.75080700	2.29038000	-0.75460600
C	2.56564600	0.99832900	-3.10687700
C	2.26773600	3.01528600	-1.82905300
C	2.65900600	2.38036500	-3.00224700
H	2.89059600	0.50653100	-4.01913800
H	2.35728400	4.09473700	-1.74571400
H	3.04821500	2.96237400	-3.83159300
C	2.00727400	-1.28659800	-2.19705600
C	3.34385100	-1.86946000	-2.67178000
H	3.29998100	-2.96215300	-2.65206700
H	3.57019600	-1.56699200	-3.69879400
H	4.17155600	-1.54566700	-2.03479600
C	1.32590700	3.01796300	0.50761100
S	-0.16795200	-1.91740000	1.14303800
H	1.79617500	-1.72258400	-1.21414300
H	1.05292900	2.26398200	1.25293800
C	0.88063900	-1.69281000	-3.15577100
H	1.08718500	-1.31564200	-4.16322300
H	0.79882600	-2.78272200	-3.21136800
H	-0.08388200	-1.28956600	-2.83516600

C	0.09609300	3.89479900	0.23704400
H	-0.25992600	4.34665000	1.16865600
H	0.35202500	4.70568000	-0.45398700
H	-0.71015900	3.30452700	-0.20518100
C	2.46552000	3.86086600	1.09246200
H	2.14165000	4.32615000	2.02806600
H	3.35287200	3.25674600	1.30177500
H	2.75701100	4.66280200	0.40692600
C	-1.19909500	-0.03039500	-0.71405000
O	-1.17398400	1.15006500	-1.12884500
C	-2.38088800	-0.89677900	-1.02316400
C	-2.30092400	-2.28504100	-1.18419100
C	-3.60786700	-0.25845600	-1.24259600
C	-3.43401000	-3.02225100	-1.52164800
H	-1.34641500	-2.79351100	-1.08464000
C	-4.73756200	-0.99465000	-1.57830100
H	-3.64986100	0.82243200	-1.13844000
C	-4.65499400	-2.38097500	-1.71324100
H	-3.35683700	-4.09710400	-1.64998700
H	-5.68566000	-0.49034500	-1.73883000
H	-5.53641100	-2.95594200	-1.97804200
C	-2.54841700	0.51304500	2.16161700
C	-3.72544400	1.15310400	1.61188300
C	-1.31365600	1.31316600	2.34327000
H	-0.47801100	0.69536300	2.68082100
H	-1.04663900	1.78807100	1.39213600
H	-1.47085100	2.12088500	3.06977000
H	-2.61959600	-0.52248800	2.47050000
O	-3.76218900	2.30419400	1.20352800
O	-4.79899500	0.33667900	1.59416700
C	-5.98346400	0.91122200	1.04746600
H	-6.72838200	0.11737600	1.04232100
H	-6.32175800	1.74882700	1.66195200
H	-5.80277200	1.26912900	0.03079000

Vibrational frequencies

25.2887	29.1024	32.7316
37.8675	44.5547	48.4523
55.1210	61.3695	67.9781
78.6904	83.2987	86.0219
90.1704	100.9213	108.7883
113.9463	121.6105	133.9251
142.2969	145.1988	164.0809
174.4771	183.7487	197.3353

206.5026 210.0341 218.7944
229.1589 234.7579 238.9953
244.1066 247.7200 256.9312
264.9605 270.7444 281.1292
287.7915 304.9185 320.0732
325.0411 338.0924 348.5635
362.9254 363.9382 387.3677
408.7640 411.1305 422.4337
447.5072 452.2563 467.5007
476.3839 486.1725 506.2465
523.8987 545.9066 561.4921
569.3254 570.7885 598.6308
620.9005 627.1092 645.3969
652.2659 665.5466 678.2857
687.9485 715.3385 718.6153
724.0492 731.1641 773.3131
788.6162 797.5591 815.3309
826.9755 828.8783 832.7468
880.5822 892.7545 897.5786
900.4832 914.2267 931.5412
931.8769 941.4978 944.8707
962.2867 964.9404 968.1328
973.9992 975.6346 984.4365
1002.7613 1005.9790 1007.0201
1008.6748 1018.6224 1032.4736
1052.4877 1063.8435 1070.4952
1073.5797 1082.7961 1095.9603
1097.8188 1114.5531 1118.7187
1120.6127 1140.5638 1144.0447
1158.7233 1160.1676 1168.3277
1171.3794 1179.4817 1181.8418
1184.0270 1186.6285 1197.4881
1206.8790 1219.6770 1235.7352
1241.9150 1246.8196 1258.3756
1281.4434 1288.1870 1293.7424
1302.1618 1313.0816 1321.7150
1336.8882 1343.4105 1345.3440
1346.9092 1357.9827 1372.8837
1380.8185 1381.3193 1394.7665
1396.2596 1400.8505 1403.3482
1404.0228 1405.5341 1416.0689
1420.8373 1422.2823 1454.9570
1457.2064 1475.1938 1476.8540
1480.4478 1482.6561 1485.1541

1488.8474	1489.3586	1490.5201
1492.2741	1492.8529	1494.5044
1495.6666	1499.1637	1502.3423
1504.2872	1505.3512	1508.5419
1512.0134	1515.2439	1522.9653
1531.0351	1544.0996	1618.4438
1673.1800	1677.1322	1680.3209
1687.6749	1689.5447	1769.5703
3047.1127	3048.7719	3054.5350
3055.8646	3057.5393	3059.4789
3061.5746	3061.9330	3064.2156
3064.7891	3085.3377	3101.0754
3102.8986	3104.6126	3112.7204
3115.3012	3117.3482	3117.4088
3130.8476	3138.9869	3142.1632
3145.4498	3145.9979	3147.5009
3148.9413	3154.0445	3158.9253
3166.6288	3167.4543	3198.6000
3201.4243	3206.4788	3209.0807
3209.8825	3220.0826	3221.1725
3222.7603	3240.8671	3254.5143

^{t}TS8-F

Zero-point correction=	0.641108
Thermal correction to Energy=	0.678432
Thermal correction to Enthalpy=	0.679376
Thermal correction to Gibbs Free Energy=	0.570391
Sum of electronic and zero-point Energies=	-1882.094202
Sum of electronic and thermal Energies=	-1882.056878
Sum of electronic and thermal Enthalpies=	-1882.055934
Sum of electronic and thermal Free Energies=	-1882.164920

Cartesian coordinates

C	-4.41675100	-1.92549700	-2.56650300
C	-3.25179100	-2.91680500	-2.63012900
C	-1.89267400	-2.28507600	-2.96209300
C	-4.37221400	-0.90522700	-1.42573600
C	-1.31799500	-1.47911500	-1.83365900
C	-3.24506700	0.13241700	-1.52660000
C	-1.89110600	-0.42948100	-1.20275300
H	-5.34780500	-2.49563500	-2.47818400
H	-3.47481900	-3.66110900	-3.40190900
H	-1.99492500	-1.64403100	-3.84807800
H	-4.28986800	-1.42634200	-0.46348900

H	-3.21986400	0.54999500	-2.54210500
C	0.09625900	-0.55665100	0.00769900
H	-4.47568800	-1.38517500	-3.52159300
H	-3.17016800	-3.45774800	-1.67909300
H	-1.18256600	-3.07174300	-3.23324600
H	-5.32370900	-0.36396400	-1.41230700
H	-3.45801900	0.96240300	-0.84959400
N	-1.11235600	0.09247000	-0.16509800
C	-1.69531600	0.89229000	0.88911900
C	-2.16541600	0.23033100	2.03430700
C	-1.80621500	2.28035000	0.72393500
C	-2.70406800	1.01257500	3.05932500
C	-2.36590700	3.01622900	1.76910100
C	-2.79959300	2.39287900	2.93378700
H	-3.06068300	0.53108100	3.96526100
H	-2.45479600	4.09441400	1.67056300
H	-3.22284000	2.98283300	3.74055800
C	-2.09764600	-1.28019600	2.19790400
C	-3.44732000	-1.86914300	2.62477700
H	-3.39330400	-2.96155800	2.62277700
H	-3.71919600	-1.55428100	3.63690600
H	-4.25010300	-1.56189800	1.94882300
C	-1.32421800	2.99262500	-0.52701400
S	0.22926300	-1.88247100	-1.12135900
H	-1.84296400	-1.72411400	1.22885700
H	-1.03917300	2.23037600	-1.25979600
C	-1.00631200	-1.66559500	3.20492000
H	-1.25855000	-1.28462000	4.20051600
H	-0.91327000	-2.75395900	3.27184300
H	-0.03492600	-1.25129000	2.92123400
C	-0.08552400	3.84306800	-0.21520000
H	0.31320700	4.28503200	-1.13406200
H	-0.34761900	4.65986900	0.46653800
H	0.69142800	3.23588400	0.25601000
C	-2.42470100	3.85410200	-1.15683800
H	-2.06009500	4.30224800	-2.08576000
H	-3.31733400	3.26620900	-1.38924100
H	-2.72114900	4.66965700	-0.48983100
C	1.14771100	-0.05241800	0.83143300
O	1.10404100	1.10516900	1.30576500
C	2.33819200	-0.91905000	1.10446400
C	2.25196200	-2.30588100	1.27274500
C	3.57733100	-0.28912000	1.27334500
C	3.39035300	-3.05184100	1.57001000

H	1.28869500	-2.80387100	1.20685600
C	4.71328100	-1.03516800	1.56521700
H	3.62589500	0.79131600	1.16682100
C	4.62344800	-2.41995000	1.70952400
H	3.30943300	-4.12541500	1.70639600
H	5.67179400	-0.54013100	1.68782900
H	5.50978000	-3.00126200	1.94217300
C	2.65042200	0.55370800	-2.19432900
C	3.79100700	1.19172000	-1.56852500
C	1.37730800	1.30615600	-2.29921300
H	0.57606800	0.69353800	-2.71826200
H	1.07697000	1.66007700	-1.30617000
H	1.50125700	2.19979900	-2.92499800
H	2.77509400	-0.43812500	-2.61039000
O	3.77470600	2.31069700	-1.07768700
O	4.89246800	0.41446100	-1.58201300
C	6.04643300	0.99352600	-0.97654000
H	6.81736400	0.22543700	-1.00334300
H	6.36804600	1.87661700	-1.53349200
H	5.83373100	1.28454600	0.05501400

Vibrational frequencies

21.6460	28.3172	30.3243
36.2089	45.0257	48.6889
49.9583	66.6264	69.4030
78.4711	83.7418	91.2046
96.3824	100.4871	104.0829
111.6646	120.2161	127.5232
133.6287	143.8366	163.0098
171.1998	187.4781	201.1884
203.5593	206.6179	218.7926
225.5320	231.0584	239.6289
242.7881	247.9587	253.9681
265.1442	270.2218	280.8141
287.3534	300.0611	319.6502
324.8513	334.4684	345.7581
361.5199	363.7361	389.3697
409.1475	410.2976	423.5739
447.4663	451.3068	468.8509
474.6397	485.3908	506.5198
524.4174	546.2725	548.7869
560.6764	569.3464	598.9067
619.6272	627.1438	645.4169
653.1587	668.3202	681.7931

686.0675 714.8967 718.7537
724.3843 729.9614 772.2382
789.0784 797.5298 816.0376
827.5007 829.7826 832.9176
885.2793 893.4695 896.9708
899.9764 914.1582 928.1361
932.3584 942.2637 944.1629
962.4510 964.9032 968.0710
973.2671 976.1530 985.0180
997.5049 1002.6808 1009.0326
1011.4148 1018.6675 1034.5265
1050.7672 1062.8450 1070.1104
1073.1320 1082.3526 1094.8144
1095.4139 1113.7649 1117.8284
1119.9355 1140.8356 1143.8919
1157.5880 1160.1917 1168.8315
1172.2336 1179.5183 1181.5112
1185.7185 1186.0401 1197.5644
1207.1362 1220.7321 1235.5623
1243.7543 1247.7417 1260.2526
1281.8648 1287.8540 1294.6978
1302.6620 1313.4957 1322.7033
1336.9335 1340.0369 1347.6354
1349.4520 1357.3237 1373.3668
1379.7778 1382.8540 1392.8924
1395.7473 1399.6667 1403.1090
1404.6000 1405.2769 1417.8967
1422.0179 1423.1733 1455.2942
1464.6216 1470.2316 1476.9692
1480.7891 1481.1237 1483.6611
1488.4503 1488.8159 1491.9568
1492.7098 1493.4898 1494.9835
1495.7392 1499.5574 1504.1678
1505.0889 1505.8578 1508.6862
1512.9845 1517.8443 1522.5051
1529.6778 1544.3750 1621.5205
1672.3893 1676.9692 1680.7684
1687.8757 1689.2614 1764.5925
3044.5913 3048.8017 3054.9842
3056.2010 3057.9519 3058.3003
3061.9208 3062.1445 3064.5360
3064.8022 3091.4826 3094.0127
3101.0746 3104.0923 3112.5786
3114.3040 3114.5626 3119.1896

3131.8354	3137.8309	3143.2883
3143.7762	3145.8088	3146.6201
3151.7127	3152.7991	3159.3304
3168.1070	3174.3004	3199.5637
3203.1541	3205.0850	3209.7114
3211.1747	3219.0153	3221.6010
3223.8907	3237.3569	3270.5516

^{os}TS5

Zero-point correction= 0.640892
Thermal correction to Energy= 0.677064
Thermal correction to Enthalpy= 0.678008
Thermal correction to Gibbs Free Energy= 0.573394
Sum of electronic and zero-point Energies= -1882.090824
Sum of electronic and thermal Energies= -1882.054652
Sum of electronic and thermal Enthalpies= -1882.053708
Sum of electronic and thermal Free Energies= -1882.158323

Cartesian coordinates

C	-4.765174	-2.173386	-1.731154
C	-3.621473	-3.177197	-1.894272
C	-2.353915	-2.599433	-2.536770
C	-4.530874	-1.050856	-0.718094
C	-1.599120	-1.663986	-1.637964
C	-3.461406	-0.023522	-1.116311
C	-2.057854	-0.549848	-1.023209
H	-5.661983	-2.723913	-1.427897
H	-3.969917	-3.999719	-2.527180
H	-2.620681	-2.066342	-3.458728
H	-4.267105	-1.480298	0.256472
H	-3.640494	0.312648	-2.146575
C	0.150096	-0.506788	-0.283507
H	-4.992023	-1.728425	-2.709764
H	-3.363069	-3.610972	-0.920315
H	-1.691096	-3.416934	-2.834044
H	-5.472220	-0.509541	-0.580864
H	-3.554651	0.856950	-0.478156
N	-1.078028	0.090468	-0.249084
C	-1.486803	0.973094	0.835090
C	-1.741474	0.378344	2.080591
C	-1.690832	2.338220	0.593926
C	-2.154662	1.213992	3.122229
C	-2.118471	3.126080	1.663452
C	-2.337990	2.575319	2.920900

H	-2.340491	0.786720	4.103101
H	-2.276765	4.189392	1.507643
H	-2.661409	3.206811	3.742043
C	-1.568888	-1.109659	2.345890
C	-2.800089	-1.716389	3.029341
H	-2.690831	-2.802649	3.093325
H	-2.918490	-1.336571	4.048443
H	-3.717382	-1.492780	2.477976
C	-1.454483	2.978849	-0.760198
S	0.074448	-1.941257	-1.250632
H	-1.445757	-1.627461	1.388046
H	-1.187420	2.185784	-1.465076
C	-0.314179	-1.359248	3.192937
H	-0.435550	-0.911865	4.185289
H	-0.146249	-2.432858	3.321997
H	0.576950	-0.923677	2.733533
C	-0.284827	3.968796	-0.685749
H	-0.052403	4.356483	-1.682856
H	-0.545063	4.819690	-0.047175
H	0.604333	3.484880	-0.274762
C	-2.713506	3.675534	-1.290228
H	-2.518879	4.091151	-2.283244
H	-3.558039	2.985394	-1.370209
H	-3.012880	4.501636	-0.637538
C	1.314450	0.111453	0.354486
O	1.230211	1.311435	0.684320
C	2.479683	-0.709854	0.816657
C	2.496477	-2.107404	0.896628
C	3.593005	0.002062	1.281980
C	3.616454	-2.773676	1.388625
H	1.627599	-2.692885	0.617227
C	4.706405	-0.663537	1.778559
H	3.565575	1.085502	1.226892
C	4.727234	-2.057207	1.826060
H	3.610514	-3.857501	1.444752
H	5.563008	-0.094787	2.127983
H	5.596764	-2.579179	2.212392
C	2.241144	0.326550	-2.126720
C	3.481274	0.914315	-1.699690
C	1.147074	1.231793	-2.563720
H	0.237134	0.675822	-2.810050
H	0.929674	1.938213	-1.754389
H	1.429780	1.826327	-3.442948
H	2.249570	-0.725352	-2.388700

O	3.643931	2.095274	-1.413920
O	4.494349	0.012083	-1.627702
C	5.755759	0.553146	-1.252579
H	6.437511	-0.293271	-1.178441
H	6.110891	1.259543	-2.007984
H	5.690417	1.067187	-0.291224

Vibrational frequencies

-540.1294	22.6216	24.8320
33.4452	39.4682	41.8149
47.8250	57.9078	77.2781
81.0047	89.2678	96.5712
99.9924	109.1022	114.2467
118.2266	124.1924	134.0677
140.6843	151.1258	163.0495
180.1898	195.8566	204.1831
213.1715	218.5812	224.1181
228.5656	234.6619	239.6054
243.9470	251.0945	260.3375
273.9227	282.0789	286.1773
293.9796	305.9189	323.6677
327.5192	338.7228	349.9955
365.1887	376.4396	381.8184
411.3877	418.4512	421.2661
439.1518	454.1762	464.9472
480.1298	493.0500	505.3524
513.4677	532.5590	556.5423
567.6206	590.3795	609.0710
627.9583	636.0015	651.1804
654.0945	660.7171	682.1123
702.5572	708.1543	720.3897
727.1483	739.3328	778.1137
787.6386	792.8988	817.5962
830.0421	831.7022	835.8574
872.6016	891.3669	896.1231
899.0035	913.4665	933.3781
935.3934	942.7667	945.9343
948.0451	957.7655	966.1876
968.2375	973.4828	974.4104
990.0857	1002.7733	1009.7250
1016.6093	1017.7660	1021.3072
1049.6099	1065.8117	1071.7091
1074.2744	1083.5474	1087.5610
1099.0061	1107.4841	1119.0355

1123.8707	1129.6147	1141.5279
1143.7624	1165.9725	1166.8333
1173.4589	1174.1751	1183.0205
1184.7702	1188.4246	1191.9445
1206.1852	1210.7550	1218.6068
1239.3372	1242.7403	1253.1665
1282.7452	1288.3788	1293.1138
1298.7048	1304.7343	1316.6444
1325.0858	1335.5334	1337.5012
1343.6100	1347.0030	1361.5830
1371.9310	1377.0936	1382.5932
1396.0513	1396.9429	1401.6377
1404.0731	1405.3132	1408.1348
1414.6663	1423.1752	1427.5779
1450.7906	1475.6022	1480.4003
1482.0677	1483.3189	1485.2867
1487.5281	1489.8040	1492.0657
1493.3482	1494.1909	1495.7022
1497.1917	1498.3138	1499.4606
1503.7250	1507.3132	1509.3051
1511.9927	1515.5361	1523.0414
1530.8992	1544.0228	1594.5938
1669.7145	1675.1159	1681.4933
1687.7409	1690.9414	1736.7574
3038.5662	3053.3095	3058.7460
3059.3138	3059.8367	3063.5281
3064.1448	3065.5277	3066.6201
3068.7990	3080.4297	3091.6497
3105.1069	3110.9632	3111.0139
3114.8955	3116.7894	3122.1205
3135.9460	3144.0554	3144.9891
3146.0207	3149.1030	3149.7019
3153.0905	3154.7301	3158.7692
3161.1622	3167.5273	3192.6084
3200.7719	3204.5302	3210.6490
3215.0127	3220.8296	3227.5950
3230.3561	3243.2089	3245.8836

M8

Zero-point correction= 0.645593
Thermal correction to Energy= 0.680895
Thermal correction to Enthalpy= 0.681839
Thermal correction to Gibbs Free Energy= 0.580995
Sum of electronic and zero-point Energies= -1882.125126

Sum of electronic and thermal Energies= -1882.089824
Sum of electronic and thermal Enthalpies= -1882.088880
Sum of electronic and thermal Free Energies= -1882.189723

Cartesian coordinates

C	5.228294	-1.635149	-1.170640
C	4.273927	-2.750701	-1.603518
C	3.062540	-2.274190	-2.418040
C	4.671948	-0.629077	-0.159156
C	2.052321	-1.535466	-1.589680
C	3.571515	0.294366	-0.711035
C	2.253509	-0.407935	-0.863551
H	6.118621	-2.099152	-0.733587
H	4.831581	-3.460923	-2.222210
H	3.400681	-1.614991	-3.227644
H	4.293703	-1.159815	0.723602
H	3.890129	0.675736	-1.689438
C	0.036947	-0.808049	-0.325431
H	5.569191	-1.091361	-2.062283
H	3.920415	-3.302721	-0.724372
H	2.577465	-3.130446	-2.893824
H	5.495702	0.006487	0.182094
H	3.444400	1.164690	-0.061962
N	1.094835	-0.010700	-0.177675
C	1.037240	1.258068	0.533676
C	1.499630	1.314996	1.853643
C	0.586056	2.373970	-0.181118
C	1.437833	2.552556	2.492477
C	0.544871	3.590318	0.507768
C	0.951968	3.677361	1.832833
H	1.774923	2.636042	3.521738
H	0.200163	4.481681	-0.006315
H	0.907901	4.630583	2.350044
C	2.070129	0.110519	2.580210
C	3.506407	0.388664	3.044054
H	3.516581	1.147582	3.832977
H	4.142451	0.746680	2.228996
H	3.952990	-0.522470	3.453431
C	0.252067	2.323452	-1.664650
S	0.430999	-2.094579	-1.374415
H	2.091448	-0.735052	1.881752
H	0.016654	1.289341	-1.936743
C	1.191381	-0.297700	3.768161
H	1.148047	0.509764	4.507685

H	1.617081	-1.178212	4.260353
H	0.184472	-0.517070	3.409310
C	-0.964360	3.174743	-2.032560
H	-1.822883	2.932941	-1.402840
H	-1.239811	2.987434	-3.074432
H	-0.745813	4.243415	-1.939149
C	1.471831	2.766875	-2.485136
H	1.735113	3.801474	-2.240936
H	1.249515	2.713281	-3.554941
H	2.345552	2.141533	-2.285697
C	-1.316242	-0.627729	0.476767
O	-1.081641	-0.120114	1.658880
C	-2.277612	0.218929	-0.409667
C	-2.504420	0.003468	-1.771542
C	-3.044245	1.171612	0.259367
C	-3.489798	0.719734	-2.447336
H	-1.923218	-0.737593	-2.316635
C	-4.045191	1.876761	-0.408820
H	-2.831193	1.325428	1.311943
C	-4.272511	1.650653	-1.764854
H	-3.654120	0.543717	-3.506230
H	-4.643146	2.607970	0.127723
H	-5.048336	2.199557	-2.289537
C	-1.944631	-2.109894	0.569772
C	-1.175095	-2.932387	1.595510
H	-1.599782	-3.934340	1.700203
H	-0.122770	-3.034397	1.315539
C	-3.378758	-1.960904	1.014185
O	-3.745566	-1.801916	2.157378
O	-4.236574	-2.009650	-0.018648
C	-5.595624	-1.715275	0.305117
H	-5.669476	-0.705933	0.717703
H	-5.983391	-2.431496	1.032047
H	-6.147812	-1.783432	-0.630373
H	-1.227076	-2.413024	2.552344
H	-1.967096	-2.586838	-0.417690

Vibrational frequencies

27.0737	41.2518	41.9613
49.7473	59.0735	70.2631
79.4209	81.5806	88.4480
90.4409	94.3018	101.2870
122.1914	123.6786	129.0910
133.3049	139.0291	147.1089

162.8248	173.1971	190.1237
206.0650	212.2683	215.9941
225.4625	236.8913	241.9449
247.1226	250.0254	254.9194
268.8471	282.1585	284.5730
294.5546	298.8485	300.1245
311.3767	319.7360	336.6223
348.9675	355.7551	357.8748
368.4132	406.8998	415.3658
420.6580	424.7186	434.7865
449.3773	475.9349	490.7604
510.5220	527.2504	534.9166
549.1780	566.3930	585.0685
615.1015	621.8487	629.0310
637.0992	653.1138	668.7102
687.1035	710.0861	723.0843
729.7422	736.4646	767.8910
780.9111	790.1311	803.2654
822.4860	829.2955	834.2154
836.5432	877.0161	883.4649
891.5702	897.1758	914.2340
916.6535	921.9048	931.2246
933.8580	938.5859	956.1243
962.1502	968.5828	973.8054
974.5969	978.3838	1001.6326
1006.9076	1011.1950	1013.6536
1015.9579	1021.3042	1052.4348
1055.6208	1067.3130	1073.0589
1084.4522	1088.1562	1099.7837
1107.5420	1118.5753	1124.6203
1135.3906	1143.5331	1145.3226
1148.7592	1168.3407	1172.2471
1173.0800	1177.2202	1183.3970
1189.7477	1190.0110	1200.7243
1209.5414	1216.5193	1235.8895
1238.5088	1252.3857	1255.6129
1258.0599	1289.1952	1293.0654
1299.7228	1307.7080	1322.1792
1329.6327	1336.9397	1338.8237
1340.3664	1343.8881	1363.1798
1373.0877	1377.0645	1384.7971
1391.3101	1392.4526	1398.2916
1400.7936	1405.5280	1406.7837
1408.3064	1416.6486	1419.9310

1425.1964	1478.1819	1480.5540
1483.8271	1485.5666	1485.9136
1488.6527	1489.8055	1491.8868
1492.7303	1495.1919	1496.4009
1496.6676	1497.4157	1498.9713
1501.1306	1504.8228	1507.4912
1508.9301	1514.1559	1518.8906
1525.9225	1533.8159	1540.4930
1675.4107	1676.2290	1685.5385
1688.0044	1688.7804	1841.7810
3051.4715	3055.0040	3060.6918
3063.8121	3066.2629	3067.8523
3069.0294	3069.5488	3072.6377
3075.5511	3078.6110	3082.0504
3086.7536	3108.6042	3111.8136
3119.5501	3121.3931	3127.6251
3132.0483	3140.0220	3140.2510
3140.6521	3147.4210	3148.3263
3148.3417	3165.5835	3171.1877
3176.6584	3180.4510	3187.7304
3191.8445	3194.9625	3199.2671
3202.4559	3208.1218	3211.5527
3224.1285	3227.1418	3230.3935

TS6

Zero-point correction= 0.644871
Thermal correction to Energy= 0.679992
Thermal correction to Enthalpy= 0.680936
Thermal correction to Gibbs Free Energy= 0.580339
Sum of electronic and zero-point Energies= -1882.114088
Sum of electronic and thermal Energies= -1882.078967
Sum of electronic and thermal Enthalpies= -1882.078023
Sum of electronic and thermal Free Energies= -1882.178620

Cartesian coordinates

C	-5.058107	-1.998053	-1.161167
C	-4.074491	-3.169035	-1.106061
C	-2.754690	-2.926148	-1.850008
C	-4.633402	-0.728208	-0.417641
C	-1.851805	-1.943400	-1.162580
C	-3.451181	0.025263	-1.049733
C	-2.133519	-0.662492	-0.831430
H	-6.012741	-2.334092	-0.742285
H	-4.555338	-4.045073	-1.553609

H	-2.971594	-2.560167	-2.862452
H	-4.393743	-0.973483	0.624693
H	-3.634267	0.119117	-2.128403
C	0.061548	-0.784988	0.016524
H	-5.254538	-1.746601	-2.212606
H	-3.856135	-3.423945	-0.061924
H	-2.222373	-3.874058	-1.969714
H	-5.488613	-0.044114	-0.393107
H	-3.398135	1.043781	-0.656361
N	-1.036585	-0.045233	-0.190478
C	-1.065390	1.374684	0.116619
C	-1.717405	1.811470	1.275756
C	-0.464230	2.250176	-0.800392
C	-1.724823	3.184219	1.530900
C	-0.492526	3.612953	-0.494106
C	-1.108902	4.076571	0.662501
H	-2.214036	3.555609	2.426910
H	-0.032979	4.321938	-1.174469
H	-1.118142	5.139703	0.881305
C	-2.409808	0.866342	2.242387
C	-3.894402	1.225356	2.395079
H	-4.007224	2.190246	2.899592
H	-4.404602	1.291084	1.430170
H	-4.404504	0.470880	3.001779
C	0.119656	1.768372	-2.120776
S	-0.248290	-2.340763	-0.636289
H	-2.340853	-0.151527	1.839546
H	0.498265	0.751710	-1.978171
C	-1.723318	0.876499	3.614173
H	-1.847630	1.853690	4.094225
H	-2.176587	0.124717	4.268067
H	-0.656123	0.677226	3.504273
C	1.291375	2.623980	-2.602896
H	2.032477	2.764726	-1.812567
H	1.782343	2.130440	-3.446351
H	0.953748	3.606415	-2.949389
C	-0.974968	1.724321	-3.196287
H	-1.407159	2.720342	-3.339333
H	-0.554449	1.392929	-4.150514
H	-1.781803	1.038863	-2.926247
C	1.583257	-0.002441	1.228110
O	1.033641	0.808142	1.993889
C	2.538736	0.538782	0.166374
C	2.864640	-0.123054	-1.021935

C	3.223376	1.710686	0.492637
C	3.866351	0.367019	-1.853941
H	2.332690	-1.029648	-1.298445
C	4.234126	2.199802	-0.335311
H	2.958175	2.222963	1.411955
C	4.562244	1.525749	-1.508325
H	4.104737	-0.157533	-2.774363
H	4.764770	3.106835	-0.062316
H	5.347677	1.903173	-2.155423
C	2.103288	-1.308136	1.932000
H	2.844571	-0.888403	2.621799
C	1.015504	-2.023578	2.723776
H	0.425750	-2.673608	2.075968
H	0.358255	-1.277065	3.174752
C	2.851848	-2.247528	1.022337
O	2.349419	-3.121706	0.346261
O	4.167378	-2.001276	1.019885
C	4.934964	-2.762057	0.083813
H	4.793429	-3.830763	0.251838
H	4.631348	-2.510598	-0.935705
H	5.972771	-2.480998	0.250401
H	1.450136	-2.635908	3.517767

Vibrational frequencies

-125.2070	32.3237	40.3404
42.6820	51.4962	58.0251
62.3729	73.5981	80.0396
82.0614	94.3620	101.5886
115.6889	118.2751	122.7612
124.6680	128.6938	139.1038
149.5111	152.0183	161.5685
172.7182	186.5218	208.5654
223.3085	229.3353	232.8384
239.0553	245.7787	246.6641
263.3994	280.9410	283.1401
292.8303	303.2419	305.8098
315.7569	323.5886	336.3771
338.5255	351.9827	357.8998
366.4716	390.6997	403.6676
410.7319	425.5201	426.7124
449.5056	470.8104	476.7009
501.6981	519.7808	529.3657
534.4818	552.4096	566.0497
582.9239	614.5682	623.9536

628.9121 650.2839 653.5388
670.0820 696.9722 717.9661
720.4457 731.4523 758.8256
780.3370 781.9497 791.4361
811.6254 813.8157 830.0190
832.7097 836.5675 869.1535
880.3405 895.5458 898.6907
916.1521 931.2772 932.8550
935.9645 942.0929 946.1893
968.0305 971.7998 975.1792
975.4316 977.7357 989.1721
1005.8659 1012.0382 1016.1358
1018.9107 1022.9430 1045.8461
1058.4667 1063.4754 1071.2497
1077.4592 1087.1509 1094.5588
1115.9625 1121.5185 1125.0748
1127.5997 1137.1093 1150.3775
1151.3538 1161.7469 1170.3060
1176.2308 1182.1671 1187.5053
1192.2058 1200.4323 1212.2052
1215.5695 1232.8527 1234.9372
1247.2063 1255.4400 1257.3897
1285.3612 1292.9759 1297.4683
1298.7473 1304.4585 1321.4011
1330.7834 1334.4351 1336.9765
1344.7183 1361.2549 1371.8056
1376.4014 1382.4702 1395.1916
1396.7191 1398.1486 1401.7360
1405.1344 1405.8808 1410.6685
1412.9803 1423.7564 1424.3132
1426.8574 1477.6002 1483.1208
1484.6190 1486.7741 1488.1512
1489.0966 1492.8580 1493.5651
1495.5650 1495.9386 1497.0565
1498.0134 1501.4649 1503.4186
1504.2826 1506.9929 1507.6507
1514.0280 1520.0072 1527.2094
1536.1173 1546.3239 1631.0995
1676.5613 1678.3314 1687.5336
1694.1489 1694.9280 1829.8659
3053.8174 3057.8763 3060.5794
3061.5898 3062.5874 3067.1794
3068.1248 3069.4129 3070.4626
3079.2138 3083.5398 3088.6179

3095.7606	3108.7809	3116.4962
3117.1628	3119.1105	3121.0851
3133.5762	3136.2835	3139.9538
3142.4944	3149.0694	3152.4853
3160.7109	3162.9791	3175.1018
3180.0897	3180.8554	3187.4867
3197.8698	3197.9873	3206.5073
3209.0850	3213.2677	3217.7907
3219.4466	3226.0258	3234.7021

P

Zero-point correction= 0.212314
Thermal correction to Energy= 0.225666
Thermal correction to Enthalpy= 0.226610
Thermal correction to Gibbs Free Energy= 0.171494
Sum of electronic and zero-point Energies= -651.614008
Sum of electronic and thermal Energies= -651.600657
Sum of electronic and thermal Enthalpies= -651.599712
Sum of electronic and thermal Free Energies= -651.654829

Cartesian coordinates

C	-0.111768	-1.336289	-0.469521
O	0.016884	-2.228942	-1.284995
C	1.045352	-0.452652	-0.116670
C	0.951399	0.600194	0.800530
C	2.267760	-0.705007	-0.749886
C	2.065769	1.387268	1.076824
H	0.019459	0.818927	1.311980
C	3.378885	0.080467	-0.472514
H	2.324754	-1.524220	-1.458387
C	3.278378	1.128754	0.442333
H	1.985305	2.201205	1.789189
H	4.323161	-0.121455	-0.967106
H	4.145679	1.743059	0.661657
C	-1.457859	-1.160546	0.237506
H	-2.151214	-1.782454	-0.339492
C	-1.418464	-1.653069	1.685612
H	-0.707692	-1.081867	2.286292
H	-1.127699	-2.704860	1.712045
C	-1.984509	0.258330	0.133918
O	-2.530702	0.866393	1.024880
O	-1.776206	0.756466	-1.087942
C	-2.208342	2.108625	-1.286746
H	-3.277735	2.196362	-1.090206

H	-1.658840	2.775372	-0.619052
H	-1.987475	2.340657	-2.325859
H	-2.407112	-1.548511	2.135084

Vibrational frequencies

34.1816	58.6397	81.7043
96.9532	136.5161	148.9115
165.1539	186.0599	197.7936
243.2190	263.5708	337.7996
394.1688	416.9199	439.3813
462.8800	492.7531	539.3993
623.9319	671.0796	703.7328
728.1349	754.4183	789.0832
831.5989	893.3626	897.8705
960.7739	985.0851	1016.5464
1025.8166	1036.9404	1044.2181
1065.0868	1087.9866	1120.3034
1135.6346	1147.7339	1176.5487
1187.9902	1206.0588	1222.6141
1278.3472	1297.1345	1314.4361
1345.8081	1362.8795	1375.4623
1421.4385	1490.9696	1496.4859
1499.3480	1500.4708	1503.5051
1504.2841	1547.3580	1673.4523
1689.8661	1821.4871	1859.4659
3093.7249	3095.9130	3104.2649
3177.9414	3182.6970	3189.7077
3213.8982	3219.5296	3226.6656
3227.5096	3233.8220	3238.7803

M19

Zero-point correction= 0.545205
Thermal correction to Energy= 0.574250
Thermal correction to Enthalpy= 0.575194
Thermal correction to Gibbs Free Energy= 0.485962
Sum of electronic and zero-point Energies= -1575.857544
Sum of electronic and thermal Energies= -1575.828500
Sum of electronic and thermal Enthalpies= -1575.827556
Sum of electronic and thermal Free Energies= -1575.916788

Cartesian coordinates

C	4.00177000	3.13778900	-0.08300700
C	2.74178600	4.00222100	0.01199600
C	1.60801100	3.57718800	-0.93010300

C	3.86433600	1.68914700	0.39305200
C	0.93466900	2.29647000	-0.52692900
C	2.96312700	0.80106600	-0.47843600
C	1.49639100	1.09823700	-0.32140300
H	4.79296400	3.61719900	0.50394400
H	3.01587700	5.03500700	-0.22980100
H	2.00750200	3.47462900	-1.94860900
H	3.49657500	1.67176500	1.42702500
H	3.24316600	0.93144500	-1.53254100
C	-0.73465300	0.52684500	0.20858500
H	4.35098400	3.13439500	-1.12517400
H	2.36855800	4.00471700	1.04345800
H	0.85916300	4.37396300	-0.97568600
H	4.86283200	1.23877000	0.40662300
H	3.14812600	-0.24853500	-0.23890400
N	0.59847600	0.09591000	0.11339100
C	0.93830200	-1.28830400	-0.09604600
C	1.56432600	-1.98655000	0.94923200
C	0.67457900	-1.87600800	-1.33884500
C	1.89023200	-3.32535500	0.73516800
C	1.00680200	-3.22388900	-1.50585200
C	1.60276800	-3.94437000	-0.47940700
H	2.37596200	-3.89427000	1.52094500
H	0.79940300	-3.71130700	-2.45478700
H	1.85673700	-4.98942600	-0.62710400
C	1.84357600	-1.29480400	2.27316900
C	2.99561600	-1.92654200	3.05457800
H	3.24171500	-1.30310000	3.91836900
H	2.72868600	-2.91839800	3.43361600
H	3.89313000	-2.02683900	2.43665000
C	0.03240000	-1.10663600	-2.48052800
S	-0.79865400	2.26101700	-0.17979000
H	2.12354200	-0.25870200	2.04794200
H	-0.06245700	-0.05765900	-2.18207300
C	0.57167000	-1.24781400	3.13125700
H	0.21415100	-2.26411100	3.33083800
H	0.77719500	-0.76295700	4.09052400
H	-0.22457600	-0.69539000	2.62639100
C	-1.37506400	-1.63975800	-2.77432000
H	-1.84994500	-1.04707700	-3.56217800
H	-1.32919400	-2.67939800	-3.11689600
H	-2.00186500	-1.60220400	-1.87909400
C	0.90721800	-1.14430300	-3.73889300
H	0.45426800	-0.54084500	-4.53112000

H	1.90750600	-0.75048200	-3.53574800
H	1.01497900	-2.16537300	-4.11833200
C	-1.82237300	-0.23793100	0.49432100
O	-1.64287600	-1.60754000	0.64773600
C	-3.21915400	0.22058900	0.51429100
C	-3.61504100	1.50575900	0.92094500
C	-4.22665000	-0.69118300	0.14748600
C	-4.95693000	1.87551700	0.91413700
H	-2.87980300	2.21287500	1.28893700
C	-5.56498100	-0.31822000	0.14463500
H	-3.94304200	-1.69687400	-0.14490200
C	-5.93993900	0.97137000	0.51997900
H	-5.23464300	2.87422000	1.23667400
H	-6.32006300	-1.03860700	-0.15520200
H	-6.98504400	1.26300500	0.51664000
H	-2.06699500	-1.87095800	1.47622900

Vibrational frequencies

22.5616	31.0177	33.4692
46.9665	54.0039	60.8483
81.8155	85.3810	92.7311
95.5210	108.7348	125.8176
133.5321	146.3160	180.3746
204.2582	209.3280	214.3076
228.8839	237.5138	241.0736
260.0198	267.2354	270.2638
278.3498	293.2326	307.3895
315.6252	326.8419	344.2870
345.0071	354.4755	365.0197
376.6308	406.5246	417.3104
422.4801	441.1408	452.3353
470.2556	496.1292	500.9368
522.4095	535.4362	554.0419
565.4743	585.3673	605.5428
614.6902	628.4811	639.0358
653.8185	661.7565	711.5536
717.3980	724.3788	772.0605
784.7157	797.7668	813.3849
829.0786	830.2332	833.7955
880.4087	888.2130	894.7415
914.4034	929.6071	933.8167
937.8532	941.6578	953.8383
964.0122	966.9381	975.6125
977.9768	984.0747	1002.0356

1006.5906	1008.3429	1012.5694
1023.3302	1065.7403	1069.9759
1074.3215	1085.1588	1095.2650
1097.3051	1118.9891	1121.2186
1133.7392	1147.2671	1151.2179
1163.7840	1170.9953	1174.6146
1180.8632	1187.4641	1204.9937
1207.6007	1210.2487	1236.6247
1250.9637	1272.2060	1281.9620
1289.9506	1293.1726	1300.1490
1308.6658	1315.5017	1331.6662
1338.7851	1342.5555	1343.9063
1360.6802	1363.7186	1372.8692
1381.4812	1383.7758	1390.7691
1396.7728	1401.5767	1404.3164
1405.0632	1413.4434	1419.9497
1423.6512	1478.8469	1481.8666
1484.2261	1488.6496	1488.7751
1490.6278	1492.2963	1495.2959
1496.3509	1497.8726	1503.8439
1507.8388	1508.7929	1513.6334
1523.3948	1529.4756	1547.5525
1655.1885	1672.1837	1678.5292
1683.0351	1703.8504	1761.2155
3047.6654	3048.9038	3051.3001
3057.6058	3058.5956	3059.7181
3060.9683	3061.8229	3061.9093
3085.2374	3101.5613	3104.0321
3104.8425	3111.8210	3114.4619
3134.3269	3135.9093	3138.0766
3142.3657	3143.2795	3144.4218
3149.7496	3164.5156	3167.9991
3195.9978	3199.5396	3207.9707
3211.6638	3225.6370	3231.3164
3234.8688	3241.3998	3827.3347

^{2}M20

Zero-point correction= 0.546333
Thermal correction to Energy= 0.575451
Thermal correction to Enthalpy= 0.576395
Thermal correction to Gibbs Free Energy= 0.484429
Sum of electronic and zero-point Energies= -1575.704424
Sum of electronic and thermal Energies= -1575.675306
Sum of electronic and thermal Enthalpies= -1575.674362

Sum of electronic and thermal Free Energies= -1575.766328

Cartesian coordinates

C	-3.628738	3.334891	0.277573
C	-2.296804	4.071104	0.441605
C	-1.359492	3.473628	1.503085
C	-3.547943	1.913645	-0.285184
C	-0.735742	2.180065	1.072218
C	-2.879744	0.889626	0.648639
C	-1.389222	1.041907	0.701658
H	-4.265416	3.928374	-0.386483
H	-2.507775	5.104614	0.733230
H	-1.917131	3.300598	2.432500
H	-3.022303	1.922655	-1.248685
H	-3.277218	1.010335	1.664578
C	0.797745	0.364104	0.368186
H	-4.140475	3.302670	1.248970
H	-1.769397	4.112696	-0.518953
H	-0.568917	4.189690	1.742016
H	-4.564689	1.561254	-0.483525
H	-3.127585	-0.124307	0.327719
N	-0.528640	0.028539	0.311349
C	-1.017425	-1.214864	-0.251278
C	-1.241000	-1.260768	-1.632791
C	-1.269239	-2.285435	0.613511
C	-1.729092	-2.460831	-2.155030
C	-1.772228	-3.455652	0.043411
C	-1.994676	-3.545118	-1.326313
H	-1.906754	-2.545583	-3.222403
H	-1.988567	-4.308667	0.679931
H	-2.380389	-4.466251	-1.750759
C	-0.937418	-0.084263	-2.545204
C	-2.062622	0.171477	-3.553007
H	-1.866214	1.098387	-4.098690
H	-2.131951	-0.635115	-4.288690
H	-3.032237	0.261479	-3.054919
C	-1.017666	-2.203172	2.108228
S	0.975943	1.994380	0.932813
H	-0.840189	0.818084	-1.929212
H	-0.535394	-1.244074	2.325728
C	0.398055	-0.305925	-3.268731
H	0.337010	-1.187777	-3.914673
H	0.643227	0.559370	-3.890720
H	1.217131	-0.464585	-2.560754

C	-0.069522	-3.313069	2.575716
H	0.144693	-3.195004	3.641584
H	-0.518841	-4.300707	2.433248
H	0.872720	-3.279882	2.023627
C	-2.340701	-2.253298	2.882359
H	-2.155733	-2.152628	3.955440
H	-3.017116	-1.451144	2.573621
H	-2.849078	-3.208110	2.713933
C	1.886667	-0.472289	0.112642
O	1.654372	-1.784325	0.011192
C	3.266994	0.012561	0.016662
C	3.583554	1.178737	-0.695984
C	4.291938	-0.741746	0.608340
C	4.906375	1.592282	-0.793756
H	2.800930	1.735234	-1.202564
C	5.611236	-0.320045	0.505277
H	4.050372	-1.636216	1.175231
C	5.919333	0.847601	-0.191773
H	5.148274	2.488528	-1.354113
H	6.398623	-0.897838	0.976579
H	6.950718	1.174231	-0.270631
H	2.434348	-2.236480	-0.346516

Vibrational frequencies

9.8690	14.8294	34.9979
43.9354	48.1827	56.7176
74.1042	77.0607	84.7485
88.7053	108.3292	116.9728
129.9399	137.5897	173.5079
189.4328	203.1499	212.9764
227.1023	230.4732	240.7121
254.4855	255.5750	264.0888
269.7319	290.0704	299.9613
321.3569	328.4481	331.2075
346.8852	358.4310	385.2237
409.2923	413.8868	415.9568
449.2424	449.3133	472.5867
487.9192	497.5674	511.4010
528.1824	547.8478	563.9492
573.6753	603.6157	613.2227
623.9211	635.6098	648.5659
655.2714	685.5157	715.7947
720.9514	728.7292	780.9681
790.3867	793.1323	817.2068

830.5879	833.2378	837.9382
881.0078	892.5817	900.7547
914.4330	928.5498	944.6604
948.3255	949.8700	962.8042
967.7827	970.1433	977.2267
979.5410	982.6405	1009.1263
1013.7274	1017.4133	1025.1701
1040.7430	1063.5699	1069.8166
1074.8129	1085.6499	1093.9029
1118.0387	1121.9035	1127.0002
1144.8956	1147.5794	1159.5343
1165.4035	1170.2695	1184.1715
1184.5557	1195.6067	1211.6842
1212.4220	1226.6252	1238.4519
1249.2267	1270.0381	1289.2270
1294.3094	1294.9591	1302.9131
1322.7324	1330.5091	1334.7265
1340.9394	1345.3373	1359.6773
1367.2411	1370.4184	1381.2668
1388.4237	1394.0594	1396.4013
1401.9307	1407.4297	1412.0308
1412.8915	1427.9087	1431.4015
1433.2697	1477.4854	1479.6942
1484.5668	1487.5238	1489.4499
1490.3677	1494.2412	1495.7927
1498.5527	1499.7728	1503.8358
1506.8390	1509.8782	1516.1640
1523.3879	1533.8634	1547.2324
1567.6955	1654.0645	1665.5768
1676.5154	1686.7380	1689.1955
3054.3629	3062.8909	3063.6713
3064.0675	3064.4174	3067.3720
3069.9942	3071.8853	3072.3858
3080.4001	3092.2012	3116.6238
3121.4907	3124.8833	3130.9017
3143.1835	3145.6795	3147.5157
3148.5037	3149.2034	3151.7348
3152.1028	3154.8351	3164.0686
3211.1448	3217.3413	3217.7093
3223.0341	3226.5843	3236.6541
3237.7342	3245.5872	3797.9597

^{2}M21

Zero-point correction= 0.532080

Thermal correction to Energy= 0.560851
Thermal correction to Enthalpy= 0.561795
Thermal correction to Gibbs Free Energy= 0.472393
Sum of electronic and zero-point Energies= -1575.364953
Sum of electronic and thermal Energies= -1575.336182
Sum of electronic and thermal Enthalpies= -1575.335238
Sum of electronic and thermal Free Energies= -1575.424641

Cartesian coordinates

C	-3.812546	3.299496	-0.218468
C	-2.501196	4.087616	-0.126230
C	-1.529358	3.580879	0.949658
C	-3.704326	1.833090	-0.650255
C	-0.857683	2.288377	0.582184
C	-2.950952	0.931828	0.339851
C	-1.458922	1.127731	0.285844
H	-4.478087	3.817656	-0.918440
H	-2.750517	5.132588	0.092407
H	-2.076393	3.465267	1.896700
H	-3.221219	1.765512	-1.633907
H	-3.311124	1.140710	1.356501
C	0.761358	0.519077	-0.285756
H	-4.309483	3.335939	0.761674
H	-1.990998	4.078926	-1.097691
H	-0.764830	4.342955	1.131630
H	-4.720548	1.439940	-0.771116
H	-3.187037	-0.115787	0.138961
N	-0.617598	0.101549	-0.182025
C	-0.943422	-1.245685	0.207511
C	-1.708401	-2.028585	-0.677390
C	-0.566526	-1.739267	1.466697
C	-2.058011	-3.324512	-0.294438
C	-0.920438	-3.049352	1.804589
C	-1.661402	-3.840356	0.935461
H	-2.640237	-3.943689	-0.971715
H	-0.615314	-3.451660	2.767604
H	-1.933728	-4.853443	1.215970
C	-2.090597	-1.509302	-2.052309
C	-3.552973	-1.777794	-2.414390
H	-3.789572	-1.315259	-3.377792
H	-3.758689	-2.849102	-2.507542
H	-4.236155	-1.366935	-1.663319
C	0.244095	-0.909077	2.445725
S	0.902294	2.203368	0.346641

H	-1.940236	-0.425833	-2.040643
H	0.282980	0.115971	2.071305
C	-1.134924	-2.099329	-3.096858
H	-1.276637	-3.184515	-3.168074
H	-1.324983	-1.668847	-4.085994
H	-0.101199	-1.903238	-2.795653
C	1.681313	-1.441075	2.514539
H	2.317194	-0.769306	3.100955
H	1.698510	-2.426131	2.996384
H	2.097203	-1.541214	1.508039
C	-0.398322	-0.862739	3.835953
H	0.185462	-0.216263	4.498764
H	-1.418014	-0.468559	3.784720
H	-0.441530	-1.854721	4.297047
C	1.747825	-0.315414	-0.751758
O	1.532511	-1.540886	-1.108856
C	3.182390	0.138438	-0.742260
C	3.633500	1.452380	-0.942145
C	4.157187	-0.861131	-0.582147
C	4.993573	1.757786	-0.933463
H	2.922493	2.246962	-1.142313
C	5.513532	-0.557839	-0.559046
H	3.806415	-1.883156	-0.484846
C	5.942982	0.758994	-0.729046
H	5.312003	2.783097	-1.100385
H	6.242631	-1.350722	-0.415645
H	7.001508	0.999782	-0.717138

Vibrational frequencies

23.3694	29.9605	36.2636
36.7965	47.9859	52.1190
72.3246	79.4218	83.1531
95.0904	105.3783	124.7192
131.6697	140.7633	182.0239
193.8257	212.4841	217.7370
231.4485	235.6198	250.0991
256.6604	262.8228	277.7762
284.2513	291.6205	311.2153
320.3519	326.9715	340.7678
350.2728	361.6735	377.9738
396.3795	409.5294	424.6556
447.5321	454.9131	468.8039
480.6746	503.5430	517.1251
538.3027	553.6372	561.8489

594.1378	615.4079	626.4091
630.5685	653.8944	660.5947
665.6075	708.6967	714.3023
725.0573	772.8692	790.8337
793.3253	805.8073	828.7330
832.3858	835.7787	884.4598
885.7147	888.9589	915.4161
932.4564	933.9383	935.1055
936.2029	949.2626	961.4614
967.3953	977.7465	981.4607
984.4794	995.7684	1002.1714
1006.0506	1013.6460	1022.0844
1061.0060	1067.7279	1074.2614
1085.8145	1095.2632	1098.7213
1109.8204	1117.9390	1143.2456
1146.7458	1151.5923	1164.8148
1169.5106	1174.9507	1181.7180
1190.8086	1192.5189	1208.8928
1216.7669	1230.2915	1245.9236
1265.8822	1286.9564	1292.2132
1297.9730	1307.2838	1311.5998
1326.8586	1336.4060	1344.6520
1353.0196	1357.3990	1369.8662
1378.0098	1381.5480	1386.3095
1394.1264	1398.9714	1401.0328
1402.1255	1404.1345	1411.9629
1420.7823	1424.3594	1482.1826
1484.6442	1486.1470	1488.2973
1490.5741	1492.1962	1492.7703
1493.8756	1494.2808	1502.2066
1506.4560	1509.8489	1514.1500
1518.4933	1526.5439	1533.0622
1536.8695	1635.2427	1665.1090
1676.0393	1677.9502	1685.4341
1748.7855	3035.0474	3039.5466
3040.5665	3046.8278	3051.0443
3054.4581	3055.8182	3056.2822
3057.2748	3093.9358	3099.9500
3100.8408	3106.8022	3113.7125
3118.0902	3123.5613	3128.5837
3133.3499	3135.6765	3139.9992
3143.3219	3149.5579	3150.9891
3160.2016	3190.2850	3190.3808
3201.2022	3201.7039	3216.4847

3220.0852	3221.1497	3226.8669

M22

Zero-point correction=	0.104854
Thermal correction to Energy=	0.112248
Thermal correction to Enthalpy=	0.113192
Thermal correction to Gibbs Free Energy=	0.072928
Sum of electronic and zero-point Energies=	-306.933451
Sum of electronic and thermal Energies=	-306.926057
Sum of electronic and thermal Enthalpies=	-306.925113
Sum of electronic and thermal Free Energies=	-306.965377

Cartesian coordinates

C	-1.19247200	-0.66109400	0.00002800
H	-1.12403800	-1.74400300	0.00011200
C	-2.53642400	0.00465100	0.00003000
H	-2.39308600	1.08991500	-0.00014800
H	-3.15712200	-0.23683400	0.87799200
C	-0.03122300	0.07162900	-0.00007500
O	0.14964400	1.31867400	-0.00014300
O	1.12972500	-0.75027500	-0.00009400
C	2.34881700	-0.04852700	0.00017600
H	3.14213700	-0.80106100	0.00051800
H	2.46139400	0.59084800	-0.88323300
H	2.46083400	0.59110000	0.88346600
H	-3.15725400	-0.23711100	-0.87776000

Vibrational frequencies

42.9161	100.3399	142.7903
198.0611	234.2573	354.0787
484.6249	591.8585	661.2527
735.5025	852.0513	1025.1988
1068.0098	1093.1437	1173.4814
1179.1949	1181.5747	1201.9684
1391.3942	1448.5033	1481.0124
1495.8848	1495.9142	1516.0286
1525.3032	1737.5942	2990.8932
3013.9392	3046.2020	3106.2631
3124.0659	3137.6037	3194.7735

M23

Zero-point correction=	0.333349
Thermal correction to Energy=	0.351928
Thermal correction to Enthalpy=	0.352872

Thermal correction to Gibbs Free Energy=	0.283380
Sum of electronic and zero-point Energies=	-940.524616
Sum of electronic and thermal Energies=	-940.506037
Sum of electronic and thermal Enthalpies=	-940.505093
Sum of electronic and thermal Free Energies=	-940.574585

Cartesian coordinates

N	1.33503000	-0.00004200	-0.00007600
C	0.66288600	1.15058600	0.02804100
C	-0.77046600	1.18419400	0.04647300
H	-1.29365000	2.12847600	0.12782600
C	-1.50085500	0.00004000	-0.00000600
C	-0.77054000	-1.18415100	-0.04654700
H	-1.29378900	-2.12839700	-0.12786500
C	0.66281600	-1.15062300	-0.02820200
C	-2.98149000	0.00007900	0.00003000
C	-3.68640300	0.99443100	-0.68714300
H	-3.14862400	1.75562100	-1.24471000
C	-5.07703700	0.99158800	-0.68760700
H	-5.61556800	1.76098000	-1.23026500
C	-5.77413300	0.00015500	0.00007700
H	-6.85899000	0.00018400	0.00010300
C	-5.07706300	-0.99131200	0.68773900
H	-5.61561800	-1.76067500	1.23041500
C	-3.68642900	-0.99423200	0.68722800
H	-3.14867300	-1.75546000	1.24476500
C	1.44374800	2.38087000	0.06571500
C	2.84215000	2.29739400	0.25308000
H	3.29370400	1.32061700	0.37540300
C	3.61169000	3.44454800	0.29324200
H	4.68264300	3.37383700	0.44581300
C	3.00718600	4.69688100	0.13843900
H	3.61303600	5.59632200	0.16776800
C	1.62725900	4.79593800	-0.05602600
H	1.16442200	5.76763200	-0.18375500
C	0.84780000	3.65237400	-0.08886200
H	-0.21729100	3.75436900	-0.25728600
C	1.44359300	-2.38094500	-0.06582600
C	2.84204200	-2.29754000	-0.25287400
H	3.29366900	-1.32077600	-0.37503300
C	3.61152800	-3.44473400	-0.29292000
H	4.68252000	-3.37408100	-0.44524800
C	3.00691200	-4.69704000	-0.13832900
H	3.61271800	-5.59651300	-0.16757500

C	1.62692500	-4.79602900	0.05577500
H	1.16401300	-5.76770800	0.18334200
C	0.84752700	-3.65242600	0.08852400
H	-0.21760000	-3.75441000	0.25670700

Vibrational frequencies

25.8585	32.1234	37.3081
46.1055	63.5914	80.3937
101.4563	104.0333	193.2883
196.7900	225.7724	238.3361
243.6548	271.1081	295.4810
383.1150	394.6661	395.5902
414.9208	423.0178	445.9523
453.7381	492.0480	577.5684
584.7196	608.8009	615.1127
624.4056	624.8477	633.8765
634.1873	680.8885	681.8542
682.5718	714.0225	722.5934
783.9853	807.7381	808.5645
816.3257	839.9354	861.2263
861.2682	880.3214	913.0336
931.0386	963.8330	981.4817
981.6654	989.1423	1000.7821
1010.8472	1012.2662	1016.5458
1025.8871	1026.0852	1037.2629
1038.0686	1048.8564	1049.1099
1056.5802	1065.8572	1074.2727
1093.6151	1125.5187	1126.4918
1133.5505	1147.6525	1182.2004
1184.6899	1187.8082	1190.6450
1215.6228	1223.7555	1253.7554
1292.1288	1317.0678	1335.1095
1344.9465	1361.1970	1364.8360
1378.4596	1380.5104	1388.9410
1416.7192	1468.8980	1491.3147
1500.1272	1513.7678	1520.2374
1532.8405	1550.1411	1558.8695
1623.5637	1627.5590	1632.5553
1633.4896	1671.2245	1688.3283
1699.7867	3210.7542	3212.7585
3216.6253	3230.8939	3230.9651
3236.0637	3238.5697	3238.8144
3240.9872	3245.5363	3245.6116
3257.4042	3257.7068	3265.6128

3266.2786 3271.4359 3273.4581

R3

Zero-point correction= 0.133881
Thermal correction to Energy= 0.142573
Thermal correction to Enthalpy= 0.143517
Thermal correction to Gibbs Free Energy= 0.099821
Sum of electronic and zero-point Energies= -455.113389
Sum of electronic and thermal Energies= -455.104697
Sum of electronic and thermal Enthalpies= -455.103753
Sum of electronic and thermal Free Energies= -455.147449

Cartesian coordinates

N	1.183741	0.000262	0.291693
C	0.561098	-1.187335	0.227663
C	-0.811116	-1.213681	0.077183
H	-1.324986	-2.164740	0.025086
C	-1.499359	0.000022	0.001562
C	-0.811321	1.213843	0.076825
H	-1.325322	2.164817	0.024486
C	0.560923	1.187735	0.227237
H	1.192388	2.063338	0.307425
H	1.192628	-2.062855	0.308340
O	2.532311	0.000496	0.505096
C	3.256555	-0.000649	-0.750562
H	4.301198	0.000187	-0.449022
H	3.018880	-0.902265	-1.317694
H	3.017980	0.899389	-1.319789
C	-2.932149	-0.000157	-0.150795
N	-4.080746	-0.000334	-0.273733

Vibrational frequencies

76.8450	86.5045	151.9635
199.3592	216.8115	335.2275
406.6730	415.6638	440.0519
519.4923	570.3508	593.6010
679.7256	714.6366	752.3408
861.1805	863.8732	883.8397
993.0133	1007.0394	1022.2176
1081.1450	1144.4864	1181.8394
1212.2100	1221.1470	1240.1307
1261.4972	1312.2582	1341.8589
1476.7961	1488.5575	1496.7373
1505.3527	1554.6589	1656.7081

1719.3939	2437.6189	3096.8761
3192.8624	3240.7101	3268.4433
3269.2129	3287.2435	3288.6353

M9

Zero-point correction= 0.708521
Thermal correction to Energy= 0.751805
Thermal correction to Enthalpy= 0.752749
Thermal correction to Gibbs Free Energy= 0.632925
Sum of electronic and zero-point Energies= -2295.433087
Sum of electronic and thermal Energies= -2295.389802
Sum of electronic and thermal Enthalpies= -2295.388858
Sum of electronic and thermal Free Energies= -2295.508682

Cartesian coordinates

C	-4.828115	-1.981769	-1.336804
C	-4.479182	-0.901618	-2.362178
C	-3.897563	0.383511	-1.760502
C	-3.638796	-2.647042	-0.641117
C	-2.502634	0.227412	-1.226647
C	-2.851497	-1.748081	0.318780
C	-2.033562	-0.682836	-0.351400
H	-5.405967	-2.762878	-1.842754
H	-5.390264	-0.634861	-2.908428
H	-4.553629	0.742720	-0.955904
H	-2.948686	-3.049423	-1.393226
H	-3.546092	-1.260430	1.018903
C	-0.071319	0.564484	-0.659647
H	-5.492637	-1.550297	-0.575053
H	-3.770924	-1.304233	-3.097760
H	-3.892884	1.167055	-2.525184
H	-4.009932	-3.501042	-0.064962
H	-2.181763	-2.370026	0.916083
N	-0.668312	-0.550427	-0.031987
C	0.126038	-1.772249	0.100137
C	0.519271	-2.447636	-1.070947
C	0.462030	-2.268710	1.372245
C	1.283282	-3.610634	-0.940728
C	1.216302	-3.440382	1.450221
C	1.635490	-4.106173	0.306251
H	1.601530	-4.137455	-1.835892
H	1.483949	-3.831616	2.428073
H	2.227930	-5.012628	0.387418
C	0.171955	-1.962727	-2.470335

C	-0.393434	-3.083146	-3.351797
H	-0.744740	-2.665853	-4.300266
H	0.364330	-3.836985	-3.586359
H	-1.233735	-3.589542	-2.868127
C	0.034076	-1.596592	2.661282
S	-1.232924	1.326229	-1.755098
H	-0.608565	-1.203721	-2.393818
H	-0.525827	-0.708546	2.372231
C	1.395547	-1.323871	-3.139741
H	2.182694	-2.072413	-3.283017
H	1.125725	-0.921639	-4.121705
H	1.804054	-0.516148	-2.527255
C	1.243420	-1.157286	3.494750
H	0.908116	-0.595797	4.374809
H	1.799506	-2.028217	3.857698
H	1.926779	-0.544447	2.905018
C	-0.880967	-2.495198	3.504166
H	-1.200628	-1.962483	4.405551
H	-1.776601	-2.804849	2.958856
H	-0.352709	-3.399553	3.823238
C	1.181317	1.006030	-0.315965
O	1.731715	0.450392	0.786804
H	2.475154	-0.254450	0.490449
C	2.016170	1.956749	-1.075482
C	1.636341	2.600469	-2.267568
C	3.311290	2.208632	-0.584355
C	2.502604	3.476386	-2.915090
H	0.676751	2.410070	-2.731444
C	4.174708	3.077180	-1.238912
H	3.623651	1.705866	0.322788
C	3.774730	3.725222	-2.406127
H	2.179416	3.958677	-3.832482
H	5.167208	3.248549	-0.833282
H	4.447049	4.407167	-2.916594
C	4.070033	-1.700837	0.921602
O	4.596979	-2.938107	0.626177
O	3.362199	-1.199416	-0.011019
O	4.346186	-1.225009	2.022209
H	4.195922	-3.191491	-0.216367
N	-2.639244	2.051869	1.400567
C	-2.273053	3.094327	0.630152
C	-0.978466	3.560942	0.709956
H	-0.674303	4.396168	0.092402
C	-0.078035	2.910411	1.561045

C	-0.506997	1.836077	2.363517
H	0.178241	1.326853	3.028907
C	-1.808080	1.417436	2.258974
C	1.259041	3.408126	1.713547
C	-4.791059	2.286653	2.229800
H	-4.819721	3.351697	1.990995
H	-4.451361	2.124691	3.254852
H	-5.767217	1.832645	2.073975
N	2.320515	3.840501	1.871246
H	-2.248069	0.599912	2.817394
H	-3.039396	3.504673	-0.015212
O	-3.924779	1.592324	1.303546

Vibrational frequencies

26.2770	31.2809	34.4976
38.2128	42.5228	46.1432
50.7679	58.0659	61.8785
66.0800	74.9748	84.3979
91.2830	96.7499	99.2154
102.1101	102.9076	103.3067
112.6788	115.7816	120.4449
129.3206	137.6327	140.2785
151.8288	156.4510	165.5547
171.0220	186.7302	192.8778
202.3019	212.3875	223.4109
230.9195	232.7838	243.2603
249.2194	260.0811	273.6790
275.5815	280.1182	295.9139
301.5197	322.4420	326.6127
333.7719	336.3864	347.6505
378.0728	386.2219	403.2169
407.9343	412.6290	415.4021
420.2170	433.7868	441.9300
453.7129	461.8978	463.8580
502.5457	513.5188	517.5968
518.5283	534.0634	561.6739
564.3601	569.7481	572.2486
576.9678	601.1557	616.1807
620.7757	627.1159	642.9389
649.9315	650.7560	672.5816
676.6608	689.5907	706.0283
708.4169	711.9195	725.1278
727.7972	774.4170	784.0060
792.1325	815.4228	824.2640

827.9656 832.1981 832.4920
839.8744 853.4098 856.0339
860.3560 885.0961 902.3130
916.1642 924.9217 930.7816
933.3034 934.7993 937.7153
965.5231 966.6011 970.2357
973.9995 976.3994 985.8897
989.2763 995.7482 998.3379
1005.7286 1010.1173 1024.3079
1024.9824 1029.9779 1069.7914
1070.5824 1072.5667 1077.8550
1083.6343 1090.5266 1097.7755
1109.9481 1122.7242 1133.5748
1141.3320 1144.0503 1145.0343
1151.3976 1166.1635 1173.5410
1174.1756 1182.5367 1186.2368
1188.2802 1202.0292 1206.9915
1216.0498 1221.7060 1223.4261
1235.2704 1241.7666 1252.0596
1259.1272 1267.4483 1269.1634
1291.5098 1294.1286 1300.8358
1303.8094 1306.1558 1317.7257
1327.5576 1333.5290 1337.4597
1342.6737 1350.5028 1353.1957
1364.9399 1369.8356 1379.8099
1385.4116 1387.4129 1398.9086
1401.7445 1405.1124 1407.4375
1409.7800 1419.5649 1425.1069
1425.9114 1474.8230 1475.0996
1477.3048 1482.7183 1487.5684
1488.6042 1489.3261 1490.1893
1490.2884 1492.6994 1499.2219
1499.8738 1502.6600 1504.5685
1506.7393 1509.0993 1514.1425
1515.0295 1517.8304 1527.6131
1539.0066 1547.2986 1558.6555
1602.3667 1612.8842 1657.3556
1675.5003 1681.1952 1688.1877
1708.6375 1719.8673 1770.5376
2162.3876 2421.7504 3045.4043
3046.6180 3053.3196 3053.5745
3059.0178 3062.5659 3063.3433
3064.1094 3065.5858 3095.6850
3105.5577 3109.6153 3111.8030

3113.7681	3121.4761	3132.0652
3137.7563	3139.2738	3149.6003
3150.7374	3159.3516	3161.1014
3167.4738	3182.8775	3189.8649
3190.2544	3197.6979	3199.6875
3201.9734	3210.7783	3216.9466
3221.8984	3233.1570	3245.7826
3250.3558	3262.6164	3268.1642
3275.5543	3278.3618	3850.7215

^{os}TS7

Zero-point correction= 0.704097
Thermal correction to Energy= 0.747448
Thermal correction to Enthalpy= 0.748392
Thermal correction to Gibbs Free Energy= 0.628248
Sum of electronic and zero-point Energies= -2295.435004
Sum of electronic and thermal Energies= -2295.391653
Sum of electronic and thermal Enthalpies= -2295.390709
Sum of electronic and thermal Free Energies= -2295.510852

Cartesian coordinates

C	4.570429	-2.287040	1.548319
C	4.284915	-1.121952	2.499238
C	3.853091	0.176061	1.803942
C	3.358880	-2.866870	0.814179
C	2.463511	0.118504	1.240042
C	2.713279	-1.934227	-0.217846
C	1.950251	-0.790995	0.383123
H	5.038041	-3.093572	2.123426
H	5.195797	-0.911805	3.069982
H	4.557356	0.414695	0.995381
H	2.594828	-3.171549	1.540502
H	3.490590	-1.519420	-0.876177
C	0.072377	0.575375	0.637683
H	5.314467	-1.965168	0.806259
H	3.513224	-1.413567	3.223454
H	3.909482	1.004419	2.517179
H	3.676167	-3.774502	0.290431
H	2.034714	-2.512007	-0.848657
N	0.608613	-0.578714	0.045101
C	-0.259623	-1.745032	-0.125619
C	-0.717546	-2.401916	1.032564
C	-0.597458	-2.206349	-1.409289
C	-1.554709	-3.510186	0.875829

C	-1.434969	-3.318597	-1.512848
C	-1.920126	-3.965014	-0.383273
H	-1.925188	-4.022386	1.759148
H	-1.713485	-3.679376	-2.499164
H	-2.576220	-4.824141	-0.484909
C	-0.378426	-1.944619	2.443721
C	0.064479	-3.103088	3.345943
H	0.425465	-2.709148	4.300582
H	-0.762959	-3.784683	3.565457
H	0.869267	-3.686294	2.889575
C	-0.077623	-1.564470	-2.679728
S	1.257770	1.296425	1.713544
H	0.459682	-1.245369	2.395574
H	0.547078	-0.728967	-2.368512
C	-1.575920	-1.217299	3.070152
H	-2.420106	-1.906983	3.181705
H	-1.314506	-0.835201	4.062409
H	-1.902669	-0.380598	2.447918
C	-1.216802	-1.013079	-3.543000
H	-0.804374	-0.508078	-4.424388
H	-1.864393	-1.821346	-3.897777
H	-1.830706	-0.315807	-2.970987
C	0.782213	-2.536923	-3.498067
H	1.176506	-2.031588	-4.385513
H	1.629945	-2.923657	-2.925396
H	0.190105	-3.392311	-3.839329
C	-1.168913	1.078759	0.237513
O	-1.723735	0.558111	-0.821946
H	-2.710711	-0.284153	-0.467950
C	-1.948241	2.069083	1.022601
C	-1.599360	2.542544	2.299392
C	-3.156340	2.518699	0.463396
C	-2.403541	3.462076	2.964286
H	-0.722725	2.169061	2.815242
C	-3.960538	3.433752	1.132072
H	-3.442854	2.134352	-0.507937
C	-3.584090	3.920027	2.382611
H	-2.110970	3.809646	3.950074
H	-4.886727	3.768670	0.674939
H	-4.209673	4.636673	2.905016
C	-4.130271	-1.548659	-1.024050
O	-4.804032	-2.646414	-0.607315
O	-3.421016	-1.007035	-0.075022
O	-4.248533	-1.165576	-2.171539

H	-4.505420	-2.841709	0.292324
N	2.881395	1.843710	-1.341047
C	2.605368	2.939150	-0.587753
C	1.358675	3.503790	-0.661279
H	1.132940	4.372229	-0.055783
C	0.380886	2.917160	-1.492617
C	0.732918	1.806184	-2.305137
H	0.006577	1.356690	-2.969931
C	1.987745	1.283761	-2.208730
C	-0.888371	3.540247	-1.669263
C	5.017408	1.919551	-2.226036
H	5.113842	2.986349	-2.010817
H	4.643440	1.763639	-3.240692
H	5.972505	1.415916	-2.090045
N	-1.908035	4.066129	-1.843987
H	2.355006	0.432556	-2.769044
H	3.410384	3.295300	0.042497
O	4.135666	1.297422	-1.269887

Vibrational frequencies

-677.1218	23.1556	28.8730
31.8624	38.6132	44.2964
50.3294	52.4536	58.3326
62.0384	64.3784	76.3439
81.8440	88.5418	93.0076
96.4133	103.2449	107.9982
112.6792	116.1774	118.6322
121.7323	129.7250	130.8412
139.3333	151.5616	155.1322
168.3557	174.7727	179.9603
192.8293	198.6135	200.5589
212.3478	221.0564	227.2996
238.1510	243.7873	250.9423
262.1336	266.4775	276.6668
293.7827	304.3096	316.4380
321.4457	329.9095	338.9274
352.5851	376.8104	395.1038
398.0045	406.3875	418.0417
424.8354	437.5783	446.4629
450.1424	452.9680	462.8958
470.5166	495.6107	505.1195
511.0052	522.1757	540.2369
542.2681	555.6343	565.4510
577.5285	580.4356	600.1998

623.9411	627.1071	629.9993
649.5073	652.3177	657.3468
672.8922	675.4695	681.5646
705.8335	712.9142	719.8447
726.2801	764.9076	774.5196
788.3594	793.1118	810.1431
812.8564	814.5529	826.9429
830.2905	831.0220	832.7295
870.3400	881.5400	889.5867
898.3211	914.8117	924.6880
927.6172	929.1917	940.6243
947.4034	961.7928	966.2317
968.9076	973.7722	974.8777
979.4383	983.8378	995.0110
1002.3929	1005.6109	1012.8855
1025.8191	1030.7062	1048.5932
1060.4498	1068.3320	1071.2954
1076.0314	1083.5449	1095.8365
1111.6224	1117.7164	1120.9912
1137.7852	1139.6017	1144.6055
1148.4345	1156.8388	1164.8391
1169.4428	1175.2793	1181.4433
1184.2338	1186.2195	1203.4596
1205.1045	1214.8222	1222.0647
1231.0560	1234.9293	1248.7794
1252.5904	1256.0477	1272.1015
1278.1259	1290.2426	1292.3026
1300.8158	1304.9143	1308.8709
1317.7531	1334.5713	1336.8001
1340.1959	1355.0326	1358.3796
1361.2240	1369.1046	1375.0657
1381.5359	1391.2575	1394.5784
1402.1224	1402.8421	1404.3577
1416.0905	1421.4960	1423.6162
1424.1935	1427.8633	1474.1041
1477.0830	1480.0594	1483.1921
1485.3136	1486.6799	1488.7794
1490.4648	1491.1630	1492.9964
1494.6878	1497.4027	1500.9505
1504.1990	1509.0188	1509.9426
1512.3579	1513.8009	1517.1884
1523.8326	1526.9682	1539.9669
1542.8372	1617.2762	1655.4311
1672.7405	1675.8076	1681.2785

1690.9710	1702.0958	1765.6744
1974.9626	2366.7017	3042.4881
3048.3057	3050.9753	3055.1756
3055.6124	3058.4155	3063.5109
3064.8228	3066.7790	3083.4746
3105.4487	3110.2700	3115.3433
3115.4943	3123.2349	3126.1051
3133.7073	3137.5336	3141.9095
3151.0429	3154.4864	3155.5333
3162.9146	3175.3847	3175.6543
3191.9568	3195.4915	3198.9191
3199.9916	3208.7030	3214.7920
3216.5765	3219.2404	3230.7556
3245.1141	3259.8533	3262.5391
3274.9412	3276.5795	3846.0473

^{2}M10

Zero-point correction=	0.130650
Thermal correction to Energy=	0.139824
Thermal correction to Enthalpy=	0.140768
Thermal correction to Gibbs Free Energy=	0.095188
Sum of electronic and zero-point Energies=	-455.257655
Sum of electronic and thermal Energies=	-455.248481
Sum of electronic and thermal Enthalpies=	-455.247537
Sum of electronic and thermal Free Energies=	-455.293118

Cartesian coordinates

N	-1.21827400	-0.00000200	-0.43241800
C	-0.56500300	-1.20840500	-0.29783900
C	0.77918200	-1.22607800	-0.10748000
H	1.28715900	-2.17982900	-0.03296700
C	1.51272800	-0.00007100	-0.01120700
C	0.77924500	1.22597400	-0.10752300
H	1.28727200	2.17970000	-0.03304100
C	-0.56494200	1.20837200	-0.29788400
H	-1.19018900	2.08699900	-0.38587800
H	-1.19029500	-2.08700200	-0.38580200
O	-2.59039600	0.00003300	-0.45135500
C	-3.11752600	0.00007500	0.88479400
H	-4.19993200	0.00010300	0.76540100
H	-2.79536300	-0.89707000	1.42089600
H	-2.79531200	0.89722300	1.42086100
C	2.90894400	-0.00013200	0.18295100
N	4.06456700	0.00017500	0.34191700

Vibrational frequencies

48.4932	110.6588	119.3212
155.4275	212.9958	262.4564
370.4554	425.3388	451.0867
484.3690	518.8612	580.3012
635.8025	669.4406	709.3919
752.5281	768.9912	818.3542
946.7715	957.6623	1003.8701
1033.2402	1125.1835	1176.7579
1194.1158	1217.3342	1249.5585
1280.8133	1284.2106	1352.2775
1417.1551	1469.3174	1486.5452
1488.9820	1510.2022	1563.8356
1739.5247	2308.8663	3070.8872
3158.2758	3200.7929	3241.9065
3242.7103	3265.9005	3267.9588

^{2}M11

Zero-point correction= 0.533230
Thermal correction to Energy= 0.562185
Thermal correction to Enthalpy= 0.563129
Thermal correction to Gibbs Free Energy= 0.471694
Sum of electronic and zero-point Energies= -1575.271146
Sum of electronic and thermal Energies= -1575.242191
Sum of electronic and thermal Enthalpies= -1575.241247
Sum of electronic and thermal Free Energies= -1575.332682

Cartesian coordinates

C	3.842271	-3.244428	0.140241
C	2.559260	-4.057262	-0.049302
C	1.405635	-3.657635	0.880709
C	3.767051	-1.766991	-0.253253
C	0.784464	-2.335242	0.534413
C	2.870917	-0.900856	0.644964
C	1.402897	-1.137591	0.431250
H	4.636127	-3.714787	-0.449948
H	2.790259	-5.111366	0.137164
H	1.769170	-3.627358	1.916886
H	3.432000	-1.674381	-1.294752
H	3.112638	-1.100149	1.697385
C	-0.777725	-0.477927	-0.082535
H	4.156415	-3.314902	1.190919
H	2.221913	-3.983817	-1.090372
H	0.632376	-4.430777	0.848817

H	4.778774	-1.349172	-0.210582
H	3.092425	0.154654	0.471120
N	0.537567	-0.096163	0.086269
C	0.942400	1.285044	0.145074
C	1.643824	1.829525	-0.938888
C	0.651285	2.015019	1.304031
C	2.035062	3.165789	-0.851027
C	1.054741	3.352404	1.342763
C	1.737544	3.925003	0.276574
H	2.570760	3.621872	-1.678538
H	0.831080	3.949854	2.222155
H	2.043760	4.965201	0.324829
C	1.932091	1.019809	-2.189886
C	3.399736	1.115192	-2.616230
H	3.587600	0.450122	-3.464271
H	3.660080	2.131306	-2.928438
H	4.071778	0.828281	-1.800777
C	-0.095971	1.413008	2.481663
S	-0.930256	-2.194036	0.213231
H	1.717976	-0.031924	-1.971622
H	-0.212677	0.338676	2.305844
C	0.990345	1.456935	-3.318844
H	1.186349	2.499153	-3.594092
H	1.141240	0.836297	-4.207379
H	-0.050381	1.378157	-2.993273
C	-1.497670	2.026157	2.594288
H	-2.066713	1.536504	3.390265
H	-1.430455	3.093155	2.832788
H	-2.046379	1.923463	1.653848
C	0.686668	1.579452	3.788599
H	0.157919	1.085840	4.609013
H	1.684878	1.139635	3.707402
H	0.800602	2.635235	4.053535
C	-1.811310	0.372919	-0.573113
O	-1.578687	1.513371	-1.039437
C	-3.222070	-0.134429	-0.556028
C	-3.769624	-0.828104	0.528186
C	-4.040043	0.177422	-1.647893
C	-5.103750	-1.229800	0.505157
H	-3.161743	-1.030478	1.405650
C	-5.367787	-0.232204	-1.675228
H	-3.614348	0.743553	-2.470385
C	-5.902225	-0.940989	-0.598786
H	-5.521711	-1.758623	1.355803

H	-5.989006	0.003789	-2.533421
H	-6.940162	-1.257597	-0.617049

Vibrational frequencies

14.4779	20.3480	35.8536
43.5421	49.6825	53.3321
61.4821	66.8007	79.9592
89.3898	109.1258	113.5619
126.2481	136.4570	168.1669
200.3992	201.9261	212.9965
227.6467	233.5501	243.3942
256.4437	258.8526	264.6155
270.4654	287.0498	298.2258
316.1359	326.1687	330.4608
344.5002	357.3234	385.5897
401.8134	410.0229	419.3839
442.3402	447.0812	469.3136
481.0337	502.3052	525.1897
553.9918	561.8635	565.1162
598.7840	612.7928	626.4046
646.0188	653.3200	664.2995
686.2451	714.8512	722.0479
724.1853	776.1940	792.0300
795.9829	816.9300	828.4974
830.4505	834.5144	883.5942
893.3438	901.2691	915.2358
933.5872	935.0728	945.3345
949.6142	958.8927	967.2653
968.7902	975.0692	976.6050
987.8677	1005.1939	1009.3020
1010.7502	1018.2751	1029.4450
1063.1592	1070.7434	1074.5758
1084.0133	1098.8673	1113.4365
1121.0136	1122.5253	1144.7951
1149.1536	1164.1089	1170.5716
1173.1047	1177.8430	1184.7029
1192.1729	1195.8018	1211.0000
1238.2465	1247.2081	1252.4757
1284.7759	1291.9965	1293.7925
1303.4767	1318.5545	1324.7714
1335.5694	1346.6176	1354.9248
1355.7051	1356.8411	1374.7830
1383.5670	1390.3841	1395.7101
1398.2461	1401.7633	1405.2749

1406.2247	1414.9861	1420.7390
1424.9326	1467.3227	1478.2217
1481.7462	1483.1236	1488.3841
1490.1030	1491.5513	1492.7592
1494.0137	1497.0735	1497.4779
1505.1499	1506.6200	1509.6206
1511.9987	1526.6674	1532.2378
1544.2859	1624.1482	1672.0651
1677.0716	1684.4568	1688.6997
1692.8933	3050.1500	3051.8575
3054.4970	3056.3675	3058.6065
3060.0372	3064.7433	3065.5332
3069.9218	3099.6531	3100.3954
3105.6038	3110.3659	3117.3942
3119.2618	3136.9063	3138.2842
3138.7498	3144.2744	3145.3699
3145.7441	3153.2976	3153.8153
3154.6473	3202.2913	3207.3671
3212.8520	3214.9701	3216.1443
3224.5082	3228.6969	3236.1922

^{2}TS8

Zero-point correction=	0.128531
Thermal correction to Energy=	0.137575
Thermal correction to Enthalpy=	0.138519
Thermal correction to Gibbs Free Energy=	0.093189
Sum of electronic and zero-point Energies=	-455.239550
Sum of electronic and thermal Energies=	-455.230506
Sum of electronic and thermal Enthalpies=	-455.229562
Sum of electronic and thermal Free Energies=	-455.274891

Cartesian coordinates

N	1.27145600	-0.00001700	-0.84756200
C	0.61837600	1.17130800	-0.65276100
C	-0.70732300	1.21048500	-0.27796900
H	-1.20811300	2.16275400	-0.15102300
C	-1.39180500	-0.00000200	-0.08392000
C	-0.70732700	-1.21049700	-0.27793500
H	-1.20812000	-2.16276000	-0.15096200
C	0.61837300	-1.17133500	-0.65272700
H	1.20249800	-2.07067500	-0.81280300
H	1.20250300	2.07064200	-0.81286400
O	2.77994100	-0.00000500	-0.00765000
C	2.47415500	0.00003000	1.36185500

H	3.43637200	0.00003700	1.88688600
H	1.91525900	0.89478700	1.67079500
H	1.91524700	-0.89470300	1.67084000
C	-2.77057600	0.00000600	0.30695400
N	-3.88551500	0.00001400	0.62175400

Vibrational frequencies

-691.5895	71.4780	72.2214
155.1529	172.5103	188.3344
265.8597	334.6700	398.1596
431.9373	462.3451	566.5707
576.3721	666.3358	726.3769
763.9348	840.8245	862.4250
940.5061	981.3443	987.8000
1055.5618	1072.1160	1130.3988
1177.9772	1189.8189	1202.8364
1249.4733	1296.3158	1339.8444
1452.4270	1465.5497	1472.7614
1500.8701	1522.4701	1582.8639
1647.1281	2407.8268	3018.5801
3085.2252	3112.4692	3231.1551
3231.7952	3253.7294	3254.1860

^{2}M12

Zero-point correction=	0.037680
Thermal correction to Energy=	0.040637
Thermal correction to Enthalpy=	0.041581
Thermal correction to Gibbs Free Energy=	0.014762
Sum of electronic and zero-point Energies=	-114.958153
Sum of electronic and thermal Energies=	-114.955196
Sum of electronic and thermal Enthalpies=	-114.954252
Sum of electronic and thermal Free Energies=	-114.981071

Cartesian coordinates

O	-0.79413300	-0.00004800	-0.00763000
C	0.57843500	-0.00020000	-0.01225700
H	0.87146200	0.00768200	1.05390700
H	1.00559500	-0.90989400	-0.45364300
H	1.00540000	0.90379600	-0.46568100

Vibrational frequencies

959.0747	974.1287	1143.4229
1388.8514	1400.5957	1528.8259
2980.9515	3058.2629	3105.4504

M13

Zero-point correction=	0.088470
Thermal correction to Energy=	0.094425
Thermal correction to Enthalpy=	0.095369
Thermal correction to Gibbs Free Energy=	0.058247
Sum of electronic and zero-point Energies=	-340.308361
Sum of electronic and thermal Energies=	-340.302406
Sum of electronic and thermal Enthalpies=	-340.301462
Sum of electronic and thermal Free Energies=	-340.338584

Cartesian coordinates

N	2.19219000	0.00000200	0.00016300
C	1.50150200	-1.14318900	0.00010300
C	0.11171000	-1.20572500	-0.00018600
H	-0.40508100	-2.15767000	-0.00001200
C	-0.59041800	-0.00000200	-0.00067300
C	0.11170700	1.20572300	-0.00018600
H	-0.40508800	2.15766700	-0.00001200
C	1.50149900	1.14319200	0.00010300
H	2.08312400	2.06076100	0.00040300
H	2.08313000	-2.06075700	0.00040300
C	-2.03237000	-0.00000400	0.00025200
N	-3.18902700	0.00000200	0.00022800

Vibrational frequencies

146.9673	164.0258	386.6537
396.7375	456.8321	573.9450
593.2823	683.1700	757.3210
786.8252	854.1008	901.9372
1009.5588	1023.3368	1031.5112
1105.1081	1125.4085	1232.9884
1258.9248	1288.5501	1361.8337
1463.7007	1551.0055	1653.6055
1688.3358	2417.1263	3215.8429
3218.6979	3242.8707	3243.5009

TEMPOH(R4)

Zero-point correction=	0.276134
Thermal correction to Energy=	0.288222
Thermal correction to Enthalpy=	0.289166
Thermal correction to Gibbs Free Energy=	0.240265
Sum of electronic and zero-point Energies=	-483.845959
Sum of electronic and thermal Energies=	-483.833871

Sum of electronic and thermal Enthalpies= -483.832927
Sum of electronic and thermal Free Energies= -483.881828

Cartesian coordinates

C	-1.270974	-0.060908	0.054007
C	-1.107985	1.409686	0.487042
C	-0.072774	2.125250	-0.371383
C	1.312097	1.512295	-0.134783
C	1.282470	-0.031459	0.047994
H	-2.086724	1.897821	0.425485
H	-0.347579	2.031668	-1.427587
H	1.971068	1.769736	-0.970379
H	-0.051628	3.194757	-0.141707
H	-0.799025	1.459421	1.538913
H	1.758452	1.952634	0.764352
N	0.013437	-0.513599	-0.546830
O	0.010653	-1.938014	-0.530556
C	-2.309470	-0.164861	-1.069006
H	-2.325506	-1.184819	-1.463910
H	-3.308967	0.076768	-0.694236
H	-2.066489	0.518595	-1.887759
C	-1.756584	-0.906948	1.239313
H	-1.022954	-0.947703	2.045931
H	-2.672132	-0.458053	1.638410
H	-1.982631	-1.927280	0.924666
C	2.422901	-0.647770	-0.768290
H	3.369066	-0.176187	-0.486418
H	2.505453	-1.722188	-0.589924
H	2.255761	-0.475751	-1.836273
C	1.479736	-0.427355	1.520159
H	1.295964	-1.497838	1.649961
H	2.511247	-0.216077	1.820397
H	0.822555	0.129691	2.192167
H	0.118282	-2.173463	-1.460148

Vibrational frequencies

93.7147	115.7975	173.0030
229.3457	242.1588	269.7976
279.3626	290.4709	310.7024
329.1856	345.2190	354.8956
371.6426	380.0955	398.2876
412.0708	462.4023	484.8174
520.1766	581.1177	606.6970
680.4653	806.3875	814.6556

853.2908	902.6304	934.8947
938.4593	944.1268	982.5015
991.6837	1001.8519	1016.0213
1052.2688	1075.9275	1082.0005
1093.4395	1125.6846	1186.8777
1223.2494	1233.4028	1252.7300
1276.2751	1285.3321	1301.2101
1332.3998	1363.9622	1375.4380
1384.9008	1391.0545	1400.1620
1401.1899	1409.6839	1414.7097
1480.1322	1487.6240	1490.1283
1492.3478	1497.1999	1499.2980
1505.0077	1508.0815	1514.5713
1518.9916	1522.4805	3058.0914
3060.5891	3062.7855	3065.0052
3068.9084	3075.2037	3076.0742
3109.0898	3113.9916	3125.8325
3141.2736	3143.0630	3145.0246
3146.3175	3154.5931	3159.2998
3162.9783	3183.0056	3861.9773

R5

Zero-point correction= 0.110593
Thermal correction to Energy= 0.120942
Thermal correction to Enthalpy= 0.121886
Thermal correction to Gibbs Free Energy= 0.073157
Sum of electronic and zero-point Energies= -752.772573
Sum of electronic and thermal Energies= -752.762224
Sum of electronic and thermal Enthalpies= -752.761280
Sum of electronic and thermal Free Energies= -752.810010

Cartesian coordinates

N	-0.241721	-0.000064	-0.584183
C	0.366339	-1.194131	-0.465884
C	1.714815	-1.215320	-0.176918
H	2.221618	-2.166089	-0.075855
C	2.389041	0.000005	-0.027385
C	1.714766	1.215289	-0.176972
H	2.221515	2.166093	-0.075963
C	0.366282	1.194015	-0.465928
H	-0.250895	2.070371	-0.617756
H	-0.250781	-2.070529	-0.617693
C	3.797811	0.000029	0.273103
N	4.926778	0.000074	0.517099

O	-1.569705	-0.000035	-0.933387
C	-2.404563	0.000028	0.201273
F	-2.181077	-1.073982	0.935144
F	-3.620532	-0.000182	-0.274837
F	-2.181298	1.074261	0.934828

Vibrational frequencies

55.9108	56.9760	77.6259
144.9636	157.4730	282.9302
318.5902	333.0457	409.3225
432.3167	487.7387	494.4985
568.0842	571.3041	578.3319
624.0742	685.0716	692.9267
735.5604	787.8489	848.5099
863.3615	895.5118	946.0463
990.4773	1001.8404	1074.2014
1146.4640	1183.9720	1217.7268
1241.1924	1275.9135	1317.1812
1323.7556	1343.9996	1402.4893
1496.8626	1551.3593	1651.3933
1714.2352	2442.6815	3272.8369
3273.5895	3286.5128	3288.1446

M14

Zero-point correction= 0.473584
Thermal correction to Energy= 0.505273
Thermal correction to Enthalpy= 0.506217
Thermal correction to Gibbs Free Energy= 0.410003
Sum of electronic and zero-point Energies= -1579.631792
Sum of electronic and thermal Energies= -1579.600102
Sum of electronic and thermal Enthalpies= -1579.599158
Sum of electronic and thermal Free Energies= -1579.695372

Cartesian coordinates

H	1.019556	2.724570	-2.274325
C	0.753620	2.015003	-0.541643
O	1.344846	2.935103	-1.389022
O	0.054539	1.131297	-1.114061
O	1.011548	2.148903	0.660879
H	-1.131569	0.215872	-0.168655
C	0.952064	-1.523876	1.446157
C	0.506831	-2.163103	0.286924
C	1.970338	-0.811863	-1.049117
C	-3.342185	0.952520	1.095861

C	-4.794079	1.362864	0.775182
C	-5.623390	0.156373	0.351072
C	-5.091077	-0.413772	-0.970030
C	-3.543086	-0.336752	-1.095644
H	-5.219875	1.847523	1.660870
H	-5.569579	-0.608799	1.132962
H	-5.413967	-1.455585	-1.069871
H	-6.678037	0.428381	0.244112
H	-4.807774	2.112100	-0.025872
H	-5.530202	0.132886	-1.812742
N	-3.012676	-0.245380	0.282183
O	-1.624998	-0.487030	0.326805
C	-3.243489	0.502794	2.558799
H	-2.256248	0.071264	2.743859
H	-3.388635	1.351578	3.234701
H	-3.999778	-0.256154	2.781097
C	-2.393655	2.142130	0.890068
H	-2.339861	2.449813	-0.156889
H	-2.763111	2.991932	1.474231
H	-1.379037	1.911423	1.224889
C	-3.028736	-1.649014	-1.694364
H	-3.547231	-1.846508	-2.637854
H	-1.954068	-1.600594	-1.890351
H	-3.218765	-2.476479	-1.005317
C	-3.126869	0.809472	-2.037870
H	-2.043466	0.961559	-2.021141
H	-3.423853	0.556474	-3.061551
H	-3.616358	1.752481	-1.781820
C	1.940950	-0.566593	1.365346
H	0.518367	-1.750004	2.411235
C	2.449764	-0.270156	-2.355402
H	1.645877	-0.396253	-3.079015
H	2.685797	0.790481	-2.264671
H	3.331239	-0.810488	-2.704809
C	1.006838	-1.806617	-0.956365
N	2.447355	-0.319346	0.121630
O	3.416800	0.658648	0.047571
H	0.625931	-2.247072	-1.868818
C	4.710467	0.128409	0.061135
C	2.438907	0.216896	2.531672
H	2.384942	1.277469	2.278434
H	1.798943	0.005964	3.387011
H	3.465162	-0.050475	2.785945
C	-0.517877	-3.171749	0.386978

N	-1.316602	-4.001890	0.476590
F	5.506611	1.167996	0.092754
F	4.903879	-0.640791	1.120393
F	4.945639	-0.599450	-1.018527

Vibrational frequencies

17.1607	25.0242	31.9920
43.2700	44.9124	53.9556
57.1608	65.2585	71.9671
84.5849	99.4582	108.7000
116.8675	119.4475	130.9237
148.8812	165.9425	176.5169
183.1268	190.2346	204.4999
219.7382	220.0267	247.8414
248.8886	264.9318	285.4488
290.5944	294.5321	297.2653
313.9352	320.7043	333.5756
339.9728	348.0822	361.5448
368.5490	382.5161	401.1493
407.7264	435.2866	442.8867
467.6531	486.2678	489.3152
494.3160	524.6239	528.2091
556.7167	564.3317	580.8873
592.4890	606.0644	607.8300
609.3878	613.6001	626.2507
666.4068	669.1818	675.6711
691.1097	735.7311	799.1293
815.2705	825.4332	838.4435
848.0132	849.3461	900.3587
900.5829	911.0921	936.2691
940.2427	941.3713	948.9157
982.2599	982.9458	990.6653
995.6007	1004.2771	1021.7910
1026.6484	1046.9402	1052.0632
1065.9689	1068.1358	1077.4864
1084.3947	1087.3013	1103.0799
1140.0408	1181.3666	1187.7747
1210.2766	1223.6974	1232.0870
1238.0558	1251.9384	1255.2779
1273.5180	1280.6202	1286.3441
1290.5680	1301.7365	1310.9589
1328.2937	1368.3598	1370.5119
1379.2307	1389.3861	1389.5107
1399.0649	1400.9743	1404.6823

1410.8709	1418.7248	1422.8305
1424.5719	1456.9527	1464.1710
1477.6817	1478.7531	1481.8038
1482.0632	1487.9394	1490.1693
1495.4792	1500.8130	1502.1973
1506.8017	1508.8464	1515.8284
1523.3504	1524.9463	1525.9099
1528.1660	1653.5505	1719.5363
1788.2150	2440.8381	3057.5985
3059.5007	3060.6818	3062.2775
3065.1081	3068.3867	3074.7254
3102.8451	3103.7852	3106.4188
3106.4393	3123.6754	3137.5696
3141.7228	3142.8948	3148.6583
3155.0297	3158.1324	3161.4019
3175.3511	3190.0189	3199.3501
3206.8953	3208.5594	3263.6022
3265.6277	3350.2741	3862.2562

^{os}TS9

Zero-point correction= 0.468237
Thermal correction to Energy= 0.499469
Thermal correction to Enthalpy= 0.500413
Thermal correction to Gibbs Free Energy= 0.406399
Sum of electronic and zero-point Energies= -1579.617740
Sum of electronic and thermal Energies= -1579.586508
Sum of electronic and thermal Enthalpies= -1579.585564
Sum of electronic and thermal Free Energies= -1579.679578

Cartesian coordinates

H	1.350988	3.611426	0.151435
C	0.810149	2.019331	1.021823
O	1.645572	3.076662	0.902486
O	-0.087461	1.978174	0.076432
O	0.964400	1.232076	1.936337
H	-0.716218	1.064039	0.115590
C	0.755881	-1.944032	0.320232
C	0.110773	-1.570087	-0.883582
C	1.862086	0.038422	-1.312598
C	-3.355157	-0.400884	1.294253
C	-4.881442	-0.290698	1.121636
C	-5.291644	-0.682838	-0.294186
C	-4.747291	0.330871	-1.308020
C	-3.332192	0.862106	-0.948255

H	-5.361437	-0.932893	1.867836
H	-4.889204	-1.676138	-0.519483
H	-4.719491	-0.130971	-2.300774
H	-6.380451	-0.748262	-0.379495
H	-5.216221	0.732757	1.330165
H	-5.427215	1.187920	-1.377581
N	-2.719367	-0.098357	-0.008043
O	-1.383413	-0.070122	0.078416
C	-2.970347	-1.841662	1.649456
H	-1.881356	-1.935145	1.661598
H	-3.358093	-2.102429	2.638797
H	-3.367369	-2.541938	0.910106
C	-2.845830	0.533364	2.401612
H	-3.115995	1.573901	2.205570
H	-3.286846	0.243404	3.360728
H	-1.757105	0.464919	2.477121
C	-2.467708	0.900603	-2.210774
H	-2.986714	1.481933	-2.978623
H	-1.497327	1.366313	-2.018761
H	-2.312019	-0.115284	-2.585846
C	-3.410829	2.292656	-0.377176
H	-2.432516	2.615669	-0.010535
H	-3.725416	2.980844	-1.168957
H	-4.137351	2.372491	0.434585
C	1.898495	-1.313782	0.722592
H	0.306131	-2.673970	0.980774
C	2.432261	1.222420	-2.028458
H	1.668426	1.617275	-2.697107
H	2.710318	1.996814	-1.310182
H	3.314768	0.962161	-2.613882
C	0.727665	-0.605925	-1.716190
N	2.453686	-0.396074	-0.143566
O	3.535206	0.323978	0.328693
H	0.245904	-0.284267	-2.630534
C	4.750377	-0.206799	-0.083900
C	2.523070	-1.507589	2.065385
H	2.589711	-0.537035	2.562725
H	1.886615	-2.167583	2.653009
H	3.519935	-1.943296	1.999663
C	-1.075582	-2.234843	-1.305584
N	-2.075481	-2.727579	-1.629858
F	5.669369	0.529755	0.498406
F	4.884502	-1.475523	0.276418
F	4.891998	-0.149626	-1.401067

Vibrational frequencies

-1543.9866	26.3889	29.9522
36.2297	41.8323	53.3431
53.8359	67.1511	73.2721
88.4226	91.1124	107.0595
119.6110	124.5895	136.8262
139.6154	146.4078	149.9023
180.1906	183.8426	199.8661
205.7566	215.5484	226.8301
244.8879	273.9416	277.3322
285.1687	290.4257	298.7460
306.3387	322.6172	335.7191
347.0696	353.3637	356.6196
371.0367	383.7146	407.2964
412.5004	430.0704	436.1903
444.8379	469.9487	485.1580
487.6364	491.7259	536.1887
538.9745	547.2791	554.3772
563.1145	571.8918	574.3605
597.7701	611.1155	612.3163
624.3045	652.9211	660.3214
665.4610	700.9633	749.7111
813.2433	819.0188	824.0517
835.9256	858.1259	875.5359
898.3267	901.4198	935.9716
940.8137	941.6973	952.3787
961.8848	980.6290	985.8927
993.4392	1003.2834	1033.8619
1036.7011	1043.8241	1060.0732
1066.0055	1068.4037	1072.3570
1089.6974	1091.1000	1116.5520
1168.7647	1184.4497	1210.5101
1223.9078	1227.5634	1234.0676
1250.4757	1256.9715	1264.7083
1268.2416	1269.8051	1275.9877
1300.1470	1307.8784	1324.0516
1338.7520	1361.4120	1363.7676
1372.1541	1374.7886	1383.5052
1390.3708	1396.1698	1402.9493
1408.1820	1413.9473	1419.0291
1427.0164	1447.7321	1469.8723
1475.5695	1480.5113	1486.6006
1488.7635	1490.0724	1493.0290

1496.7294	1499.5927	1500.3105
1506.1439	1508.1639	1508.8360
1516.3862	1518.0907	1521.8935
1525.4846	1568.1672	1613.2903
1720.9340	1892.8457	2367.1380
3062.7256	3063.9042	3065.6521
3066.7336	3068.5357	3070.9424
3083.6621	3099.2961	3102.8376
3109.5750	3112.1650	3133.5366
3143.3268	3148.5990	3151.2190
3154.4385	3162.9682	3167.4829
3167.8135	3171.9212	3183.4248
3189.1739	3200.6712	3206.1090
3252.3732	3255.1797	3851.1032

^{2}M15

Zero-point correction=	0.164289
Thermal correction to Energy=	0.177941
Thermal correction to Enthalpy=	0.178885
Thermal correction to Gibbs Free Energy=	0.121982
Sum of electronic and zero-point Energies=	-831.477358
Sum of electronic and thermal Energies=	-831.463706
Sum of electronic and thermal Enthalpies=	-831.462762
Sum of electronic and thermal Free Energies=	-831.519665

Cartesian coordinates

N	0.16448300	0.00017500	-0.04399200
C	-0.52714500	1.22758600	-0.14863200
C	-1.88415900	1.21607500	-0.05208100
H	-2.40631300	2.16563700	-0.05781700
C	-2.61312000	0.00000300	0.04233500
C	-1.88402000	-1.21601500	-0.05177700
H	-2.40606900	-2.16563700	-0.05737900
C	-0.52701200	-1.22737400	-0.14832100
C	-4.02261300	-0.00007600	0.15711200
N	-5.18262500	-0.00029500	0.25726300
O	1.39577500	-0.00006800	-0.74197400
C	2.46742800	-0.00006000	0.11564100
F	2.49065300	1.07227600	0.89995800
F	3.54260400	-0.00505800	-0.65130000
F	2.48524700	-1.06748000	0.90667300
C	0.27033500	2.48573900	-0.28392200
H	0.84346300	2.69379100	0.62240900
H	0.97235900	2.42491800	-1.11880000

H	-0.41380900	3.31493600	-0.46222800
C	0.27060400	-2.48541500	-0.28400600
H	0.84468600	-2.69327000	0.62175000
H	-0.41356200	-3.31478000	-0.46145600
H	0.97171800	-2.42464200	-1.11967000

Vibrational frequencies

22.2224	30.3290	103.4892
113.8517	141.0198	149.7697
191.6523	243.8799	268.6099
270.6559	291.0396	312.9977
354.6519	410.9756	442.8122
481.3790	481.6561	519.6323
544.6532	550.6247	555.8824
585.5561	614.0603	651.5822
654.5666	696.2053	798.9794
878.2457	886.0582	937.6963
962.0395	968.4527	1039.7873
1057.3720	1059.3892	1064.4203
1127.6113	1172.3556	1259.9632
1265.4386	1286.6803	1320.0002
1332.2665	1350.1006	1420.6233
1421.7599	1422.9562	1440.2121
1482.4613	1483.1573	1499.7123
1506.7672	1590.3935	1726.4551
2328.7380	3087.7389	3088.0757
3162.8313	3162.9292	3187.5620
3187.6726	3231.7050	3232.1273

^{2}M16

Zero-point correction=	0.264354
Thermal correction to Energy=	0.276309
Thermal correction to Enthalpy=	0.277253
Thermal correction to Gibbs Free Energy=	0.226748
Sum of electronic and zero-point Energies=	-483.247034
Sum of electronic and thermal Energies=	-483.235080
Sum of electronic and thermal Enthalpies=	-483.234136
Sum of electronic and thermal Free Energies=	-483.284641

Cartesian coordinates

C	-1.30575500	-0.07558300	0.07380900
C	-1.11291100	1.38440200	0.50713000
C	-0.07169900	2.07183200	-0.36709400
C	1.31039600	1.48362500	-0.08218800

C	1.31982800	-0.06394600	0.05454400
H	-2.08423500	1.88610200	0.45083700
H	-0.32846500	1.93302100	-1.42346200
H	2.00758400	1.78229500	-0.87074400
H	-0.05777000	3.14954700	-0.18344700
H	-0.79410600	1.42940400	1.55657100
H	1.69265800	1.90896400	0.85246200
N	0.00616500	-0.63365300	-0.36391800
O	-0.00643900	-1.85408600	-0.73432600
C	-2.24699600	-0.16171700	-1.13197100
H	-2.27919400	-1.18840200	-1.50089500
H	-3.25386200	0.14242300	-0.83408300
H	-1.91189500	0.48961800	-1.94398500
C	-1.86219000	-0.92923100	1.21683000
H	-1.19806600	-0.91190500	2.08495200
H	-2.83689400	-0.53823800	1.52303000
H	-1.98305500	-1.96298600	0.88608000
C	2.39006000	-0.65863600	-0.85957100
H	3.35260700	-0.20301700	-0.61194000
H	2.46305400	-1.73894700	-0.73454400
H	2.16020200	-0.43930900	-1.90614200
C	1.59015300	-0.49488800	1.50388500
H	1.48742400	-1.58032100	1.59399600
H	2.60762200	-0.21118200	1.78918900
H	0.89943200	-0.01396900	2.20191800

Vibrational frequencies

24.8292	95.9958	190.2531
222.2025	239.7165	259.3434
272.0343	286.9597	307.0189
322.5372	332.5900	352.0129
386.8087	401.8220	407.5099
448.5373	481.2821	542.6958
560.5976	597.6460	648.8842
816.6022	817.9164	857.7967
906.2297	943.8143	948.3823
949.1861	990.1343	996.0447
1008.0300	1023.7004	1055.9151
1091.7911	1095.0733	1120.0459
1179.8161	1217.1444	1225.5851
1253.0337	1267.9000	1284.0104
1303.3266	1331.2778	1375.2010
1387.6105	1395.9856	1399.1962
1402.5181	1412.2923	1416.5444

1479.0222	1484.7004	1490.4439
1491.8650	1495.8937	1497.1450
1501.6379	1504.9133	1506.7697
1514.3432	1516.3933	1521.1945
3062.8551	3067.6094	3070.5938
3073.4626	3074.5334	3077.0880
3078.7401	3117.6675	3120.2250
3129.0691	3151.7616	3153.2064
3156.0047	3157.5513	3161.0249
3168.8948	3174.2672	3185.9330

^{2}TS10

Zero-point correction=	0.162741
Thermal correction to Energy=	0.175913
Thermal correction to Enthalpy=	0.176857
Thermal correction to Gibbs Free Energy=	0.121822
Sum of electronic and zero-point Energies=	-831.476397
Sum of electronic and thermal Energies=	-831.463225
Sum of electronic and thermal Enthalpies=	-831.462281
Sum of electronic and thermal Free Energies=	-831.517316

Cartesian coordinates

N	-0.12758200	0.00034200	-0.24821400
C	0.55749700	1.20932300	-0.15432200
C	1.92404500	1.20925800	-0.03485100
H	2.44610100	2.15886400	-0.01482700
C	2.63969800	-0.00017700	0.03226400
C	1.92354700	-1.20934900	-0.03416900
H	2.44521400	-2.15916200	-0.01376700
C	0.55705200	-1.20888200	-0.15427100
C	4.06001200	-0.00043100	0.16119800
N	5.21541200	-0.00064300	0.26661400
O	-1.31070200	0.00078800	0.78213400
C	-2.50380600	-0.00004000	0.14938700
F	-2.69060600	1.07030400	-0.62860100
F	-3.44552000	0.00036700	1.09001300
F	-2.68994000	-1.07171900	-0.62692400
C	-0.24032000	-2.47055900	-0.25086900
H	-0.80683800	-2.49729500	-1.18447500
H	0.43074900	-3.32848700	-0.21562400
H	-0.95340700	-2.54727200	0.57342300
C	-0.23939400	2.47134300	-0.25038800
H	-0.80536100	2.49900700	-1.18436400

H	-0.95296000	2.54763500	0.57342900
H	0.43191500	3.32903000	-0.21394100

Vibrational frequencies

-530.7758	33.2748	51.5340
114.1137	133.6636	169.7175
173.3901	204.6767	241.3243
248.1406	310.1226	317.6061
329.5405	408.4403	437.4933
444.8161	462.5964	476.9048
531.5051	539.7286	567.3337
589.6395	608.5698	629.9574
639.0353	669.7173	707.6745
853.7937	902.5263	904.0540
944.7146	975.9969	979.1891
1044.7488	1060.8109	1062.8499
1066.2953	1176.2576	1255.8605
1266.7996	1268.0825	1298.8874
1303.8196	1309.6624	1418.9023
1420.4713	1437.9107	1484.0206
1491.0846	1491.6872	1514.7906
1521.6472	1545.1229	1675.7664
2374.6428	3087.1775	3087.5080
3162.8668	3163.0850	3188.3735
3188.4924	3233.1913	3233.2977

^{2}M17

Zero-point correction=	0.016438
Thermal correction to Energy=	0.020723
Thermal correction to Enthalpy=	0.021667
Thermal correction to Gibbs Free Energy=	-0.011739
Sum of electronic and zero-point Energies=	-412.619846
Sum of electronic and thermal Energies=	-412.615561
Sum of electronic and thermal Enthalpies=	-412.614617
Sum of electronic and thermal Free Energies=	-412.648023

Cartesian coordinates

O	0.78403000	-0.00490300	-1.14972700
C	0.00535800	-0.00020000	-0.03395000
F	-0.77018100	1.07533600	0.02345700
F	0.84685500	-0.00036800	0.99324900
F	-0.77716100	-1.07047600	0.02790700

Vibrational frequencies

179.5016	411.8124	581.7699
596.6682	625.3662	933.8322
1267.5493	1291.4738	1327.5976

M18

Zero-point correction=	0.143632
Thermal correction to Energy=	0.153092
Thermal correction to Enthalpy=	0.154036
Thermal correction to Gibbs Free Energy=	0.108726
Sum of electronic and zero-point Energies=	-418.857541
Sum of electronic and thermal Energies=	-418.848081
Sum of electronic and thermal Enthalpies=	-418.847137
Sum of electronic and thermal Free Energies=	-418.892447

Cartesian coordinates

N	-1.61916800	-0.00001700	-0.00000400
C	-0.94659200	-1.15728500	-0.00000900
C	0.44840800	-1.20697600	0.00000800
H	0.97384800	-2.15468700	0.00001900
C	1.14493400	0.00002000	0.00001800
C	0.44837800	1.20699700	0.00001300
H	0.97379400	2.15472200	0.00001700
C	-0.94662100	1.15726900	0.00000700
C	2.58706300	0.00003800	0.00000000
N	3.74386200	0.00000800	-0.00001700
C	-1.77243400	-2.41389300	0.00000200
H	-2.41843600	-2.43522500	0.88136200
H	-2.41831300	-2.43529300	-0.88145300
H	-1.14531600	-3.30616000	0.00005200
C	-1.77249600	2.41385500	-0.00000600
H	-2.41839400	2.43524800	0.88143000
H	-1.14540200	3.30613800	-0.00009600
H	-2.41847900	2.43515800	-0.88138600

Vibrational frequencies

92.8823	94.3035	128.1880
137.2670	200.9631	213.6939
282.2307	408.8231	410.2044
457.2133	545.6244	561.9481
586.4317	600.3949	635.3244
747.0467	896.1111	906.3242
942.9911	977.4522	1018.2713
1036.1439	1061.4236	1068.2720
1068.5980	1181.3687	1250.7657

1290.9143	1356.9072	1415.7264
1427.1032	1463.0458	1470.1688
1486.4592	1487.2621	1506.6844
1523.5001	1659.5065	1688.4456
2415.2940	3088.4342	3088.8975
3162.3658	3162.4028	3187.8160
3187.9816	3233.9352	3234.0068

^{2}M24

Zero-point correction= 0.262094
Thermal correction to Energy= 0.273696
Thermal correction to Enthalpy= 0.274640
Thermal correction to Gibbs Free Energy= 0.226687
Sum of electronic and zero-point Energies= -483.320612
Sum of electronic and thermal Energies= -483.309010
Sum of electronic and thermal Enthalpies= -483.308066
Sum of electronic and thermal Free Energies= -483.356019

Cartesian coordinates

C	-1.249902	-0.076807	0.040356
C	-1.118035	1.384015	0.513437
C	-0.068890	2.124301	-0.304893
C	1.301513	1.503976	-0.021985
C	1.265063	-0.051357	0.032670
H	-2.097487	1.876630	0.456560
H	-0.307648	2.037393	-1.370478
H	2.018324	1.837395	-0.782380
H	-0.058361	3.193153	-0.062138
H	-0.816481	1.410913	1.570483
H	1.673204	1.887047	0.937834
N	0.014897	-0.539366	-0.595617
O	0.019904	-1.941295	-0.668466
C	-2.295076	-0.164364	-1.081660
H	-2.224112	-1.163411	-1.518445
H	-3.312354	0.004876	-0.709077
H	-2.084087	0.571991	-1.864881
C	-1.737830	-0.961504	1.197414
H	-1.076564	-0.900726	2.065209
H	-2.739952	-0.649812	1.515690
H	-1.757546	-1.995521	0.852464
C	2.414482	-0.595127	-0.822578
H	3.374184	-0.195772	-0.473834
H	2.422409	-1.684040	-0.774317
H	2.272036	-0.293602	-1.866318

C	1.470885	-0.576240	1.465297
H	1.178240	-1.630337	1.458318
H	2.518047	-0.488322	1.779793
H	0.861376	-0.033296	2.194216

Vibrational frequencies

84.2494	147.2351	210.7397
229.3624	243.8278	267.4714
279.8619	302.1546	325.9771
329.1391	358.4862	367.5699
388.4091	399.4792	412.2112
467.7801	488.7664	514.9156
584.0561	604.8123	686.7027
794.0695	798.7779	847.1039
899.1969	927.5731	931.8916
937.1035	969.0504	973.5450
990.6637	999.2415	1044.1520
1072.4635	1079.9155	1088.6034
1114.7773	1174.4369	1205.4011
1228.8304	1243.2043	1259.8983
1272.8344	1287.6334	1316.3731
1354.4441	1362.4585	1367.7789
1376.4858	1381.9196	1383.2333
1393.8312	1472.5825	1475.8836
1483.5364	1489.2818	1493.6122
1501.1295	1504.8002	1506.6003
1510.4270	1522.3008	1525.0423
3038.2306	3041.4355	3042.7609
3045.0629	3051.6284	3056.0478
3065.7359	3083.1690	3085.3899
3112.6770	3115.1401	3116.5332
3123.3251	3143.9840	3155.3874
3157.1789	3176.6072	3180.3472

^{2}M25

Zero-point correction=	0.086936
Thermal correction to Energy=	0.093089
Thermal correction to Enthalpy=	0.094033
Thermal correction to Gibbs Free Energy=	0.055983
Sum of electronic and zero-point Energies=	-340.038078
Sum of electronic and thermal Energies=	-340.031925
Sum of electronic and thermal Enthalpies=	-340.030981
Sum of electronic and thermal Free Energies=	-340.069031

Cartesian coordinates

N	2.03471400	0.00001400	0.00036200
C	1.51718300	-1.20282200	-0.00005600
C	0.12147500	-1.22239400	-0.00011200
H	-0.39450500	-2.17488400	-0.00003000
C	-0.55864900	-0.00001300	-0.00023800
C	0.12145200	1.22238300	-0.00011200
H	-0.39454600	2.17486200	-0.00003000
C	1.51716100	1.20284000	-0.00005600
H	2.16101400	2.07630800	-0.00022100
H	2.16105300	-2.07627700	-0.00022100
C	-2.00026600	-0.00003200	0.00009300
N	-3.15516400	0.00001700	0.00012300

Vibrational frequencies

148.0551	163.9362	385.5168
386.0175	469.0202	510.9555
564.7753	618.1961	685.4817
719.8314	771.5708	839.9497
977.2048	995.7298	1004.4513
1098.2544	1116.7171	1184.6980
1230.9313	1289.2634	1320.5375
1438.4129	1492.4012	1615.5698
1666.8316	2435.3606	3249.6802
3252.9008	3262.6248	3265.7763

^{2}M26

Zero-point correction=	0.036648
Thermal correction to Energy=	0.039542
Thermal correction to Enthalpy=	0.040486
Thermal correction to Gibbs Free Energy=	0.014416
Sum of electronic and zero-point Energies=	-115.091355
Sum of electronic and thermal Energies=	-115.088462
Sum of electronic and thermal Enthalpies=	-115.087518
Sum of electronic and thermal Free Energies=	-115.113588

Cartesian coordinates

O	-0.79653600	-0.00003500	-0.00004900
C	0.53868200	-0.00007100	-0.00016500
H	1.04744200	-0.96402100	-0.31805700
H	1.04690700	0.75837800	-0.67483900
H	1.04584400	0.20635000	0.99427600

Vibrational frequencies

1208.6810	1223.6375	1226.6429
1482.4803	1486.1651	1558.7057
2599.2091	2602.6124	2698.5779

^{2}M27

Zero-point correction=	0.142435
Thermal correction to Energy=	0.152216
Thermal correction to Enthalpy=	0.153160
Thermal correction to Gibbs Free Energy=	0.106480
Sum of electronic and zero-point Energies=	-418.596079
Sum of electronic and thermal Energies=	-418.586298
Sum of electronic and thermal Enthalpies=	-418.585354
Sum of electronic and thermal Free Energies=	-418.632034

Cartesian coordinates

N	-1.44190000	0.00000700	-0.00082300
C	-0.94500300	-1.21883400	-0.00412800
C	0.45581900	-1.22240700	-0.00161400
H	0.97856200	-2.17190100	-0.00414500
C	1.13220200	-0.00000400	0.00097200
C	0.45584000	1.22239400	-0.00158200
H	0.97858800	2.17188500	-0.00413600
C	-0.94499500	1.21882900	-0.00414400
C	2.57444600	-0.00001000	0.00110300
N	3.72951100	-0.00002400	0.00155100
C	-1.83525300	-2.42266500	0.00123100
H	-2.31284700	-2.51385900	0.97930500
H	-2.60825500	-2.31813100	-0.76091600
H	-1.23777100	-3.31056200	-0.19598100
C	-1.83520900	2.42269400	0.00121400
H	-2.31082600	2.51527800	0.98012300
H	-1.23808300	3.31029300	-0.19840600
H	-2.60971800	2.31714000	-0.75924000

Vibrational frequencies

87.3698	92.1838	117.7722
136.9437	180.6598	196.8981
247.5646	375.0125	404.7427
466.8402	495.0128	512.9134
580.4494	591.9745	593.6192
682.4453	849.7889	896.2353
922.0613	958.4750	1002.4886
1031.0521	1059.5227	1060.4526
1072.5654	1178.5109	1246.1740

1282.1020	1357.1335	1405.0994
1410.3854	1418.6009	1453.3421
1470.9078	1473.5548	1485.3748
1500.2068	1626.0887	1660.6427
2433.5172	3101.6253	3101.9084
3189.8951	3190.1005	3216.1395
3216.5130	3244.3260	3244.3555

^{2}M28

Zero-point correction=	0.016513
Thermal correction to Energy=	0.020500
Thermal correction to Enthalpy=	0.021444
Thermal correction to Gibbs Free Energy=	-0.010652
Sum of electronic and zero-point Energies=	-412.852716
Sum of electronic and thermal Energies=	-412.848729
Sum of electronic and thermal Enthalpies=	-412.847785
Sum of electronic and thermal Free Energies=	-412.879881

Cartesian coordinates

O	-1.40360200	-0.02422200	-0.00526500
C	-0.17358000	-0.00295700	-0.00039300
F	0.43553300	1.18652400	-0.43198300
F	0.47428700	-0.95702600	-0.80216400
F	0.45354700	-0.20599600	1.23908900

Vibrational frequencies

428.8719	430.1694	610.3217
612.1685	619.6118	868.6780
1012.1179	1014.3334	1652.2408

^{2}M29

Sum of electronic and zero-point Energies	-1122.545755
Thermal correction to Energy	0.251118
Thermal correction to Gibbs Free Energy	0.189516
Thermal correction to Enthalpy	0.252063
Zero-point correction	0.235508
Sum of electronic and thermal Energies	-1122.530145
Sum of electronic and thermal Enthalpies	-1122.529201
Sum of electronic and thermal Free Energies	-1122.591747

Cartesian coordinates

N	2.244942	-0.256455	-0.834583
C	2.631404	-1.514411	-0.357519
C	3.878174	-1.702458	0.152257

H	4.149545	-2.700795	0.477464
C	4.800191	-0.628667	0.256310
C	4.371185	0.642771	-0.180077
H	5.031149	1.501747	-0.119231
C	3.121325	0.835804	-0.692364
H	2.743451	1.782785	-1.055668
H	5.787792	-0.775578	0.671954
N	0.879168	-0.040022	-0.956802
H	0.663547	0.487949	-1.804320
S	0.162573	0.735533	0.406228
O	0.271650	2.189951	0.311217
O	0.734110	0.050485	1.559337
C	-1.529338	0.279756	0.186156
C	-2.467776	1.261059	-0.109078
C	-1.885248	-1.061261	0.332281
C	-3.798937	0.883578	-0.262469
H	-2.158463	2.295653	-0.208878
C	-3.215902	-1.415188	0.173767
H	-1.130969	-1.806410	0.565761
C	-4.188651	-0.450629	-0.127172
H	-4.545447	1.639083	-0.487301
H	-3.511429	-2.454091	0.286181
C	-5.624079	-0.860687	-0.317389
H	-5.937539	-1.559524	0.462010
H	-6.289337	0.004192	-0.299960
H	-5.750600	-1.365768	-1.280060
H	1.878193	-2.283922	-0.460552

Vibrational frequencies

20.7839	26.3026	47.1524
58.7083	73.6534	99.1828
150.5216	176.9276	198.4646
266.5398	277.2469	318.4216
333.5142	355.2092	409.7870
415.5800	445.0268	457.6568
481.9826	507.2037	537.5701
582.2175	624.7250	633.6567
642.6623	648.6134	664.3413
694.8516	718.4546	750.9351
775.3267	821.7913	829.4614
839.1214	861.4922	884.8611
961.3875	964.3390	984.5965
1002.3898	1012.6322	1015.0086
1024.6440	1034.3685	1063.9085

1100.3158	1106.9348	1118.1710
1140.4526	1173.8066	1207.2660
1208.9889	1253.0655	1253.9637
1317.4699	1327.6992	1345.7367
1350.3519	1364.3390	1373.9224
1421.1452	1450.4377	1454.5717
1490.4207	1492.7905	1499.1561
1551.5387	1569.0017	1669.9206
1692.6507	1698.2538	3074.2537
3145.0735	3172.9679	3204.7943
3213.7793	3222.8915	3223.7633
3224.8195	3234.7935	3264.0333
3274.4225	3280.1389	3514.8466

^{2}TS11

Sum of electronic and zero-point Energies	-1122.531902
Thermal correction to Energy	0.249406
Thermal correction to Gibbs Free Energy	0.188959
Thermal correction to Enthalpy	0.250350
Zero-point correction	0.234121
Sum of electronic and thermal Energies	-1122.516617
Sum of electronic and thermal Enthalpies	-1122.515673
Sum of electronic and thermal Free Energies	-1122.577065

Cartesian coordinates

N	-2.479170	0.168029	-1.149883
C	-2.841723	1.421545	-0.738328
C	-3.869025	1.618544	0.156539
H	-4.136190	2.633050	0.430594
C	-4.556314	0.520240	0.685863
C	-4.189567	-0.757501	0.254085
H	-4.712018	-1.640426	0.605565
C	-3.166045	-0.910640	-0.657100
H	-2.853788	-1.878612	-1.032645
H	-5.354188	0.656989	1.405422
N	-0.794986	0.031279	-1.153617
H	-0.620885	-0.653793	-1.893290
S	-0.206852	-0.569229	0.294029
O	-0.370177	-2.022322	0.390969
O	-0.793962	0.268838	1.337968
C	1.524857	-0.217915	0.170936
C	2.421565	-1.254850	-0.065650
C	1.952882	1.102023	0.307103
C	3.776772	-0.956185	-0.165722

H	2.058890	-2.273039	-0.155891
C	3.308526	1.378948	0.202514
H	1.233091	1.891360	0.499389
C	4.237016	0.357355	-0.037875
H	4.489447	-1.756658	-0.340792
H	3.657520	2.401385	0.313076
C	5.701956	0.674009	-0.179074
H	5.937979	0.927339	-1.217731
H	5.982883	1.528147	0.440691
H	6.319413	-0.181476	0.102149
H	-2.265723	2.232669	-1.167742

Vibrational frequencies

-738.1799	26.5774	33.4981
53.0186	70.4820	78.2611
95.0827	153.1163	173.5496
218.9033	244.3643	273.8824
323.8619	337.4126	376.3300
406.7600	413.6527	440.8894
452.3971	501.9348	527.5301
554.1925	574.1502	641.5965
644.9958	674.6176	683.3971
713.0728	724.4536	756.9766
827.7137	838.0068	849.6231
868.3713	870.0348	906.4900
952.7584	982.4511	988.1000
1001.8493	1006.7517	1021.6885
1029.7591	1033.6505	1067.1290
1070.2442	1107.6382	1114.7727
1135.3898	1159.7180	1166.8699
1205.0271	1212.4201	1229.7321
1252.4912	1308.9330	1324.7394
1339.0548	1359.4620	1367.5559
1424.3769	1451.7040	1481.8798
1492.0929	1497.3448	1499.3304
1547.2900	1594.2273	1646.9583
1667.9518	1688.2839	3081.3360
3153.2269	3176.8414	3207.0038
3212.1892	3223.3842	3229.9089
3232.9771	3233.5848	3242.1564
3244.5237	3254.3865	3516.7228

^{2}M30

Sum of electronic and zero-point Energies -874.454393

Thermal correction to Energy	0.152077
Thermal correction to Gibbs Free Energy	0.105766
Thermal correction to Enthalpy	0.153022
Zero-point correction	0.142202
Sum of electronic and thermal Energies	-874.444517
Sum of electronic and thermal Enthalpies	-874.443573
Sum of electronic and thermal Free Energies	-874.490829

Cartesian coordinates

N	-2.454363	0.117181	1.497236
H	-1.710505	0.554902	2.060799
S	-1.911759	-0.020386	-0.089900
O	-2.387137	1.202728	-0.730939
O	-2.371012	-1.318350	-0.560984
C	-0.145662	-0.013647	-0.066343
C	0.527114	1.208064	-0.081018
C	0.534146	-1.227036	-0.022173
C	1.914139	1.201279	-0.045570
H	-0.028548	2.138555	-0.134555
C	1.924126	-1.209324	0.012726
H	-0.016321	-2.161568	-0.027774
C	2.629529	-0.002538	0.004947
H	2.454619	2.142920	-0.065009
H	2.469583	-2.147449	0.040824
C	4.133256	0.014263	0.060108
H	4.474013	0.342399	1.046968
H	4.548688	-0.976852	-0.129208
H	4.542469	0.711603	-0.674974

Vibrational frequencies

-18.6515	49.7529	85.9781
164.9673	198.7572	243.9514
286.8421	325.4834	341.1287
375.2608	414.1598	442.1202
462.8722	522.4331	539.4413
640.4540	648.0800	711.6882
769.8225	829.4595	840.3788
867.7138	991.0976	1007.5099
1016.8240	1033.8283	1065.5208
1100.4363	1120.0204	1140.5995
1177.5131	1209.8556	1252.5545
1327.2933	1347.5801	1363.0399
1421.5576	1453.1458	1490.9097
1499.7789	1547.2246	1668.4625

1687.5480	3076.9585	3149.0245
3175.9294	3209.1428	3213.0706
3230.8111	3234.7712	3446.6875

^{2}M31

Sum of electronic and zero-point Energies	-248.093354
Thermal correction to Energy	0.094015
Thermal correction to Gibbs Free Energy	0.062380
Thermal correction to Enthalpy	0.094959
Zero-point correction	0.089768
Sum of electronic and thermal Energies	-248.089106
Sum of electronic and thermal Enthalpies	-248.088162
Sum of electronic and thermal Free Energies	-248.120741

Cartesian coordinates

N	0.003047	-1.417447	-0.000197
C	-1.139084	-0.722536	-0.000018
C	-1.197606	0.668757	0.000175
H	-2.156614	1.174347	0.000271
C	-0.002913	1.381672	-0.000219
C	1.194737	0.673744	-0.000061
H	2.151690	1.183229	-0.000020
C	1.142097	-0.717830	0.000189
H	2.061936	-1.298295	0.000481
H	-0.005262	2.466912	0.000214
H	-2.056470	-1.306908	0.000040

Vibrational frequencies

390.9716	418.3935	611.7711
666.5186	724.3971	769.2946
911.2864	984.9293	1020.1786
1027.5539	1038.3710	1063.0689
1099.3458	1105.1070	1166.7906
1251.6463	1306.0053	1389.7308
1494.4265	1538.5569	1675.0904
1684.7610	3196.5723	3199.0882
3211.6739	3225.6259	3232.2508

M5′

Zero-point correction= 1.072737
Thermal correction to Energy= 1.128466
Thermal correction to Enthalpy= 1.129410
Thermal correction to Gibbs Free Energy= 0.988252
Sum of electronic and zero-point Energies= -3150.491817

Sum of electronic and thermal Energies= -3150.436088
Sum of electronic and thermal Enthalpies= -3150.435144
Sum of electronic and thermal Free Energies= -3150.576302

Cartesian coordinates
C -6.743384 -0.558164 -1.989576
C -6.009001 0.597036 -2.670742
C -5.354595 1.587360 -1.702299
C -5.848609 -1.558852 -1.256858
C -4.158186 1.048068 -0.970574
C -5.191105 -1.036051 0.030653
C -4.065350 -0.066726 -0.208289
H -7.308268 -1.103110 -2.753318
H -6.725560 1.156407 -3.280803
H -6.095623 1.912350 -0.959830
H -5.073511 -1.920993 -1.942319
H -5.957434 -0.534103 0.637100
C -1.923001 0.781861 0.102349
H -7.484120 -0.151749 -1.287358
H -5.247448 0.202948 -3.354289
H -5.053762 2.485277 -2.249518
H -6.455729 -2.427777 -0.981434
H -4.830282 -1.875188 0.628007
N -2.787235 -0.202747 0.380780
C -2.520819 -1.368099 1.222530
C -2.392033 -2.614171 0.600013
C -2.563941 -1.207863 2.616666
C -2.238672 -3.730341 1.431953
C -2.417496 -2.352291 3.395873
C -2.245188 -3.605567 2.811382
H -2.114574 -4.710610 0.981290
H -2.434043 -2.267131 4.477140
H -2.127741 -4.484362 3.437989
C -2.438263 -2.821628 -0.907047
C -3.409287 -3.950907 -1.280947
H -3.581678 -3.952380 -2.361579
H -2.990649 -4.926934 -1.016421
H -4.376233 -3.853460 -0.778763
C -2.793975 0.150606 3.252880
S -2.655819 1.895097 -0.965950
H -2.794201 -1.897166 -1.375911
H -2.288096 0.893906 2.633039
C -1.047866 -3.117908 -1.479589
H -0.627391 -4.014759 -1.011039

H -1.126103 -3.313479 -2.555655
H -0.367367 -2.275980 -1.327401
C -2.195090 0.267943 4.654905
H -2.225541 1.312708 4.977489
H -2.757327 -0.321819 5.386818
H -1.152866 -0.061903 4.670861
C -4.292028 0.484664 3.293311
H -4.452037 1.456969 3.769282
H -4.727071 0.528801 2.290836
H -4.837423 -0.271594 3.868120
C -0.481857 0.922802 0.699366
O -0.154773 -0.120507 1.423785
C -0.464814 2.247161 1.551045
C -0.913463 3.521324 1.177856
C 0.058468 2.107644 2.843012
C -0.825426 4.605993 2.049548
H -1.325144 3.704420 0.192878
C 0.150223 3.184868 3.719839
H 0.380929 1.111018 3.122306
C -0.291721 4.445756 3.325879
H -1.179928 5.579775 1.724867
H 0.562383 3.037375 4.714270
H -0.227926 5.291136 4.004152
C 6.743658 -0.558474 1.989106
C 6.009457 0.596869 2.670227
C 5.354984 1.587105 1.701742
C 5.848709 -1.559196 1.256645
C 4.158418 1.047809 0.970277
C 5.191048 -1.036507 -0.030835
C 4.065387 -0.067078 0.208146
H 7.308614 -1.103362 2.752837
H 6.726145 1.156275 3.280103
H 6.095925 1.911915 0.959109
H 5.073695 -1.921206 1.942268
H 5.957327 -0.534673 -0.637439
C 1.923089 0.781676 -0.102341
H 7.484322 -0.152203 1.286729
H 5.247977 0.202930 3.353941
H 5.054314 2.485134 2.248868
H 6.455731 -2.428193 0.981234
H 4.830099 -1.875691 -0.628047
N 2.787173 -0.203071 -0.380714
C 2.520509 -1.368483 -1.222299
C 2.391538 -2.614464 -0.599635

C 2.563571 -1.208410 -2.616451
C 2.238025 -3.730710 -1.431447
C 2.416978 -2.352906 -3.395529
C 2.244541 -3.606095 -2.810893
H 2.113767 -4.710906 -0.980670
H 2.433509 -2.267860 -4.476807
H 2.126962 -4.484944 -3.437399
C 2.437594 -2.821731 0.907456
C 3.408757 -3.950786 1.281647
H 3.580980 -3.952083 2.362306
H 2.990332 -4.926923 1.017192
H 4.375766 -3.853230 0.779599
C 2.793775 0.149955 -3.252818
S 2.656135 1.894995 0.965709
H 2.793305 -1.897150 1.376255
H 2.287951 0.893390 -2.633089
C 1.047163 -3.118178 1.479831
H 0.626974 -4.015237 1.011422
H 1.125272 -3.313479 2.555955
H 0.366488 -2.276447 1.327323
C 2.194965 0.267174 -4.654886
H 2.225583 1.311885 -4.977627
H 2.757152 -0.322781 -5.386684
H 1.152694 -0.062524 -4.670838
C 4.291869 0.483825 -3.293211
H 4.452022 1.456062 -3.769270
H 4.726872 0.528000 -2.290719
H 4.837193 -0.272559 -3.867920
C 0.481950 0.922727 -0.699353
O 0.154796 -0.120557 -1.423768
C 0.465095 2.247057 -1.551082
C 0.913728 3.521221 -1.177880
C -0.057870 2.107465 -2.843168
C 0.825933 4.605832 -2.049666
H 1.325215 3.704359 -0.192827
C -0.149387 3.184634 -3.720088
H -0.380289 1.110828 -3.122482
C 0.292506 4.445533 -3.326107
H 1.180411 5.579619 -1.724972
H -0.561318 3.037082 -4.714606
H 0.228911 5.290868 -4.004455

Vibrational frequencies
22.1440 24.8187 36.4987

38.7568 46.6528 58.1038
59.7020 59.8817 69.0557
73.5106 77.7629 80.9017
81.0843 84.8607 85.3253
92.1040 94.8808 99.4290
108.2294 110.4054 117.5818
126.5919 135.6383 140.6575
142.5495 144.7722 148.7495
153.7511 162.1202 167.5614
169.3604 172.0005 176.4754
195.3993 206.9911 216.7358
222.7072 225.0516 230.9885
241.6846 243.7602 246.1988
246.6147 252.2047 259.1630
259.9998 268.2545 268.7501
279.3883 286.8747 288.7897
292.1601 300.8225 306.3756
311.6231 312.9379 318.9925
326.9157 328.0446 331.0870
333.5142 337.3078 341.5662
353.7328 358.3272 361.0244
363.4743 381.8343 390.5076
400.1643 404.8256 417.7930
421.3919 429.8373 433.7450
437.4460 441.8937 445.8400
460.9175 464.3478 472.2094
480.4521 494.3359 495.7185
504.2255 506.8196 511.5367
526.8734 534.4634 536.2445
543.5467 564.6977 567.8730
571.6783 585.5758 585.7138
606.1562 609.9139 616.2392
618.4992 628.7556 629.3129
646.7519 656.8969 659.5633
669.9996 678.8049 683.4000
711.7401 713.0950 718.1787
722.9474 729.5906 732.7151
743.8806 753.8317 781.4852
782.0943 793.0009 794.1730
811.9497 818.9358 819.8879
823.6782 834.2511 834.7109
836.0574 838.8629 839.9144
874.9008 887.8582 888.0879
891.9582 892.1585 901.8139

907.1453 918.5946 919.9922
926.9932 927.5195 929.2221
934.8726 938.7151 939.1030
948.8389 949.1010 961.0222
962.2784 969.4938 972.2648
975.1453 976.3371 980.8859
982.1039 982.2381 982.3505
983.8071 995.9726 1000.0993
1000.5002 1012.0272 1014.8005
1015.5305 1016.1855 1016.9797
1017.0775 1028.7576 1029.6414
1054.3768 1058.4066 1068.5931
1069.7313 1074.5063 1075.3892
1084.0540 1085.2880 1088.9468
1095.0461 1097.8239 1100.5190
1105.0229 1106.1450 1127.6369
1127.8612 1135.5695 1135.6572
1145.0647 1147.0602 1148.8760
1150.8296 1152.1953 1153.9853
1167.4977 1167.6660 1169.9200
1170.5956 1174.7585 1174.7958
1180.4859 1180.5904 1192.0726
1192.7247 1202.0579 1203.3970
1212.5419 1213.3655 1239.3428
1240.0692 1247.7523 1249.3340
1260.2018 1260.2785 1281.5719
1286.7460 1286.9079 1291.6113
1292.3971 1297.5702 1298.3996
1305.9486 1308.2725 1308.4957
1327.3400 1327.4822 1329.5355
1330.1971 1330.9157 1331.2067
1333.0461 1334.1785 1338.8423
1340.6006 1352.8159 1353.6109
1373.4062 1373.6993 1381.6105
1381.6377 1385.1649 1385.1690
1390.9981 1391.2159 1402.4981
1402.5918 1405.6151 1405.7408
1406.6653 1406.7191 1414.4050
1415.3036 1417.0175 1417.0639
1421.3537 1421.3696 1432.7613
1434.3683 1457.0706 1459.1517
1480.7014 1480.7861 1482.4872
1484.0236 1485.1790 1485.6018
1485.6441 1486.3896 1486.9701

1489.3228 1490.2082 1491.2173
1491.6090 1494.7810 1496.1446
1498.2196 1498.2284 1499.7460
1503.2179 1503.5359 1508.1303
1508.2132 1512.4710 1512.8844
1515.9518 1517.0948 1517.9976
1520.0795 1528.4713 1531.1808
1532.9205 1535.4782 1536.1061
1594.2297 1662.0979 1663.5432
1676.2003 1676.2510 1683.6519
1683.7499 1686.8899 1687.1828
1694.4122 1694.7300 3044.8391
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3076.6586 3076.6818 3090.7736
3090.7911 3110.9753 3110.9820
3117.7696 3117.7861 3118.6685
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3126.2370 3126.2545 3133.6313
3133.6477 3137.4515 3137.5283
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3149.0671 3151.1444 3151.1647
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3157.7498 3160.1365 3160.1639
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3198.6612 3199.3770 3199.4034
3209.3873 3209.4318 3220.2360
3220.4396 3226.3695 3226.3934
3231.2881 3231.3149 3234.7058
3234.7643 3245.7677 3246.9833

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